openforcefield Documentation

Release 0.4.1

Open Force Field Consortium

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A modern, extensible library for molecular mechanics force field science from the Open Force Field Initiative

CHAPTER

ONE

USER GUIDE

1.1 Installation

1.1.1 Installing via *conda*

The simplest way to install the Open Forcefield Toolkit is via the conda package manager. Packages are provided on the omnia Anaconda Cloud channel for Linux, OS X, and Win platforms. The openforcefield Anaconda Cloud page has useful instructions and download statistics.

If you are using the anaconda scientific Python distribution, you already have the `conda` package manager installed. If not, the quickest way to get started is to install the miniconda distribution, a lightweight minimal installation of Anaconda Python.

On `linux`, you can install the Python 3 version into `$HOME/miniconda3` with (on `bash` systems):

```
$ wget https://repo.continuum.io/miniconda/Miniconda3-latest-Linux-x86_64.sh
$ bash ./Miniconda3-latest-Linux-x86_64.sh -b -p $HOME/miniconda3
$ source ~/miniconda3/etc/profile.d/conda.sh
$ conda activate base
```

On `osx`, you want to use the `osx` binary

```
$ curl https://repo.continuum.io/miniconda/Miniconda3-latest-MacOSX-x86_64.sh -O
$ bash ./Miniconda3-latest-MacOSX-x86_64.sh -b -p $HOME/miniconda3
$ source ~/miniconda3/etc/profile.d/conda.sh
$ conda activate base
```

You may want to add the new `source ~/miniconda3/etc/profile.d/conda.sh` line to your `~/.bashrc` file to ensure Anaconda Python can enabled in subsequent terminal sessions. `conda activate base` will need to be run in each subsequent terminal session to return to the environment where the toolkit will be installed.

Note that `openforcefield` will be installed into this local Python installation, so that you will not need to worry about disrupting existing Python installations.

Note: Installation via the conda package manager is the preferred method since all dependencies are automatically fetched and installed for you.

1.1.2 Required dependencies

The `openforcefield` toolkit makes use of the Omnia and Conda Forge free and open source community package repositories:

```
$ conda config --add channels omnia --add channels conda-forge
$ conda update --all
```

This only needs to be done once.

Note: If automation is required, provide the `--yes` argument to `conda update` and `conda install` comamnds. More information on the `conda` command-line API can be found in the conda online documentation.

Release build

You can install the latest stable release build of `openforcefield` via the `conda` package with

```
$ conda config --add channels omnia --add channels conda-forge
$ conda install openforcefield
```

This version is recommended for all users not actively developing new forcefield parameterization algorithms.

Note: The conda package manager will install dependencies from binary packages automatically, including difficult-to-install packages such as OpenMM, numpy, and scipy. This is really the easiest way to get started.

Upgrading your installation

To update an earlier `conda` installation of `openforcefield` to the latest release version, you can use `conda update`:

```
$ conda update openforcefield
```

Optional dependencies

This toolkit can optionally make use of the OpenEye toolkit if the user has a license key installed. Academic laboratories intending to release results into the public domain can obtain a free license key, while other users (including academics intending to use the software for purposes of generating protected intellectual property) must pay to obtain a license.

To install the OpenEye toolkits (provided you have a valid license file):

```
$ conda install --yes -c openeye openeye-toolkits
```

No essential `openforcefield` release capabilities *require* the OpenEye toolkit, but the Open Force Field developers make use of it in parameterizing new open source force fields. It is known that there are certain differences in toolkit behavior between RDKit and OpenEye when reading a small fraction of molecules, and we encourage you to report any unexpected behavior that may be caused by toolkit differences to our issue tracker.

1.2 Release History

Releases follow the `major.minor.micro` scheme recommended by PEP440, where

- `major` increments denote a change that may break API compatibility with previous `major` releases
- `minor` increments add features but do not break API compatibility
- `micro` increments represent bugfix releases or improvements in documentation

1.2.1 0.4.1 - Bugfix Release

This update fixes several toolkit bugs that have been reported by the community. Details of these bugfixes are provided below.

It also refactors how `ParameterType` and `ParameterHandler` store their attributes, by introducing `ParameterAttribute` and `IndexedParameterAttribute`. These new attribute-handling classes provide a consistent backend which should simplify manipulation of parameters and implementation of new handlers.

Bug fixes

- PR #329: Fixed a bug where the two `BondType` parameter attributes `k` and `length` were treated as indexed attributes. (`k` and `length` values that correspond to specific bond orders will be indexed under `k_bondorder1`, `k_bondorder2`, etc when implemented in the future)
- PR #329: Fixed a bug that allowed setting indexed attributes to single values instead of strictly lists.
- PR #370: Fixed a bug in the API where `BondHandler`, `ProperTorsionHandler` , and `ImproperTorsionHandler` exposed non-functional indexed parameters.
- PR #351: Fixes Issue #344, in which the main `FrozenMolecule` constructor and several other Molecule-construction functions ignored or did not expose the `allow_undefined_stereo` keyword argument.
- PR #351: Fixes a bug where a molecule which previously generated a SMILES using one cheminformatics toolkit returns the same SMILES, even though a different toolkit (which would generate a different SMILES for the molecule) is explicitly called.
- PR #354: Fixes the error message that is printed if an unexpected parameter attribute is found while loading data into a `ForceField` (now instructs users to specify `allow_cosmetic_attributes` instead of `permit_cosmetic_attributes`)
- PR #364: Fixes Issue #362 by modifying `OpenEyeToolkitWrapper.from_smiles` and `RDKitToolkitWrapper.from_smiles` to make implicit hydrogens explicit before molecule creation. These functions also now raise an error if the optional keyword `hydrogens_are_explicit=True` but the SMILES are interpreted by the backend cheminformatic toolkit as having implicit hydrogens.

- PR #371: Fixes error when reading early SMIRNOFF 0.1 spec files enclosed by a top-level `SMIRFF` tag.

Note: The enclosing `SMIRFF` tag is present only in legacy files. Since developing a formal specification, the only acceptable top-level tag value in a SMIRNOFF data structure is `SMIRNOFF`.

Code enhancements

- PR #329: `ParameterType` was refactored to improve its extensibility. It is now possible to create new parameter types by using the new descriptors `ParameterAttribute` and `IndexedParameterAttribute`.
- PR #357: Addresses Issue #356 by raising an informative error message if a user attempts to load an OpenMM topology which is probably missing connectivity information.

Force fields added

- PR #368: Temporarily adds `test_forcefields/smirnoff99frosst_experimental.offxml` to address hierarchy problems, redundancies, SMIRKS pattern typos etc., as documented in issue #367. Will ultimately be propagated to an updated forcefield in the `openforcefield/smirnoff99frosst` repo.
- PR #371: Adds `test_forcefields/smirff99Frosst_reference_0_1_spec.offxml`, a SMIRNOFF 0.1 spec file enclosed by the legacy `SMIRFF` tag. This file is used in backwards-compatibility testing.

1.2.2 0.4.0 - Performance optimizations and support for SMIRNOFF 0.3 specification

This update contains performance enhancements that significantly reduce the time to create OpenMM systems for topologies containing many molecules via `ForceField.create_openmm_system`.

This update also introduces the SMIRNOFF 0.3 specification. The spec update is the result of discussions about how to handle the evolution of data and parameter types as further functional forms are added to the SMIRNOFF spec.

We provide methods to convert SMIRNOFF 0.1 and 0.2 forcefields written with the XML serialization (`.offxml`) to the SMIRNOFF 0.3 specification. These methods are called automatically when loading a serialized SMIRNOFF data representation written in the 0.1 or 0.2 specification. This functionality allows the toolkit to continue to read files containing SMIRNOFF 0.2 spec force fields, and also implements backwards-compatibility for SMIRNOFF 0.1 spec force fields.

Warning: The SMIRNOFF 0.1 spec did not contain fields for several energy-determining parameters that are exposed in later SMIRNOFF specs. Thus, when reading SMIRNOFF 0.1 spec data, the toolkit must make assumptions about the values that should be added for the newly-required fields. The values that are added include 1-2, 1-3 and 1-5 scaling factors, cutoffs, and long-range treatments for nonbonded interactions. Each assumption is printed as a warning during the conversion process. Please carefully review the warning messages to ensure that the conversion is providing your desired behavior.

SMIRNOFF 0.3 specification updates

- The SMIRNOFF 0.3 spec introduces versioning for each individual parameter section, allowing asynchronous updates to the features of each parameter class. The top-level `SMIRNOFF` tag, containing information like `aromaticity_model`, `Author`, and `Date`, still has a version (currently 0.3). But, to allow

for independent development of individual parameter types, each section (such as `Bonds`, `Angles`, etc) now has its own version as well (currently all 0.3).

- All units are now stored in expressions with their corresponding values. For example, distances are now stored as `1.526*angstrom`, instead of storing the unit separately in the section header.
- The current allowed value of the `potential` field for `ProperTorsions` and `ImproperTorsions` tags is no longer `charmm`, but is rather `k*(1+cos(periodicity*theta-phase))`. It was pointed out to us that CHARMM-style torsions deviate from this formula when the periodicity of a torsion term is 0, and we do not intend to reproduce that behavior.
- SMIRNOFF spec documentation has been updated with tables of keywords and their defaults for each parameter section and parameter type. These tables will track the allowed keywords and default behavior as updated versions of individual parameter sections are released.

Performance improvements and bugfixes

- PR #329: Performance improvements when creating systems for topologies with many atoms.
- PR #347: Fixes bug in charge assignment that occurs when charges are read from file, and reference and charge molecules have different atom orderings.

New features

- PR #311: Several new experimental functions.
  - Adds `convert_0_2_smirnoff_to_0_3`, which takes a SMIRNOFF 0.2-spec data dict, and updates it to 0.3. This function is called automatically when creating a `ForceField` from a SMIRNOFF 0.2 spec OFFXML file.
  - Adds `convert_0_1_smirnoff_to_0_2`, which takes a SMIRNOFF 0.1-spec data dict, and updates it to 0.2. This function is called automatically when creating a `ForceField` from a SMIRNOFF 0.1 spec OFFXML file.
  - NOTE: The format of the "SMIRNOFF data dict" above is likely to change significantly in the future. Users that require a stable serialized ForceField object should use the output of `ForceField.to_string('XML')` instead.
  - Adds `ParameterHandler` and `ParameterType` `add_cosmetic_attribute` and `delete_cosmetic_attribute` functions. Once created, cosmetic attributes can be accessed and modified as attributes of the underlying object (eg. `ParameterType.my_cosmetic_attrib = 'blue'`) These functions are experimental, and we are interested in feedback on how cosmetic attribute handling could be improved. (See Issue #338) Note that if a new cosmetic attribute is added to an object without using these functions, it will not be recognized by the toolkit and will not be written out during serialization.
  - Values for the top-level `Author` and `Date` tags are now kept during SMIRNOFF data I/O. If multiple data sources containing these fields are read, the values are concatenated using "AND" as a separator.

API-breaking changes

- `ForceField.to_string` and `ForceField.to_file` have had the default value of their `discard_cosmetic_attributes` kwarg set to False.
- `ParameterHandler` and `ParameterType` constructors now expect the `version` kwarg (per the SMIRNOFF spec change above) This requirement can be skipped by providing the kwarg `skip_version_check=True`

- `ParameterHandler` and `ParameterType` functions no longer handle `X_unit` attributes in SMIRNOFF data (per the SMIRNOFF spec change above).
- The scripts in `utilities/convert_frosst` are now deprecated. This functionality is important for provenance and will be migrated to the `openforcefield/smirnoff99Frosst` repository in the coming weeks.
- `ParameterType._SMIRNOFF_ATTRIBS` is now `ParameterType._REQUIRED_SPEC_ATTRIBS`, to better parallel the structure of the `ParameterHandler` class.
- `ParameterType._OPTIONAL_ATTRIBS` is now `ParameterType._OPTIONAL_SPEC_ATTRIBS`, to better parallel the structure of the `ParameterHandler` class.
- Added class-level dictionaries `ParameterHandler._DEFAULT_SPEC_ATTRIBS` and `ParameterType._DEFAULT_SPEC_ATTRIBS`.

1.2.3 0.3.0 - API Improvements

Several improvements and changes to public API.

New features

- PR #292: Implement `Topology.to_openmm` and remove `ToolkitRegistry.toolkit_is_available`
- PR #322: Install directories for the lookup of OFFXML files through the entry point group `openforcefield.smirnoff_forcefield_directory`. The `ForceField` class doesn't search in the `data/forcefield/` folder anymore (now renamed `data/test_forcefields/`), but only in `data/`.

API-breaking Changes

- PR #278: Standardize variable/method names
- PR #291: Remove `ForceField.load/to_smirnoff_data`, add `ForceField.to_file/string` and `ParameterHandler.add_parameters`. Change behavior of `ForceField.register_X_handler` functions.

Bugfixes

- PR #327: Fix units in tip3p.offxml (note that this file is still not loadable by current toolkit)
- PR #325: Fix solvent box for provided test system to resolve periodic clashes.
- PR #325: Add informative message containing Hill formula when a molecule can't be matched in `Topology.from_openmm`.
- PR #325: Provide warning or error message as appropriate when a molecule is missing stereochemistry.
- PR #316: Fix formatting issues in GBSA section of SMIRNOFF spec
- PR #308: Cache molecule SMILES to improve system creation speed
- PR #306: Allow single-atom molecules with all zero coordinates to be converted to OE/RDK mols
- PR #313: Fix issue where constraints are applied twice to constrained bonds

1.2.4 0.2.2 - Bugfix release

This release modifies an example to show how to parameterize a solvated system, cleans up backend code, and makes several improvements to the README.

Bugfixes

- PR #279: Cleanup of unused code/warnings in main package `__init__`
- PR #259: Update T4 Lysozyme + toluene example to show how to set up solvated systems
- PR #256 and PR #274: Add functionality to ensure that links in READMEs resolve successfully

1.2.5 0.2.1 - Bugfix release

This release features various documentation fixes, minor bugfixes, and code cleanup.

Bugfixes

- PR #267: Add neglected `<ToolkitAM1BCC>` documentation to the SMIRNOFF 0.2 spec
- PR #258: General cleanup and removal of unused/inaccessible code.
- PR #244: Improvements and typo fixes for BRD4:inhibitor benchmark

1.2.6 0.2.0 - Initial RDKit support

This version of the toolkit introduces many new features on the way to a 1.0.0 release.

New features

- Major overhaul, resulting in the creation of the SMIRNOFF 0.2 specification and its XML representation
- Updated API and infrastructure for reference SMIRNOFF `ForceField` implementation
- Implementation of modular `ParameterHandler` classes which process the topology to add all necessary forces to the system.
- Implementation of modular `ParameterIOHandler` classes for reading/writing different serialized SMIRNOFF forcefield representations
- Introduction of `Molecule` and `Topology` classes for representing molecules and biomolecular systems
- New `ToolkitWrapper` interface to RDKit, OpenEye, and AmberTools toolkits, managed by `ToolkitRegistry`
- API improvements to more closely follow PEP8 guidelines
- Improved documentation and examples

1.2.7 0.1.0

This is an early preview release of the toolkit that matches the functionality described in the preprint describing the SMIRNOFF v0.1 force field format: [DOI].

New features

This release features additional documentation, code comments, and support for automated testing.

Bugfixes

Treatment of improper torsions

A significant (though currently unused) problem in handling of improper torsions was corrected. Previously, non-planar impropers did not behave correctly, as six-fold impropers have two potential chiralities. To remedy this, SMIRNOFF impropers are now implemented as three-fold impropers with consistent chirality. However, current force fields in the SMIRNOFF format had no non-planar impropers, so this change is mainly aimed at future work.

1.3 The SMIRks Native Open Force Field (SMIRNOFF) specification

SMIRNOFF is a specification for encoding molecular mechanics force fields from the Open Force Field Initiative based on direct chemical perception using the broadly-supported SMARTS language, utilizing atom tagging extensions from SMIRKS.

1.3.1 Authors and acknowledgments

The SMIRNOFF specification was designed by the Open Force Field Initiative.

Primary contributors include:

- Caitlin C. Bannan (University of California, Irvine) <bannanc@uci.edu>
- Christopher I. Bayly (OpenEye Software) <bayly@eyesopen.com>
- John D. Chodera (Memorial Sloan Kettering Cancer Center) <john.chodera@choderalab.org>
- David L. Mobley (University of California, Irvine) <dmobley@uci.edu>

SMIRNOFF and its reference implementation in the `openforcefield` toolkit was heavily inspired by the ForceField class from the OpenMM molecular simulation package, and its associated XML format, developed by Peter K. Eastman (Stanford University).

1.3.2 Representations and encodings

A force field in the SMIRNOFF format can be encoded in multiple representations. Currently, only an XML representation is supported by the reference implementation of the openforcefield toolkit.

XML representation

A SMIRNOFF force field can be described in an XML representation, which provides a human- and machine-readable form for encoding the parameter set and its typing rules. This document focuses on describing the XML representation of the force field.

- By convention, XML-encoded SMIRNOFF force fields use an `.offxml` extension if written to a file to prevent confusion with other file formats.
- In XML, numeric quantities appear as strings, like `"1"` or `"2.3"`.

- Integers should always be written without a decimal point, such as `"1"`, `"9"`.
- Non-integral numbers, such as parameter values, should be written with a decimal point, such as `"1.23"`, `"2."`.
- In XML, certain special characters that occur in valid SMARTS/SMIRKS patterns (such as ampersand symbols `&`) must be specially encoded. See this list of XML and HTML character entity references for more details.

Future representations: JSON, MessagePack, YAML, and TOML

We are considering supporting JSON, MessagePack, YAML, and TOML representations as well.

1.3.3 Reference implementation

A reference implementation of the SMIRNOFF XML specification is provided in the openforcefield toolkit.

1.3.4 Support for molecular simulation packages

The reference implementation currently generates parameterized molecular mechanics systems for the GPU-accelerated OpenMM molecular simulation toolkit. Parameterized systems can subsequently be converted for use in other popular molecular dynamics simulation packages (including AMBER, CHARMM, NAMD, Desmond, and LAMMPS) via ParmEd and InterMol. See Converting SMIRNOFF parameterized systems to other simulation packages for more details.

1.3.5 Basic structure

A reference implementation of a SMIRNOFF force field parser that can process XML representations (denoted by `.offxml` file extensions) can be found in the `ForceField` class of the `openforcefield.typing.engines.smirnoff` module.

Below, we describe the main structure of such an XML representation.

The enclosing <SMIRNOFF> tag

A SMIRNOFF forcefield XML specification always is enclosed in a `<SMIRNOFF>` tag, with certain required attributes provided. The required and permitted attributes defined in the `<SMIRNOFF>` are recorded in the version attribute, which describes the top-level attributes that are expected or permitted to be defined.

```
<SMIRNOFF version="0.3" aromaticity_model="OEAroModel_MDL">
...
</SMIRNOFF>
```

Versioning

The SMIRNOFF force field format supports versioning via the `version` attribute to the root `<SMIRNOFF>` tag, e.g.:

```
<SMIRNOFF version="0.3" aromaticity_model="OEAroModel_MDL">
...
</SMIRNOFF>
```

The version format is `x.y`, where `x` denotes the major version and `y` denotes the minor version. SMIRNOFF versions are guaranteed to be backward-compatible within the *same major version number series*, but it is possible major version increments will break backwards-compatibility.

SMIRNOFF tag version	Required attributes	Optional attributes
0.1	`aromaticity_model`	`Date`, `Author`
0.2	`aromaticity_model`	`Date`, `Author`
0.3	`aromaticity_model`	`Date`, `Author`

The SMIRNOFF tag versions describe the required and allowed force field-wide settings. The list of keywords is as follows:

Aromaticity model

The `aromaticity_model` specifies the aromaticity model used for chemical perception (here, `OEAroModel_MDL`).

Currently, the only supported model is `OEAroModel_MDL`, which is implemented in both the RDKit and the OpenEye Toolkit.

Note: Add link to complete open specification of *OEAroModel_MDL* aromaticity model.

Metadata

Typically, date and author information is included:

```
<Date>2016-05-25</Date>
<Author>J. D. Chodera (MSKCC) charge increment tests</Author>
```

The `<Date>` tag should conform to ISO 8601 date formatting guidelines, such as `2018-07-14` or `2018-07-14T08:50:48+00:00` (UTC time).

Parameter generators

Within the `<SMIRNOFF>` tag, top-level tags encode parameters for a force field based on a SMARTS/SMIRKS-based specification describing the chemical environment the parameters are to be applied to. The file has tags corresponding to OpenMM force terms (`Bonds`, `Angles`, `ProperTorsions`, etc., as discussed in more detail below); these specify functional form and other information for individual force terms.

```
<Angles version="0.3" potential="harmonic">
   ...
</Angles>
```

which introduces the following `Angle` child elements which will use a harmonic potential.

Specifying parameters

Under each of these force terms, there are tags for individual parameter lines such as these:

```
<Angles version="0.3" potential="harmonic">
   <Angle smirks="[a,A:1]-[#6X4:2]-[a,A:3]" angle="109.50*degree" k="100.0*kilocalorie_per_mole/
↪radian**2"/>
   <Angle smirks="[#1:1]-[#6X4:2]-[#1:3]" angle="109.50*degree" k="70.0*kilocalorie_per_mole/radian**2"/
↪>
</Angles>
```

The first of these specifies the `smirks` attribute as `[a,A:1]-[#6X4:2]-[a,A:3]`, specifying a SMIRKS pattern that matches three connected atoms specifying an angle. This particular SMIRKS pattern matches a tetravalent carbon at the center with single bonds to two atoms of any type. This pattern is essentially a SMARTS string with numerical atom tags commonly used in SMIRKS to identify atoms in chemically unique environments—these can be thought of as tagged regular expressions for identifying chemical environments, and atoms within those environments. Here, `[a,A]` denotes any atom—either aromatic (`a`) or aliphatic (`A`), while `[#6X4]` denotes a carbon by element number (`#6`) that with four substituents (`X4`). The symbol `-` joining these groups denotes a single bond. The strings `:1`, `:2`, and `:2` label these atoms as indices 1, 2, and 3, with 2 being the central atom. Equilibrium angles are provided as the `angle` attribute, along with force constants as the `k` attribute (with corresponding units included in the expression).

Note: The reference implementation of the SMIRNOFF specification implemented in the Open Force Field toolkit will, by default, raise an exception if an unexpected attribute is encountered. The toolkit can be configured to accept non-spec keywords, but these are considered "cosmetic" and will not be evaluated. For example, providing an *<Angle>* tag that also specifies a second force constant *k2* will result in an exception, unless the user specifies that "cosmetic" attributes should be accepted by the parser.

SMIRNOFF parameter specification is hierarchical

Parameters that appear later in a SMIRNOFF specification override those which come earlier if they match the same pattern. This can be seen in the example above, where the first line provides a generic angle parameter for any tetravalent carbon (single bond) angle, and the second line overrides this for the specific case of a hydrogen-(tetravalent carbon)-hydrogen angle. This hierarchical structure means that a typical parameter file will tend to have generic parameters early in the section for each force type, with more specialized parameters assigned later.

Multiple SMIRNOFF representations can be processed in sequence

Multiple SMIRNOFF data sources (e.g. multiple OFFXML files) can be loaded by the openforcefield `ForceField` in sequence. If these files each contain unique top-level tags (such as `<Bonds>`, `<Angles>`, etc.), the resulting forcefield will be independent of the order in which the files are loaded. If, however, the same tag occurs in multiple files, the contents of the tags are merged, with the tags read later taking precedence over the parameters read earlier, provided the top-level tags have compatible attributes. The resulting force field will therefore depend on the order in which parameters are read.

This behavior is intended for limited use in appending very specific parameters, such as parameters specifying solvent models, to override standard parameters.

1.3.6 Units

To minimize the potential for unit conversion errors, SMIRNOFF forcefields explicitly specify units in a form readable to both humans and computers for all unit-bearing quantities. Allowed values for units are given in simtk.unit (though in the future this may change to the more widely-used Python pint library). For example,

for the `angle` (equilibrium angle) and `k` (force constant) parameters in the `<Angle>` example block above, both attributes are specified as a mathematical expression

```
<Angle smirks="[#1:1]-[#6X4:2]-[#1:3]" angle="109.50*degree" k="70.0*kilocalorie_per_mole/radian**2"/>
```

For more information, see the standard OpenMM unit system.

1.3.7 SMIRNOFF independently applies parameters to each class of potential energy terms

The SMIRNOFF uses direct chemical perception to assign parameters for potential energy terms independently for each term. Rather than first applying atom typing rules and then looking up combinations of the resulting atom types for each force term, the rules for directly applying parameters to atoms is compartmentalized in separate sections. The file consists of multiple top-level tags defining individual components of the potential energy (in addition to charge models or modifiers), with each section specifying the typing rules used to assign parameters for that potential term:

```
<Bonds version="0.3" potential="harmonic">
   <Bond smirks="[#6X4:1]-[#6X4:2]" length="1.526*angstrom" k="620.0*kilocalories_per_mole/angstrom**2"/
↪>
   <Bond smirks="[#6X4:1]-[#1:2]" length="1.090*angstrom" k="680.0*kilocalories_per_mole/angstrom**2"/>
   ...
</Bonds>

<Angles version="0.3" potential="harmonic">
   <Angle smirks="[a,A:1]-[#6X4:2]-[a,A:3]" angle="109.50*degree" k="100.0*kilocalories_per_mole/
↪radian**2"/>
   <Angle smirks="[#1:1]-[#6X4:2]-[#1:3]" angle="109.50*degree" k="70.0*kilocalories_per_mole/radian**2
↪"/>
   ...
</Angles>
```

Each top-level tag specifying a class of potential energy terms has an attribute `potential` for specifying the functional form for the interaction. Common defaults are defined, but the goal is to eventually allow these to be overridden by alternative choices or even algebraic expressions in the future, once more molecular simulation packages support general expressions. We distinguish between functional forms available in all common molecular simulation packages (specified by keywords) and support for general functional forms available in a few packages (especially OpenMM, which supports a flexible set of custom forces defined by algebraic expressions) with an **EXPERIMENTAL** label.

Many of the specific forces are implemented as discussed in the OpenMM Documentation; see especially Section 19 on Standard Forces for mathematical descriptions of these functional forms. Some top-level tags provide attributes that modify the functional form used to be consistent with packages such as AMBER or CHARMM.

1.3.8 Partial charge and electrostatics models

SMIRNOFF supports several approaches to specifying electrostatic models. Currently, only classical fixed point charge models are supported, but future extensions to the specification will support point multipoles, point polarizable dipoles, Drude oscillators, charge equilibration methods, and so on.

<LibraryCharges>: Library charges for polymeric residues and special solvent models

Warning: This functionality is not yet implemented and will appear in a future version of the toolkit. Please see [Issue 25 on the Open Force Field Toolkit issue tracker](https://github.com/openforcefield/openforcefield/issues/25).

A mechanism is provided for specifying library charges that can be applied to molecules or residues that match provided templates. Library charges are applied first, and atoms for which library charges are applied will be excluded from alternative charging schemes listed below.

For example, to assign partial charges for a non-terminal ALA residue from the AMBER ff14SB parameter set:

```
<LibraryCharges version="0.3">
   <!-- match a non-terminal alanine residue with AMBER ff14SB partial charges-->
   <LibraryCharge name="ALA" smirks="[NX3:1]([#1:2])([#6])[#6H1:3]([#1:4])([#6:5]([#1:6])([#1:7])[
↪#1:8])[#6:9](=[#8:10])[#7]" charge1="-0.4157*elementary_charge" charge2="0.2719*elementary_charge"␣
↪charge3="0.0337*elementary_charge" charge4="0.0823*elementary_charge" charge5="-0.1825*elementary_
↪charge" charge6="0.0603*elementary_charge" charge7="0.0603*elementary_charge" charge8="0.
↪0603*elementary_charge" charge9="0.5973*elementary_charge" charge10="-0.5679*elementary_charge">
   ...
</LibraryCharges>
```

In this case, a SMIRKS string defining the residue tags each atom that should receive a partial charge, with the charges specified by attributes `charge1`, `charge2`, etc. The `name` attribute is optional. Note that, for a given template, chemically equivalent atoms should be assigned the same charge to avoid undefined behavior. If the template matches multiple non-overlapping sets of atoms, all such matches will be assigned the provided charges. If multiple templates match the same set of atoms, the last template specified will be used.

Solvent models or excipients can also have partial charges specified via the `<LibraryCharges>` tag. For example, to ensure water molecules are assigned partial charges for TIP3P water, we can specify a library charge entry:

```
<LibraryCharges version="0.3">
   <!-- TIP3P water oxygen with charge override -->
   <LibraryCharge name="TIP3P" smirks="[#1:1]-[#8X2H2+0:2]-[#1:3]" charge1="+0.417*elementary_charge"␣
↪charge2="-0.834*elementary_charge" charge3="+0.417*elementary_charge"/>
</LibraryCharges>
```

<ChargeIncrementModel>: Small molecule and fragment charges

Warning: This functionality is not yet implemented and will appear in a future version of the toolkit. This area of the SMIRNOFF spec is under further consideration. Please see [Issue 208 on the Open Force Field Toolkit issue tracker](https://github.com/openforcefield/openforcefield/issues/208).

In keeping with the AMBER force field philosophy, especially as implemented in small molecule force fields such as GAFF, GAFF2, and parm@Frosst, partial charges for small molecules are usually assigned using a quantum chemical method (usually a semiempirical method such as AM1) and a partial charge determination scheme (such as CM2 or RESP), then subsequently corrected via charge increment rules, as in the highly successful AM1-BCC approach.

Here is an example:

```
<ChargeIncrementModel version="0.3" number_of_conformers="10" quantum_chemical_method="AM1" partial_
↪charge_method="CM2">
  <!-- A fractional charge can be moved along a single bond -->
  <ChargeIncrement smirks="[#6X4:1]-[#6X3a:2]" chargeincrement1="-0.0073*elementary_charge"␣
↪chargeincrement2="+0.0073*elementary_charge"/>
  <ChargeIncrement smirks="[#6X4:1]-[#6X3a:2]-[#7]" chargeincrement1="+0.0943*elementary_charge"␣
↪chargeincrement2="-0.0943*elementary_charge"/>
  <ChargeIncrement smirks="[#6X4:1]-[#8:2]" chargeincrement1="-0.0718*elementary_charge"␣
↪chargeincrement2="+0.0718*elementary_charge"/>
  <!--- Alternatively, factional charges can be redistributed among any number of bonded atoms -->
  <ChargeIncrement smirks="[N:1](H:2)(H:3)" chargeincrement1="+0.02*elementary_charge" chargeincrement2=
↪"-0.01*elementary_charge" chargeincrement3="-0.01*elementary_charge"/>
</ChargeIncrementModel>
```

The sum of formal charges for the molecule or fragment will be used to determine the total charge the molecule or fragment will possess.

`<ChargeIncrementModel>` provides several optional attributes to control its behavior:

- The `number_of_conformers` attribute (default: `"10"`) is used to specify how many conformers will be generated for the molecule (or capped fragment) prior to charging.
- The `quantum_chemical_method` attribute (default: `"AM1"`) is used to specify the quantum chemical method applied to the molecule or capped fragment.
- The `partial_charge_method` attribute (default: `"CM2"`) is used to specify how uncorrected partial charges are to be generated from the quantum chemical wavefunction. Later additions will add restrained electrostatic potential fitting (RESP) capabilities.

The `<ChargeIncrement>` tags specify how the quantum chemical derived charges are to be corrected to produce the final charges. The `chargeincrement#` attributes specify how much the charge on the associated tagged atom index (replacing #) should be modified. The sum of charge increments should equal zero.

Note that atoms for which library charges have already been applied are excluded from charging via `<ChargeIncrementModel>`.

Future additions will provide options for intelligently fragmenting large molecules and biopolymers, as well as a `capping` attribute to specify how fragments with dangling bonds are to be capped to allow these groups to be charged.

<ToolkitAM1BCC>: Temporary support for toolkit-based AM1-BCC partial charges

Warning: Until *<ChargeIncrementModel>* is implemented, support for the *<ToolkitAM1BCC>* tag has been enabled in the toolkit. This tag is not permanent and may be phased out in future versions of the spec.

This tag calculates partial charges using the default settings of the highest-priority cheminformatics toolkit that can perform AM1-BCC charge assignment. Currently, if the OpenEye toolkit is licensed and available, this will use QuacPac configured to generate charges using AM1-BCC ELF10 for each unique molecule in the topology. Otherwise RDKit will be used for initial conformer generation and the AmberTools antechamber/sqm software will be used for charge calculation.

If this tag is specified for a force field, conformer generation will be performed regardless of whether conformations of the input molecule were provided. If RDKit/AmberTools are used as the toolkit backend for this calculation, only the first conformer is used for AM1-BCC calculation.

The charges generated by this tag may differ depending on which toolkits are available.

Note that atoms for which prespecified or library charges have already been applied are excluded from charging via <ToolkitAM1BCC>.

Prespecified charges (reference implementation only)

In our reference implementation of SMIRNOFF in the openforcefield toolkit, we also provide a method for specifying user-defined partial charges during system creation. This functionality is accessed by using the charge_from_molecules optional argument during system creation, such as in ForceField.create_openmm_system(topology, charge_from_molecules=molecule_list). When this optional keyword is provided, all matching molecules will have their charges set by the entries in molecule_list. This method is provided solely for convenience in developing and exploring alternative charging schemes; actual force field releases for distribution will use one of the other mechanisms specified above.

1.3.9 Parameter sections

A SMIRNOFF force field consists of one or more force field term definition sections. For the most part, these sections independently define how a specific component of the potential energy function for a molecular system is supposed to be computed (such as bond stretch energies, or Lennard-Jones interactions), as well as how parameters are to be assigned for this particular term. Each parameter section contains a version, which encodes the behavior of the section, as well as the required and optional attributes the top-level tag and SMIRKS-based parameters. This decoupling of how parameters are assigned for each term provides a great deal of flexibility in composing new force fields while allowing a minimal number of parameters to be used to achieve accurate modeling of intramolecular forces.

Below, we describe the specification for each force field term definition using the XML representation of a SMIRNOFF force field.

As an example of a complete SMIRNOFF force field specification, see the prototype SMIRNOFF99Frosst offxml.

Note: Not all parameter sections *must* be specified in a SMIRNOFF force field. A wide variety of force field terms are provided in the specification, but a particular force field only needs to define a subset of those terms.

<vdW>

van der Waals force parameters, which include repulsive forces arising from Pauli exclusion and attractive forces arising from dispersion, are specified via the <vdW> tag with sub-tags for individual Atom entries, such as:

```
<vdW version="0.3" potential="Lennard-Jones-12-6" combining_rules="Lorentz-Berthelot" scale12="0.0"␣
↪scale13="0.0" scale14="0.5" scale15="1.0" switch_width="8.0*angstrom" cutoff="9.0*angstrom" long_
↪range_dispersion="isotropic">
   <Atom smirks="[#1:1]" sigma="1.4870*angstrom" epsilon="0.0157*kilocalories_per_mole"/>
   <Atom smirks="[#1:1]-[#6]" sigma="1.4870*angstrom" epsilon="0.0157*kilocalories_per_mole"/>
   ...
</vdW>
```

For standard Lennard-Jones 12-6 potentials (specified via potential="Lennard-Jones-12-6"), the epsilon parameter denotes the well depth, while the size property can be specified either via providing the sigma

attribute, such as `sigma="1.3*angstrom"`, or via the `r_0/2` (`rmin/2`) values used in AMBER force fields (here denoted `rmin_half` as in the example above). The two are related by `r0 = 2^(1/6)*sigma` and conversion is done internally in `ForceField` into the `sigma` values used in OpenMM.

Attributes in the <vdW> tag specify the scaling terms applied to the energies of 1-2 (`scale12`, default: 0), 1-3 (`scale13`, default: 0), 1-4 (`scale14`, default: 0.5), and 1-5 (`scale15`, default: 1.0) interactions, as well as the distance at which a switching function is applied (`switch_width`, default: `"1.0*angstrom"`), the cutoff (`cutoff`, default: `"9.0*angstroms"`), and long-range dispersion treatment scheme (`long_range_dispersion`, default: `"isotropic"`).

The `potential` attribute (default: `"none"`) specifies the potential energy function to use. Currently, only `potential="Lennard-Jones-12-6"` is supported:

```
U(r) = 4*epsilon*((sigma/r)^12 - (sigma/r)^6)
```

The `combining_rules` attribute (default: `"none"`) currently only supports `"Lorentz-Berthelot"`, which specifies the geometric mean of `epsilon` and arithmetic mean of `sigma`. Support for other Lennard-Jones mixing schemes will be added later: `Waldman-Hagler`, `Fender-Halsey`, `Kong`, `Tang-Toennies`, `Pena`, `Hudson-McCoubrey`, `Sikora`.

Later revisions will add support for additional potential types (e.g., `Buckingham-exp-6`), as well as the ability to support arbitrary algebraic functional forms using a scheme such as

```
<vdW version="0.3" potential="4*epsilon*((sigma/r)^12-(sigma/r)^6)" scale12="0.0" scale13="0.0" scale14=
↪"0.5" scale15="1" switch_width="8.0*angstrom" cutoff="9.0*angstrom" long_range_dispersion="isotropic">
   <CombiningRules>
      <CombiningRule parameter="sigma" function="(sigma1+sigma2)/2"/>
      <CombiningRule parameter="epsilon" function="sqrt(epsilon1*epsilon2)"/>
   </CombiningRules>
   <Atom smirks="[#1:1]" sigma="1.4870*angstrom" epsilon="0.0157*kilocalories_per_mole"/>
   <Atom smirks="[#1:1]-[#6]" sigma="1.4870*angstrom" epsilon="0.0157*kilocalories_per_mole"/>
   ...
</vdW>
```

If the <CombiningRules> tag is provided, it overrides the `combining_rules` attribute.

Later revisions will also provide support for special interactions using the <AtomPair> tag:

```
<vdW version="0.3" potential="Lennard-Jones-12-6" combining_rules="Lorentz-Berthelot" scale12="0.0"␣
↪scale13="0.0" scale14="0.5" scale15="1">
   <AtomPair smirks1="[#1:1]" smirks2="[#6:2]" sigma="1.4870*angstrom" epsilon="0.0157*kilocalories_per_
↪mole"/>
   ...
</vdW>
```

vdW section tag version	Tag attributes and default values	Required parameter attributes	Optional parameter attributes
0.3	potential="Lennard-Jones-12-6", combining_rules="Lorentz-Berthelot", scale12="0", scale13="0", scale14="0.5", scale15="1.0", cutoff="9.0*angstrom", switch_width="1.0*angstrom", method="cutoff"	smirks, epsilon, (sigma OR rmin_half)	id, parent_id

<Electrostatics>

Electrostatic interactions are specified via the <Electrostatics> tag.

```
<Electrostatics version="0.3" method="PME" scale12="0.0" scale13="0.0" scale14="0.833333" scale15="1.0"/
↪>
```

The method attribute specifies the manner in which electrostatic interactions are to be computed:

- PME - particle mesh Ewald should be used (DEFAULT); can only apply to periodic systems
- reaction-field - reaction-field electrostatics should be used; can only apply to periodic systems
- Coulomb - direct Coulomb interactions (with no reaction-field attenuation) should be used

The interaction scaling parameters applied to atoms connected by a few bonds are

- scale12 (default: 0) specifies the scaling applied to 1-2 bonds
- scale13 (default: 0) specifies the scaling applied to 1-3 bonds
- scale14 (default: 0.833333) specifies the scaling applied to 1-4 bonds
- scale15 (default: 1.0) specifies the scaling applied to 1-5 bonds

Currently, no child tags are used because the charge model is specified via different means (currently library charges or BCCs).

For methods where the cutoff is not simply an implementation detail but determines the potential energy of the system (reaction-field and Coulomb), the cutoff distance must also be specified, and a switch_width if a switching function is to be used.

Electrostatics section tag version	Tag attributes and default values	Required parameter attributes	Optional parameter attributes
0.3	scale12="0", scale13="0", scale14="0.833333", scale15="1.0", cutoff="9.0*angstrom", switch_width="0*angstrom", method="PME"	N/A	N/A

<Bonds>

Bond parameters are specified via a <Bonds>...</Bonds> block, with individual <Bond> tags containing attributes specifying the equilibrium bond length (length) and force constant (k) values for specific bonds. For example:

```
<Bonds version="0.3" potential="harmonic">
  <Bond smirks="[#6X4:1]-[#6X4:2]" length="1.526*angstrom" k="620.0*kilocalories_per_mole/angstrom**2"/
↪>
  <Bond smirks="[#6X4:1]-[#1:2]" length="1.090*angstrom" k="680.0*kilocalories_per_mole/angstrom**2"/>
  ...
</Bonds>
```

Currently, only potential="harmonic" is supported, where we utilize the standard harmonic functional form:

```
U(r) = (k/2)*(r-length)^2
```

Later revisions will add support for additional potential types and the ability to support arbitrary algebraic functional forms. If the potential attribute is omitted, it defaults to harmonic.

Note that AMBER and CHARMM define a modified functional form, such that `U(r) = k*(r-length)^2`, so that force constants would need to be multiplied by two in order to be used in the SMIRNOFF format.

Constrained bonds are handled by a separate `<Constraints>` tag, which can either specify constraint distances or draw them from equilibrium distances specified in `<Bonds>`.

Fractional bond orders (EXPERIMENTAL)

Warning: This functionality is not yet implemented and will appear in a future version of the toolkit.

Fractional bond orders can be used to allow interpolation of bond parameters. For example, these parameters:

```
<Bonds version="0.3" potential="harmonic">
    <Bond smirks="[#6X3:1]-[#6X3:2]" k="820.0*kilocalories_per_mole/angstrom**2" length="1.45*angstrom"/
↪>
    <Bond smirks="[#6X3:1]:[#6X3:2]" k="938.0*kilocalories_per_mole/angstrom**2" length="1.40*angstrom"/
↪>
    <Bond smirks="[#6X3:1]=[#6X3:2]" k="1098.0*kilocalories_per_mole/angstrom**2" length="1.35*angstrom
↪"/>
    ...
```

can be replaced by a single parameter line by first invoking the `fractional_bondorder_method` attribute to specify a method for computing the fractional bond order and `fractional_bondorder_interpolation` for specifying the procedure for interpolating parameters between specified integral bond orders:

```
<Bonds version="0.3" potential="harmonic" fractional_bondorder_method="Wiberg" fractional_bondorder_
↪interpolation="linear">
    <Bond smirks="[#6X3:1]!#[#6X3:2]" k_bondorder1="820.0*kilocalories_per_mole/angstrom**2" k_
↪bondorder2="1098*kilocalories_per_mole/angstrom**2" length_bondorder1="1.45*angstrom" length_
↪bondorder2="1.35*angstrom"/>
    ...
```

This allows specification of force constants and lengths for bond orders 1 and 2, and then interpolation between those based on the partial bond order.

- `fractional_bondorder_method` defaults to `none`, but the `Wiberg` method is supported.
- `fractional_bondorder_interpolation` defaults to `linear`, which is the only supported scheme for now.

Bonds section tag version	Tag attributes and default values	Required parameter attributes	Optional parameter attributes
0.3	`potential="harmonic"`, `fractional_bondorder_method="none"`, `fractional_bondorder_interpolation="linear"`	`smirks`, `length`, `k`	`id`, `parent_id`

`<Angles>`

Angle parameters are specified via an `<Angles>...</Angles>` block, with individual `<Angle>` tags containing attributes specifying the equilibrium angle (`angle`) and force constant (`k`), as in this example:

```
<Angles version="0.3" potential="harmonic">
   <Angle smirks="[a,A:1]-[#6X4:2]-[a,A:3]" angle="109.50*degree" k="100.0*kilocalories_per_mole/
↪radian**2"/>
   <Angle smirks="[#1:1]-[#6X4:2]-[#1:3]" angle="109.50*degree" k="70.0*kilocalories_per_mole/radian**2
↪"/>
   ...
</Angles>
```

Currently, only `potential="harmonic"` is supported, where we utilize the standard harmonic functional form:

```
U(r) = (k/2)*(theta-angle)^2
```

Later revisions will add support for additional potential types and the ability to support arbitrary algebraic functional forms. If the `potential` attribute is omitted, it defaults to `harmonic`.

Note that AMBER and CHARMM define a modified functional form, such that `U(r) = k*(theta-angle)^2`, so that force constants would need to be multiplied by two in order to be used in the SMIRNOFF format.

Angles section tag version	Tag attributes and default values	Required parameter attributes	Optional parameter attributes
0.3	`potential="harmonic"`	`smirks`, `angle`, `k`	`id`, `parent_id`

<ProperTorsions>

Proper torsions are specified via a `<ProperTorsions>...</ProperTorsions>` block, with individual `<Proper>` tags containing attributes specifying the periodicity (`periodicity#`), phase (`phase#`), and barrier height (`k#`).

```
<ProperTorsions version="0.3" potential="k*(1+cos(periodicity*theta-phase))">
   <Proper smirks="[a,A:1]-[#6X4:2]-[#6X4:3]-[a,A:4]" idivf1="9" periodicity1="3" phase1="0.0*degree"␣
↪k1="1.40*kilocalories_per_mole"/>
   <Proper smirks="[#6X4:1]-[#6X4:2]-[#8X2:3]-[#6X4:4]" idivf1="1" periodicity1="3" phase1="0.0*degree"␣
↪k1="0.383*kilocalories_per_mole" idivf2="1" periodicity2="2" phase2="180.0*degree" k2="0.
↪1*kilocalories_per_mole"/>
   ...
</ProperTorsions>
```

Here, child `Proper` tags specify at least `k1`, `phase1`, and `periodicity1` attributes for the corresponding parameters of the first force term applied to this torsion. However, additional values are allowed in the form `k#`, `phase#`, and `periodicity#`, where all `#` values must be consecutive (e.g., it is impermissible to specify `k1` and `k3` values without a `k2` value) but `#` can go as high as necessary.

For convenience, and optional attribute specifies a torsion multiplicity by which the barrier height should be divided (`idivf#`). The default behavior of this attribute can be controlled by the top-level attribute `default_idivf` (default: `"auto"`) for `<ProperTorsions>`, which can be an integer (such as `"1"`) controlling the value of `idivf` if not specified or `"auto"` if the barrier height should be divided by the number of torsions impinging on the central bond. For example:

```
<ProperTorsions version="0.3" potential="k*(1+cos(periodicity*theta-phase))" default_idivf="auto">
   <Proper smirks="[a,A:1]-[#6X4:2]-[#6X4:3]-[a,A:4]" periodicity1="3" phase1="0.0*degree" k1="1.
↪40*kilocalories_per_mole"/>
   ...
</ProperTorsions>
```

Currently, only `potential="k*(1+cos(periodicity*theta-phase))"` is supported, where we utilize the functional form:

```
U = \sum_{i=1}^N k_i * (1 + cos(periodicity_i * phi - phase_i))
```

Note: **AMBER defines a modified functional form**, such that *U = sum_{i=1}^N (k_i/2) * (1 + cos(periodicity_i * phi - phase_i))*, so that barrier heights would need to be divided by two in order to be used in the SMIRNOFF format.

If the `potential` attribute is omitted, it defaults to `k*(1+cos(periodicity*theta-phase))`.

ProperTorsions section tag version	Tag attributes and default values	Required parameter attributes	Optional parameter attributes
0.3	`potential="k*(1+cos(periodicity*theta-phase))"`, `default_idivf="auto"`	`smirks`, k, phase, periodicity	`idivf`, `id`, `parent_id`

<ImproperTorsions>

Improper torsions are specified via an `<ImproperTorsions>...</ImproperTorsions>` block, with individual `<Improper>` tags containing attributes that specify the same properties as `<ProperTorsions>`:

```
<ImproperTorsions version="0.3" potential="k*(1+cos(periodicity*theta-phase))">
    <Improper smirks="[*:1]~[#6X3:2](=[#7X2,#7X3+1:3])~[#7:4]" k1="10.5*kilocalories_per_mole"␣
↪periodicity1="2" phase1="180.*degree"/>
    ...
</ImproperTorsions>
```

Currently, only `potential="charmm"` is supported, where we utilize the functional form:

```
U = \sum_{i=1}^N k_i * (1 + cos(periodicity_i * phi - phase_i))
```

Note: **AMBER defines a modified functional form**, such that *U = sum_{i=1}^N (k_i/2) * (1 + cos(periodicity_i * phi - phase_i))*, so that barrier heights would need to be divided by two in order to be used in the SMIRNOFF format.

If the `potential` attribute is omitted, it defaults to `charmm`.

The improper torsion energy is computed as the average over all three impropers (all with the same handedness) in a trefoil. This avoids the dependence on arbitrary atom orderings that occur in more traditional typing engines such as those used in AMBER. The *second* atom in an improper (in the example above, the trivalent carbon) is the central atom in the trefoil.

ImproperTorsions section tag version	Tag attributes and default values	Required parameter attributes	Optional parameter attributes
0.3	`potential="k*(1+cos(periodicity*theta-phase))"`, `default_idivf="auto"`	`smirks`, k, phase, periodicity	`idivf`, `id`, `parent_id`

<GBSA>

Warning: This functionality is not yet implemented and will appear in a future version of the toolkit.

Generalized-Born surface area (GBSA) implicit solvent parameters are optionally specified via a <GBSA>...</GBSA> using <Atom> tags with GBSA model specific attributes:

```
<GBSA version="0.3" gb_model="OBC1" solvent_dielectric="78.5" solute_dielectric="1" sa_model="ACE"␣
↪surface_area_penalty="5.4*calories/mole/angstroms**2" solvent_radius="1.4*angstroms">
  <Atom smirks="[#1:1]" radius="0.12*nanometer" scale="0.85"/>
  <Atom smirks="[#1:1]~[#6]" radius="0.13*nanometer" scale="0.85"/>
  <Atom smirks="[#1:1]~[#8]" radius="0.08*nanometer" scale="0.85"/>
  <Atom smirks="[#1:1]~[#16]" radius="0.08*nanometer" scale="0.85"/>
  <Atom smirks="[#6:1]" radius="0.22*nanometer" scale="0.72"/>
  <Atom smirks="[#7:1]" radius="0.155*nanometer" scale="0.79"/>
  <Atom smirks="[#8:1]" radius="0.15*nanometer" scale="0.85"/>
  <Atom smirks="[#9:1]" radius="0.15*nanometer" scale="0.88"/>
  <Atom smirks="[#14:1]" radius="0.21*nanometer" scale="0.8"/>
  <Atom smirks="[#15:1]" radius="0.185*nanometer" scale="0.86"/>
  <Atom smirks="[#16:1]" radius="0.18*nanometer" scale="0.96"/>
  <Atom smirks="[#17:1]" radius="0.17*nanometer" scale="0.8"/>
</GBSA>
```

Supported Generalized Born (GB) models

In the <GBSA> tag, gb_model selects which GB model is used. Currently, this can be selected from a subset of the GBSA models available in OpenMM:

- HCT : Hawkins-Cramer-Truhlar (corresponding to igb=1 in AMBER): requires parameters [radius, scale]
- OBC1 : Onufriev-Bashford-Case using the GB(OBC)I parameters (corresponding to igb=2 in AMBER): requires parameters [radius, scale]
- OBC2 : Onufriev-Bashford-Case using the GB(OBC)II parameters (corresponding to igb=5 in AMBER): requires parameters [radius, scale]

If the gb_model attribute is omitted, it defaults to OBC1.

The attributes solvent_dielectric and solute_dielectric specify solvent and solute dielectric constants used by the GB model. In this example, radius and scale are per-particle parameters of the OBC1 GB model supported by OpenMM. Units are for these per-particle parameters (such as radius_units) specified in the <GBSA> tag.

Surface area (SA) penalty model

The sa_model attribute specifies the solvent-accessible surface area model ("SA" part of GBSA) if one should be included; if omitted, no SA term is included.

Currently, only the analytical continuum electrostatics (ACE) model, designated ACE, can be specified, but there are plans to add more models in the future, such as the Gaussian solvation energy component of EEF1. If sa_model is not specified, it defaults to ACE.

The ACE model permits two additional parameters to be specified:

- The surface_area_penalty attribute specifies the surface area penalty for the ACE model. (Default: 5.4 calories/mole/angstroms**2)
- The solvent_radius attribute specifies the solvent radius. (Default: 1.4 angstroms)

GBSA section tag version	Tag attributes and default values	Required parameter attributes	Optional parameter attributes
0.3	gb_model="OBC1", solvent_dielectric="78.5", solute_dielectric="1", sa_model="ACE", surface_area_penalty="5.4*calories/mole/angstrom**2", solvent_radius="1.4*angstrom"	smirks, radius, scale	id, parent_id

<Constraints>

Bond length or angle constraints can be specified through a <Constraints> block, which can constrain bonds to their equilibrium lengths or specify an interatomic constraint distance. Two atoms must be tagged in the smirks attribute of each <Constraint> record.

To constrain the separation between two atoms to their equilibrium bond length, it is critical that a <Bonds> record be specified for those atoms:

```
<Constraints version="0.3" >
  <!-- constrain all bonds to hydrogen to their equilibrium bond length -->
  <Constraint smirks="[#1:1]-[*:2]" />
</Constraints>
```

Note that the two atoms must be bonded in the specified Topology for the equilibrium bond length to be used.

To specify the constraint distance, or constrain two atoms that are not directly bonded (such as the hydrogens in rigid water models), specify the distance attribute (and optional distance_unit attribute for the <Constraints> tag):

```
<Constraints version="0.3">
  <!-- constrain water O-H bond to equilibrium bond length (overrides earlier constraint) -->
  <Constraint smirks="[#1:1]-[#8X2H2:2]-[#1]" distance="0.9572*angstrom"/>
  <!-- constrain water H...H, calculating equilibrium length from H-O-H equilibrium angle and H-O␣
↪equilibrium bond lengths -->
  <Constraint smirks="[#1:1]-[#8X2H2]-[#1:2]" distance="1.8532*angstrom"/>
</Constraints>
```

Typical molecular simulation practice is to constrain all bonds to hydrogen to their equilibrium bond lengths and enforce rigid TIP3P geometry on water molecules:

```
<Constraints version="0.3">
  <!-- constrain all bonds to hydrogen to their equilibrium bond length -->
  <Constraint smirks="[#1:1]-[*:2]" />
  <!-- TIP3P rigid water -->
  <Constraint smirks="[#1:1]-[#8X2H2:2]-[#1]" distance="0.9572*angstrom"/>
  <Constraint smirks="[#1:1]-[#8X2H2]-[#1:2]" distance="1.8532*angstrom"/>
</Constraints>
```

Constraint section tag version	Required tag attributes and default values	Required parameter attributes	Optional parameter attributes
0.3		smirks	distance

1.3.10 Advanced features

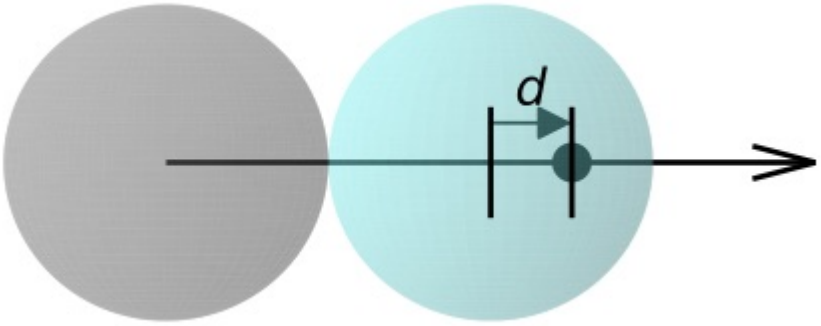
Standard usage is expected to rely primarily on the features documented above and potentially new features. However, some advanced features will also be supported.

`<VirtualSites>`: Virtual sites for off-atom charges

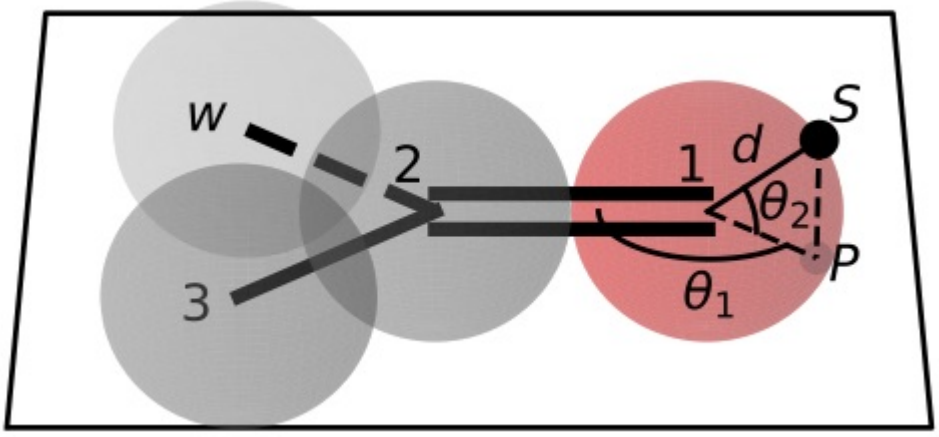
Warning: This functionality is not yet implemented and will appear in a future version of the toolkit

We will implement experimental support for placement of off-atom (off-center) charges in a variety of contexts which may be chemically important in order to allow easy exploration of when these will be warranted. We will support the following different types or geometries of off-center charges (as diagrammed below):

- `BondCharge`: This supports placement of a virtual site `S` along a vector between two specified atoms, e.g. to allow for a sigma hole for halogens or similar contexts. With positive values of the distance, the virtual site lies outside the first indexed atom (green in this image).

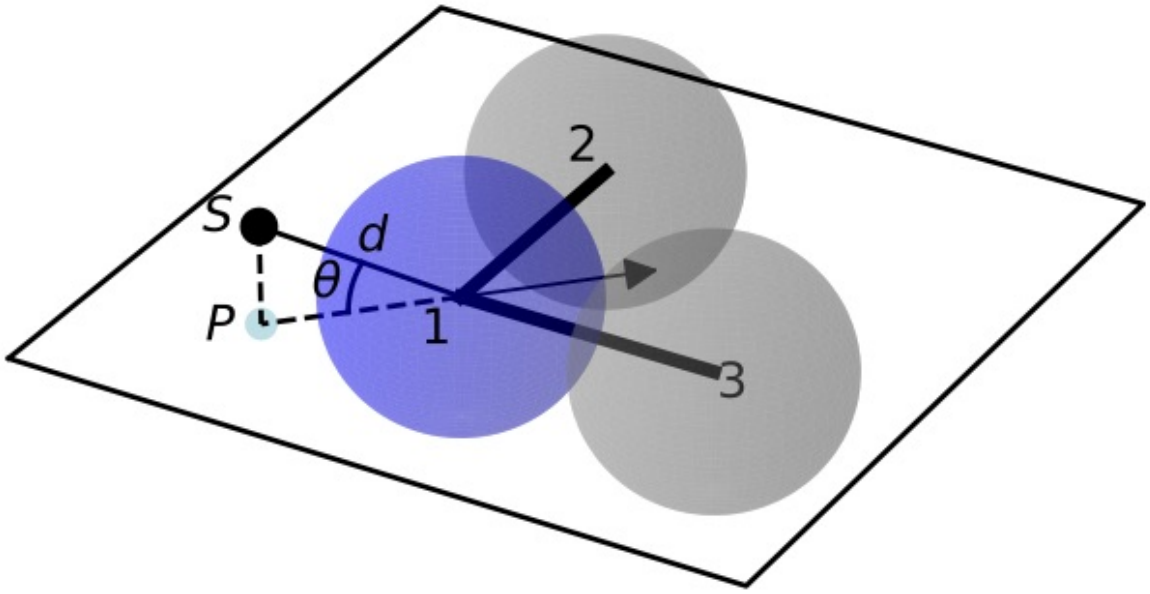


- `MonovalentLonePair`: This is originally intended for situations like a carbonyl, and allows placement of a virtual site `S` at a specified distance `d`, `inPlaneAngle` (theta 1 in the diagram), and `outOfPlaneAngle` (theta 2 in the diagram) relative to a central atom and two connected atoms.

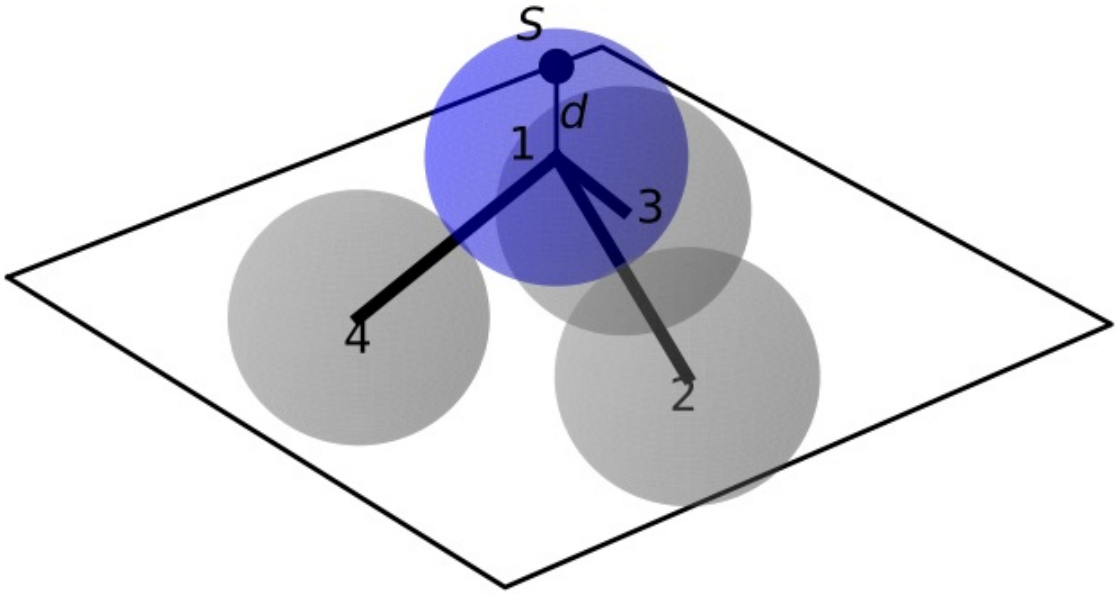


- `DivalentLonePair`: This is suitable for cases like four-point and five-point water models as well as pyrimidine; a charge site `S` lies a specified distance `d` from the central atom among three atoms (blue) along the bisector of the angle between the atoms (if `outOfPlaneAngle` is zero) or out of the plane by

the specified angle (if `outOfPlaneAngle` is nonzero) with its projection along the bisector. For positive values fo the distance `d` the virtual site lies outside the 2-1-3 angle and for negative values it lies inside.



- `TrivalentLonePair`: This is suitable for planar or tetrahedral nitrogen lone pairs; a charge site `S` lies above the central atom (e.g. nitrogen, blue) a distance `d` along the vector perpendicular to the plane of the three connected atoms (2,3,4). With positive values of `d` the site lies above the nitrogen and with negative values it lies below the nitrogen.



Each virtual site receives charge which is transferred from the desired atoms specified in the SMIRKS pattern via a `chargeincrement#` parameter, e.g., if `chargeincrement1=+0.1*elementary_charge` then the virtual site will receive a charge of -0.1 and the atom labeled `1` will have its charge adjusted upwards by +0.1. N may index any indexed atom. Increments which are left unspecified default to zero. Additionally, each virtual site can bear Lennard-Jones parameters, specified by `sigma` and `epsilon` or `rmin_half` and `epsilon`.

If unspecified these also default to zero.

In the SMIRNOFF format, these are encoded as:

```
<VirtualSites version="0.3">
    <!-- sigma hole for halogens: "distance" denotes distance along the 2->1 bond vector, measured from␣
↪atom 2 -->
    <!-- Specify that 0.2 charge from atom 1 and 0.1 charge units from atom 2 are to be moved to the␣
↪virtual site, and a small Lennard-Jones site is to be added (sigma = 0.1*angstroms, epsilon=0.05*kcal/
↪mol) -->
    <VirtualSite type="BondCharge" smirks="[Cl:1]-[C:2]" distance="0.30*angstrom" chargeincrement1="+0.
↪2*elementary_charge" chargeincrement2="+0.1*elementary_charge" sigma="0.1*angstrom" epsilon="0.
↪05*kilocalories_per_mole" />
    <!-- Charge increments can extend out to as many atoms as are labeled, e.g. with a third atom: -->
    <VirtualSite type="BondCharge" smirks="[Cl:1]-[C:2]~[*:3]" distance="0.30*angstrom"␣
↪chargeincrement1="+0.1*elementary_charge" chargeincrement2="+0.1*elementary_charge" chargeincrement3=
↪"+0.05*elementary_charge" sigma="0.1*angstrom" epsilon="0.05*kilocalories_per_mole" />
    <!-- monovalent lone pairs: carbonyl -->
    <!-- X denotes the charge site, and P denotes the projection of the charge site into the plane of 1␣
↪and 2. -->
    <!-- inPlaneAngle is angle point P makes with 1 and 2, i.e. P-1-2 -->
    <!-- outOfPlaneAngle is angle charge site (X) makes out of the plane of 2-1-3 (and P) measured from␣
↪1 -->
    <!-- Since unspecified here, sigma and epsilon for the virtual site default to zero -->
    <VirtualSite type="MonovalentLonePair" smirks="[O:1]=[C:2]-[*:3]" distance="0.30*angstrom"␣
↪outOfPlaneAngle="0*degree" inPlaneAngle="120*degree" chargeincrement1="+0.2*elementary_charge" />
    <!-- divalent lone pair: pyrimidine, TIP4P, TIP5P -->
    <!-- The atoms 2-1-3 define the X-Y plane, with Z perpendicular. If outOfPlaneAngle is 0, the␣
↪charge site is a specified distance along the in-plane vector which bisects the angle left by taking␣
↪360 degrees minus angle(2,1,3). If outOfPlaneAngle is nonzero, the charge sites lie out of the plane␣
↪by the specified angle (at the specified distance) and their in-plane projection lines along the angle
↪'s bisector. -->
    <VirtualSite type="DivalentLonePair" smirks="[*:2]~[#7X2:1]~[*:3]" distance="0.30*angstrom"␣
↪outOfPlaneAngle="0.0*degree" chargeincrement1="+0.1*elementary_charge" />
    <!-- trivalent nitrogen lone pair -->
    <!-- charge sites lie above and below the nitrogen at specified distances from the nitrogen, along␣
↪the vector perpendicular to the plane of (2,3,4) that passes through the nitrogen. If the nitrogen is␣
↪co-planar with the connected atom, charge sites are simply above and below the plane-->
    <!-- Positive and negative values refer to above or below the nitrogen as measured relative to the␣
↪plane of (2,3,4), i.e. below the nitrogen means nearer the 2,3,4 plane unless they are co-planar -->
    <VirtualSite type="TrivalentLonePair" smirks="[*:2]~[#7X3:1](~[*:4])~[*:3]" distance="0.30*angstrom
↪" chargeincrement1="+0.1*elementary_charge"/>
    <VirtualSite type="TrivalentLonePair" smirks="[*:2]~[#7X3:1](~[*:4])~[*:3]" distance="-0.30*angstrom
↪" chargeincrement1="+0.1*elementary_charge"/>
</VirtualSites>
```

Aromaticity models

Before conducting SMIRKS substructure searches, molecules are prepared using one of the supported aromaticity models, which must be specified with the `aromaticity_model` attribute. The only aromaticity model currently widely supported (by both the OpenEye toolkit and RDKit) is the `OEAroModel_MDL` model.

Additional plans for future development

See the openforcefield GitHub issue tracker to propose changes to this specification, or read through proposed changes currently being discussed.

1.3.11 The `openforcefield` reference implementation

A Python reference implementation of a parameterization engine implementing the SMIRNOFF force field specification can be found online. This implementation can use either the free-for-academics (but commercially supported) OpenEye toolkit or the free and open source RDKit cheminformatics toolkit. See the installation instructions for information on how to install this implementation and its dependencies.

Examples

A relatively extensive set of examples is made available on the reference implementation repository under examples/.

Parameterizing a system

Consider parameterizing a simple system containing a the drug imatinib.

```
# Create a molecule from a mol2 file
from openforcefield.topology import Molecule
molecule = Molecule.from_file('imatinib.mol2')

# Create a Topology specifying the system to be parameterized containing just the molecule
topology = molecule.to_topology()

# Load the smirnoff99Frosst forcefield
from openforcefield.typing.engines import smirnoff
forcefield = smirnoff.ForceField('test_forcefields/smirnoff99Frosst.offxml')

# Create an OpenMM System from the topology
system = forcefield.create_openmm_system(topology)
```

See `examples/SMIRNOFF_simulation/` for an extension of this example illustrating to simulate this molecule in the gas phase.

The `topology` object provided to `create_openmm_system()` can contain any number of molecules of different types, including biopolymers, ions, buffer molecules, or solvent molecules. The openforcefield toolkit provides a number of convenient methods for importing or constructing topologies given PDB files, Sybyl mol2 files, SDF files, SMILES strings, and IUPAC names; see the toolkit documentation for more information. Notably, this `topology` object differs from those found in OpenMM or MDTraj in that it contains information on the *chemical identity* of the molecules constituting the system, rather than this atomic elements and covalent connectivity; this additional chemical information is required for the direct chemical perception features of SMIRNOFF typing.

Using SMIRNOFF small molecule forcefields with traditional biopolymer force fields

While SMIRNOFF format force fields can cover a wide range of biological systems, our initial focus is on gneral small molecule force fields, meaning that users may have considerable interest in combining SMIRNOFF small molecule parameters to systems in combination with traditional biopolymer parameters from conventional force fields, such as the AMBER family of protein/nucleic acid force fields. Thus, we provide an example of setting up a mixed protein-ligand system in examples/mixedFF_structure, where an AMBER family force field is used for a protein and smirnoff99Frosst for a small molecule.

The optional `id` and `parent_id` attributes and other XML attributes

In general, additional optional XML attributes can be specified and will be ignored by `ForceField` unless they are specifically handled by the parser (and specified in this document).

One attribute we have found helpful in parameter file development is the `id` attribute for a specific parameter line, and we *recommend* that SMIRNOFF force fields utilize this as effectively a parameter serial number, such as in:

```
<Bond smirks="[#6X3:1]-[#6X3:2]" id="b5" k="820.0*kilocalorie_per_mole/angstrom**2" length="1.
↪45*angstrom"/>
```

Some functionality in `ForceField`, such as `ForceField.label_molecules`, looks for the `id` attribute. Without this attribute, there is no way to uniquely identify a specific parameter line in the XML file without referring to it by its smirks string, and since some smirks strings can become long and relatively unwieldy (especially for torsions) this provides a more human- and search-friendly way of referring to specific sets of parameters.

The `parent_id` attribute is also frequently used to denote parameters from which the current parameter is derived in some manner.

A remark about parameter availability

`ForceField` will currently raise an exception if any parameters are missing where expected for your system—i.e. if a bond is assigned no parameters, an exception will be raised. However, use of generic parameters (i.e. `[*:1]~[*:2]` for a bond) in your `.offxml` will result in parameters being assigned everywhere, bypassing this exception. We recommend generics be used sparingly unless it is your intention to provide true universal generic parameters.

1.3.12 Version history

0.3

This is a backwards-incompatible update to the SMIRNOFF 0.2 draft specification. However, the Open Force Field Toolkit version accompanying this update is capable of converting 0.1 spec SMIRNOFF data to 0.2 spec, and subsequently 0.2 spec to 0.3 spec. The 0.1-to-0.2 spec conversion makes a number of assumptions about settings such as long-range nonbonded handling. Warnings are printed about each assumption that is made during this spec conversion. No mechanism to convert backwards in spec is provided.

Key changes in this version of the spec are:

- Section headers now contain individual versions, instead of relying on the `<SMIRNOFF>`-level tag.
- Section headers no longer contain `X_unit` attributes.
- All physical quantities are now written as expressions containing the appropriate units.
- The default potential for `<ProperTorsions>` and `<ImproperTorsions>` was changed from `charmm` to `k*(1+cos(periodicity*theta-phase))`, as CHARMM interprets torsion terms with perioidicity 0 as having a quadratic potential, while the Open Force Field Toolkit would interpret a zero periodicity literally.

0.2

This is a backwards-incompatible overhaul of the SMIRNOFF 0.1 draft specification along with `ForceField` implementation refactor:

- Aromaticity model now defaults to `OEAroModel_MDL`, and aromaticity model names drop OpenEye-specific prefixes
- Top-level tags are now required to specify units for any unit-bearing quantities to avoid the potential for mistakes from implied units.
- Potential energy component definitions were renamed to be more general:
  - `<NonbondedForce>` was renamed to `<vdW>`
  - `<HarmonicBondForce>` was renamed to `<Bonds>`
  - `<HarmonicAngleForce>` was renamed to `<Angles>`
  - `<BondChargeCorrections>` was renamed to `<ChargeIncrementModel>` and generalized to accommodate an arbitrary number of tagged atoms
  - `<GBSAForce>` was renamed to `<GBSA>`
- `<PeriodicTorsionForce>` was split into `<ProperTorsions>` and `<ImproperTorsions>`
- `<vdW>` now specifies 1-2, 1-3, 1-4, and 1-5 scaling factors via `scale12` (default: 0), `scale13` (default: 0), `scale14` (default: 0.5), and `scale15` (default 1.0) attributes. It also specifies the long-range vdW method to use, currently supporting `cutoff` (default) and `PME`. Coulomb scaling parameters have been removed from `StericsForce`.
- Added the `<Electrostatics>` tag to separately specify 1-2, 1-3, 1-4, and 1-5 scaling factors for electrostatics, as well as the method used to compute electrostatics (`PME`, `reaction-field`, `Coulomb`) since this has a huge effect on the energetics of the system.
- Made it clear that `<Constraint>` entries do not have to be between bonded atoms.
- `<VirtualSites>` has been added, and the specification of charge increments harmonized with `<ChargeIncrementModel>`
- The `potential` attribute was added to most forces to allow flexibility in extending forces to additional functional forms (or algebraic expressions) in the future. `potential` defaults to the current recommended scheme if omitted.
- `<GBSA>` now has defaults specified for `gb_method` and `sa_method`
- Changes to how fractional bond orders are handled:
  - Use of fractional bond order is now are specified at the force tag level, rather than the root level
  - The fractional bond order method is specified via the `fractional_bondorder_method` attribute
  - The fractional bond order interpolation scheme is specified via the `fractional_bondorder_interpolation`
- Section heading names were cleaned up.
- Example was updated to reflect use of the new `openforcefield.topology.Topology` class
- Eliminated "Requirements" section, since it specified requirements for the software, rather than described an aspect of the SMIRNOFF specification
- Fractional bond orders are described in `<Bonds>`, since they currently only apply to this term.

0.1

Initial draft specification.

1.4 Examples using SMIRNOFF with the toolkit

The following examples are available in the openforcefield toolkit repository:

1.4.1 Index of provided examples

- SMIRNOFF_simulation - simulation of a molecule in the gas phase with the SMIRNOFF forcefield format
- forcefield_modification - modify forcefield parameters and evaluate how system energy changes
- using_smirnoff_in_amber_or_gromacs - convert a System generated with the Open Forcefield Toolkit, which can be simulated natively with OpenMM, into AMBER prmtop/inpcrd and GROMACS top/gro input files through the ParmEd library.
- inspect_assigned_parameters - check which parameters are used in which molecules and generate parameter usage statistics.
- using_smirnoff_with_amber_protein_forcefield - use SMIRNOFF parameters for small molecules in combination with more conventional force fields for proteins and other components of your system (using ParmEd to combine parameterized structures)

1.5 Developing for the toolkit

1.5.1 Style guide

Development for the `openforcefield` toolkit conforms to the recommendations given by the Software Development Best Practices for Computational Chemistry guide.

The naming conventions of classes, functions, and variables follows PEP8, consistently with the best practices guide. The naming conventions used in this library not covered by PEP8 are: - Use `file_path`, `file_name`, and `file_stem` to indicate `path/to/stem.extension`, `stem.extension`, and `stem` respectively, consistently with the variables in the standard `pathlib` library. - Use `n_x` to abbreviate "number of X' (e.g. *n_atoms*, *n_molecules*).

1.5.2 Contributing

We always welcome GitHub pull requests. For bug fixes, major feature additions, or refactoring, please raise an issue on the GitHub issue tracker first to ensure the design will be amenable to current developer plans.

1.5.3 How can I become a developer?

If you would like to contribute, please post an issue on the GitHub issue tracker describing the contribution you would like to make to start a discussion.

1.6 Frequently asked questions (FAQ)

1.6.1 Input files for applying SMIRNOFF parameters

SMIRNOFF force fields use direct chemical perception meaning that, unlike many molecular mechanics (MM) force fields, they apply parameters based on substructure searches acting directly on molecules. This creates unique opportunities and allows them to encode a great deal of chemistry quite simply, but it also means that the *starting point* for parameter assignment must be well-defined chemically, giving not just the elements and connectivity for all of the atoms of all of the components of your system, but also providing the formal charges and bond orders.

Specifically, to apply SMIRNOFF to a system, you must either:

1. Provide Open Force Field Toolkit `Molecule` objects corresponding to the components of your system, or
2. Provide an OpenMM `Topology` which includes bond orders and thus can be converted to molecules corresponding to the components of your system

Without this information, our direct chemical perception cannot be applied to your molecule, as it requires the chemical identity of the molecules in your system – that is, bond order and formal charge as well as atoms and connectivity. Unless you provide the full chemical identity in this sense, we must attempt to guess or infer the chemical identity of your molecules, which is a recipe for trouble. Different molecules can have the same chemical graph but differ in bond order and formal charge, or different resonance structures may be treated rather differently by some force fields (e.g. `c1cc(ccc1c2cc[nH+]cc2)[O-]` vs `C1=CC(C=CC1=C2C=CNC=C2)=O`, where the central bond is rotatable in one resonance structure but not in the other) even though they have identical formal charge and connectivity (chemical graph). A force field which uses the chemical identity of molecules to assign parameters needs to know the exact chemical identity of the molecule you are intending to parameterize.

1.6.2 Can I use an AMBER (or GROMACS) topology/coordinate file as a starting point for applying a SMIRNOFF force field?

In a word, “no”.

Parameter files used by typical molecular dynamics simulation packages do not currently encode enough information to identify the molecules chemically present, or at least not without drawing inferences. For example, one could take a structure file and infer bond orders based on bond lengths, or attempt to infer bond orders from force constants in a parameter file. Such inference work is outside the scope of SMIRNOFF.

If you have such an inference problem, we recommend that you use pre-existing cheminformatics tools available elsewhere (such as via the OpenEye toolkits, such as the `OEPerceiveBondOrders` functionality offered there) to solve this problem and identify your molecules before beginning your work with SMIRNOFF.

1.6.3 What about starting from a PDB file?

PDB files do not in general provide the chemical identity of small molecules contained therein, and thus do not provide suitable starting points for applying SMIROFF to small molecules. This is especially problematic for PDB files from X-ray crystallography which typically do not include proteins, making the problem even worse. For our purposes here, however, we assume you begin with the coordinates of all atoms present and the full topology of your system.

Given a PDB file of a hypothetical biomolecular system of interest containing a small molecule, there are several routes available to you for treating the small molecule present:

- Use a cheminformatics toolkit (see above) to infer bond orders

- Identify your ligand from a database; e.g. if it is in the Protein Data Bank (PDB), it will be present in the Ligand Expo meaning that it has a database entry and code you can use to look up its putative chemical identity
- Identify your ligand by name or SMILES string (or similar) from the literature or your collaborators

1.6.4 What do you recommend as a starting point?

For application of SMIRNOFF force fields, we recommend that you begin your work with formats which provide the chemical identity of your small molecule (including formal charge and bond order). This means we recommend one of the following or equivalent:

- A `.mol2` file or files for the molecules comprising your system, with correct bond orders and formal charges. (Note: Do NOT generate this from a simulation package or tool which does not have access to bond order information; you may end up with a `.mol2` file, but the bond orders will be incorrect)
- Isomeric SMILES strings for the components of your system
- InCHI strings for the components of your system
- Chemical Identity Registry numbers for the components of your system
- IUPAC names for the components of your system

Essentially, anything which provides the full identity of what you want to simulate (including stereochemistry) should work, though it may require more or less work to get it into an acceptable format.

CHAPTER

TWO

API DOCUMENTATION

2.1 Molecular topology representations

This module provides pure-Python classes for representing molecules and molecular systems. These classes offer several advantages over corresponding `Topology` objects in OpenMM and MDTraj, including offering serialization to a variety of standard formats (including XML, JSON, YAML, BSON, TOML, and MessagePack).

2.1.1 Primary objects

`FrozenMolecule`	Immutable chemical representation of a molecule, such as a small molecule or biopolymer.
`Molecule`	Mutable chemical representation of a molecule, such as a small molecule or biopolymer.
`Topology`	A Topology is a chemical representation of a system containing one or more molecules appearing in a specified order.

openforcefield.topology.FrozenMolecule

class openforcefield.topology.**FrozenMolecule**(*other=None*, *file_format=None*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object>*, *allow_undefined_stereo=False*)

Immutable chemical representation of a molecule, such as a small molecule or biopolymer.

Examples

Create a molecule from a sdf file

```
>>> from openforcefield.utils import get_data_file_path
>>> sdf_filepath = get_data_file_path('molecules/ethanol.sdf')
>>> molecule = FrozenMolecule.from_file(sdf_filepath)
```

Convert to OpenEye OEMol object

```
>>> oemol = molecule.to_openeye()
```

Create a molecule from an OpenEye molecule

```
>>> molecule = FrozenMolecule.from_openeye(oemol)
```

Convert to RDKit Mol object

```
>>> rdmol = molecule.to_rdkit()
```

Create a molecule from an RDKit molecule

```
>>> molecule = FrozenMolecule.from_rdkit(rdmol)
```

Create a molecule from IUPAC name (requires the OpenEye toolkit)

```
>>> molecule = FrozenMolecule.from_iupac('imatinib')
```

Create a molecule from SMILES

```
>>> molecule = FrozenMolecule.from_smiles('Cc1ccccc1')
```

Warning: This API is experimental and subject to change.

Attributes

`angles` Get an iterator over all i-j-k angles.

`atoms` Iterate over all Atom objects.

`bonds` Iterate over all Bond objects.

`conformers` Iterate over all conformers in this molecule.

`impropers` Iterate over all proper torsions in the molecule

`n_angles` int: number of angles in the Molecule.

`n_atoms` The number of Atom objects.

`n_bonds` The number of Bond objects.

`n_conformers` Iterate over all Atom objects.

`n_impropers` int: number of improper torsions in the Molecule.

`n_particles` The number of Particle objects, which corresponds to how many positions must be used.

`n_propers` int: number of proper torsions in the Molecule.

`n_virtual_sites` The number of VirtualSite objects.

`name` The name (or title) of the molecule

`partial_charges` Returns the partial charges (if present) on the molecule

`particles` Iterate over all Particle objects.

`propers` Iterate over all proper torsions in the molecule

`properties` The properties dictionary of the molecule

`torsions` Get an iterator over all i-j-k-l torsions.

`total_charge` Return the total charge on the molecule

virtual_sites Iterate over all VirtualSite objects.

Methods

chemical_environment_matches(self, query[, ...])	Retrieve all matches for a given chemical environment query.
compute_partial_charges(self[, toolkit_registry])	**Warning! Not Implemented!** Calculate partial atomic charges for this molecule using an underlying toolkit
compute_partial_charges_am1bcc(self[, ...])	Calculate partial atomic charges for this molecule using AM1-BCC run by an underlying toolkit
compute_wiberg_bond_orders(self[, ...])	Calculate wiberg bond orders for this molecule using an underlying toolkit
from_bson(serialized)	Instantiate an object from a BSON serialized representation.
from_dict(molecule_dict)	Create a new Molecule from a dictionary representation
from_file(file_path[, file_format, ...])	Create one or more molecules from a file
from_iupac(iupac_name, **kwargs)	Generate a molecule from IUPAC or common name
from_json(serialized)	Instantiate an object from a JSON serialized representation.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.
from_openeye(oemol[, allow_undefined_stereo])	Create a Molecule from an OpenEye molecule.
from_pickle(serialized)	Instantiate an object from a pickle serialized representation.
from_rdkit(rdmol[, allow_undefined_stereo])	Create a Molecule from an RDKit molecule.
from_smiles(smiles[, ...])	Construct a Molecule from a SMILES representation
from_toml(serialized)	Instantiate an object from a TOML serialized representation.
from_topology(topology)	Return a Molecule representation of an openforcefield Topology containing a single Molecule object.
from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
generate_conformers(self[, ...])	Generate conformers for this molecule using an underlying toolkit
get_bond_between(self, i, j)	Returns the bond between two atoms
get_fractional_bond_orders(self[, method, ...])	Get fractional bond orders.
is_isomorphic(self, other[, ...])	Determines whether the molecules are isomorphic by comparing their graphs.
to_bson(self)	Return a BSON serialized representation.
to_dict(self)	Return a dictionary representation of the molecule.

Continued on next page

Table 2 – continued from previous page

to_file(self, file_path, file_format[, ...])	Write the current molecule to a file or file-like object
to_iupac(self)	Generate IUPAC name from Molecule
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_networkx(self)	Generate a NetworkX undirected graph from the Molecule.
to_openeye(self[, aromaticity_model])	Create an OpenEye molecule
to_pickle(self)	Return a pickle serialized representation.
to_rdkit(self[, aromaticity_model])	Create an RDKit molecule
to_smiles(self[, toolkit_registry])	Return a canonical isomeric SMILES representation of the current molecule
to_toml(self)	Return a TOML serialized representation.
to_topology(self)	Return an openforcefield Topology representation containing one copy of this molecule
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.

__init__(*self*, *other=None*, *file_format=None*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*, *allow_undefined_stereo=False*)

Create a new FrozenMolecule object

Parameters

other [optional, default=None] If specified, attempt to construct a copy of the Molecule from the specified object. This can be any one of the following:

- a Molecule object
- a file that can be used to construct a Molecule object
- an openeye.oechem.OEMol
- an rdkit.Chem.rdchem.Mol
- a serialized Molecule object

file_format [str, optional, default=None] If providing a file-like object, you must specify the format of the data. If providing a file, the file format will attempt to be guessed from the suffix.

toolkit_registry [a ToolkitRegistry or ToolkitWrapper object, optional, default=GLOBAL_TOOLKIT_REGISTRY] ToolkitRegistry or ToolkitWrapper to use for I/O operations

allow_undefined_stereo [bool, default=False] If loaded from a file and False, raises an exception if undefined stereochemistry is detected during the molecule's construction.

Examples

Create an empty molecule:

```
>>> empty_molecule = FrozenMolecule()
```

Create a molecule from a file that can be used to construct a molecule, using either a filename or file-like object:

```
>>> from openforcefield.utils import get_data_file_path
>>> sdf_filepath = get_data_file_path('molecules/ethanol.sdf')
>>> molecule = FrozenMolecule(sdf_filepath)
>>> molecule = FrozenMolecule(open(sdf_filepath, 'r'), file_format='sdf')
```

```
>>> import gzip
>>> mol2_gz_filepath = get_data_file_path('molecules/toluene.mol2.gz')
>>> molecule = FrozenMolecule(gzip.GzipFile(mol2_gz_filepath, 'r'), file_format='mol2')
```

Create a molecule from another molecule:

```
>>> molecule_copy = FrozenMolecule(molecule)
```

Convert to OpenEye OEMol object

```
>>> oemol = molecule.to_openeye()
```

Create a molecule from an OpenEye molecule:

```
>>> molecule = FrozenMolecule(oemol)
```

Convert to RDKit Mol object

```
>>> rdmol = molecule.to_rdkit()
```

Create a molecule from an RDKit molecule:

```
>>> molecule = FrozenMolecule(rdmol)
```

Create a molecule from a serialized molecule object:

```
>>> serialized_molecule = molecule.__getstate__()
>>> molecule_copy = Molecule(serialized_molecule)
```

Methods

`__init__`(self[, other, file_format, ...])	Create a new FrozenMolecule object
`chemical_environment_matches`(self, query[, ...])	Retrieve all matches for a given chemical environment query.
`compute_partial_charges`(self[, toolkit_registry])	**Warning! Not Implemented!** Calculate partial atomic charges for this molecule using an underlying toolkit
`compute_partial_charges_am1bcc`(self[, ...])	Calculate partial atomic charges for this molecule using AM1-BCC run by an underlying toolkit
`compute_wiberg_bond_orders`(self[, ...])	Calculate wiberg bond orders for this molecule using an underlying toolkit
`from_bson`(serialized)	Instantiate an object from a BSON serialized representation.
`from_dict`(molecule_dict)	Create a new Molecule from a dictionary representation
`from_file`(file_path[, file_format, ...])	Create one or more molecules from a file

Continued on next page

Table 3 – continued from previous page

from_iupac(iupac_name, **kwargs)	Generate a molecule from IUPAC or common name
from_json(serialized)	Instantiate an object from a JSON serialized representation.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.
from_openeye(oemol[, allow_undefined_stereo])	Create a Molecule from an OpenEye molecule.
from_pickle(serialized)	Instantiate an object from a pickle serialized representation.
from_rdkit(rdmol[, allow_undefined_stereo])	Create a Molecule from an RDKit molecule.
from_smiles(smiles[, ...])	Construct a Molecule from a SMILES representation
from_toml(serialized)	Instantiate an object from a TOML serialized representation.
from_topology(topology)	Return a Molecule representation of an openforcefield Topology containing a single Molecule object.
from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
generate_conformers(self[, ...])	Generate conformers for this molecule using an underlying toolkit
get_bond_between(self, i, j)	Returns the bond between two atoms
get_fractional_bond_orders(self[, method, ...])	Get fractional bond orders.
is_isomorphic(self, other[, ...])	Determines whether the molecules are isomorphic by comparing their graphs.
to_bson(self)	Return a BSON serialized representation.
to_dict(self)	Return a dictionary representation of the molecule.
to_file(self, file_path, file_format[, ...])	Write the current molecule to a file or file-like object
to_iupac(self)	Generate IUPAC name from Molecule
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_networkx(self)	Generate a NetworkX undirected graph from the Molecule.
to_openeye(self[, aromaticity_model])	Create an OpenEye molecule
to_pickle(self)	Return a pickle serialized representation.
to_rdkit(self[, aromaticity_model])	Create an RDKit molecule
to_smiles(self[, toolkit_registry])	Return a canonical isomeric SMILES representation of the current molecule
to_toml(self)	Return a TOML serialized representation.
to_topology(self)	Return an openforcefield Topology representation containing one copy of this molecule
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.

Attributes

angles	Get an iterator over all i-j-k angles.
atoms	Iterate over all Atom objects.
bonds	Iterate over all Bond objects.
conformers	Iterate over all conformers in this molecule.
impropers	Iterate over all proper torsions in the molecule
n_angles	int: number of angles in the Molecule.
n_atoms	The number of Atom objects.
n_bonds	The number of Bond objects.
n_conformers	Iterate over all Atom objects.
n_impropers	int: number of improper torsions in the Molecule.
n_particles	The number of Particle objects, which corresponds to how many positions must be used.
n_propers	int: number of proper torsions in the Molecule.
n_virtual_sites	The number of VirtualSite objects.
name	The name (or title) of the molecule
partial_charges	Returns the partial charges (if present) on the molecule
particles	Iterate over all Particle objects.
propers	Iterate over all proper torsions in the molecule
properties	The properties dictionary of the molecule
torsions	Get an iterator over all i-j-k-l torsions.
total_charge	Return the total charge on the molecule
virtual_sites	Iterate over all VirtualSite objects.

to_dict(*self*)

Return a dictionary representation of the molecule.

Returns

molecule_dict [OrderedDict] A dictionary representation of the molecule.

classmethod from_dict(*molecule_dict*)

Create a new Molecule from a dictionary representation

Parameters

molecule_dict [OrderedDict] A dictionary representation of the molecule.

Returns

molecule [Molecule] A Molecule created from the dictionary representation

to_smiles(*self*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*)

Return a canonical isomeric SMILES representation of the current molecule

Note: RDKit and OpenEye versions will not necessarily return the same representation.

Parameters

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper, optional, default=None] `ToolkitRegistry`

or `ToolkitWrapper` to use for SMILES conversion

Returns

smiles [str] Canonical isomeric explicit-hydrogen SMILES

Examples

```
>>> from openforcefield.utils import get_data_file_path
>>> sdf_filepath = get_data_file_path('molecules/ethanol.sdf')
>>> molecule = Molecule(sdf_filepath)
>>> smiles = molecule.to_smiles()
```

static from_smiles(*smiles*, *hydrogens_are_explicit=False*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*, *allow_undefined_stereo=False*)

Construct a Molecule from a SMILES representation

Parameters

smiles [str] The SMILES representation of the molecule.

hydrogens_are_explicit [bool, default = False] If False, the cheminformatics toolkit will perform hydrogen addition

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper, optional, default=None] `ToolkitRegistry` or `ToolkitWrapper` to use for SMILES-to-molecule conversion

allow_undefined_stereo [bool, default=False] Whether to accept SMILES with undefined stereochemistry. If False, an exception will be raised if a SMILES with undefined stereochemistry is passed into this function.

Returns

molecule [openforcefield.topology.Molecule]

Examples

```
>>> molecule = Molecule.from_smiles('Cc1ccccc1')
```

is_isomorphic(*self*, *other*, *compare_atom_stereochemistry=True*, *compare_bond_stereochemistry=True*)

Determines whether the molecules are isomorphic by comparing their graphs.

Parameters

other [an openforcefield.topology.molecule.FrozenMolecule] The molecule to test for isomorphism.

compare_atom_stereochemistry [bool, optional] If `False`, atoms' stereochemistry is ignored for the purpose of determining equality. Default is `True`.

compare_bond_stereochemistry [bool, optional] If `False`, bonds' stereochemistry is ignored for the purpose of determining equality. Default is `True`.

Returns

molecules_are_isomorphic [bool]

generate_conformers(*self*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*, *n_conformers=10*, *clear_existing=True*)

Generate conformers for this molecule using an underlying toolkit

Parameters

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper, optional, default=None] `ToolkitRegistry` or `ToolkitWrapper` to use for SMILES-to-molecule conversion

n_conformers [int, default=1] The maximum number of conformers to produce

clear_existing [bool, default=True] Whether to overwrite existing conformers for the molecule

Raises

InvalidToolkitError If an invalid object is passed as the toolkit_registry parameter

Examples

```
>>> molecule = Molecule.from_smiles('CCCCCC')
>>> molecule.generate_conformers()
```

compute_partial_charges_am1bcc(*self*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*)

Calculate partial atomic charges for this molecule using AM1-BCC run by an underlying toolkit

Parameters

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper, optional, default=None] `ToolkitRegistry` or `ToolkitWrapper` to use for the calculation

Raises

InvalidToolkitError If an invalid object is passed as the toolkit_registry parameter

Examples

```
>>> molecule = Molecule.from_smiles('CCCCCC')
>>> molecule.generate_conformers()
>>> molecule.compute_partial_charges_am1bcc()
```

compute_partial_charges(*self*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*)

Warning! Not Implemented! Calculate partial atomic charges for this molecule using an underlying toolkit

Parameters

quantum_chemical_method [string, default='AM1-BCC'] The quantum chemical method to use for partial charge calculation.

partial_charge_method [string, default='None'] The partial charge calculation method to use for partial charge calculation.

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper, optional, default=None] `ToolkitRegistry` or `ToolkitWrapper` to use for SMILES-to-molecule conversion

Raises

InvalidToolkitError If an invalid object is passed as the toolkit_registry parameter

Examples

```
>>> molecule = Molecule.from_smiles('CCCCCC')
>>> molecule.generate_conformers()
```

compute_wiberg_bond_orders(*self*, *charge_model=None*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*)

Calculate wiberg bond orders for this molecule using an underlying toolkit

Parameters

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper, optional, default=None] `ToolkitRegistry` or `ToolkitWrapper` to use for SMILES-to-molecule conversion

charge_model [string, optional] The charge model to use for partial charge calculation

Raises

InvalidToolkitError If an invalid object is passed as the toolkit_registry parameter

Examples

```
>>> molecule = Molecule.from_smiles('CCCCCC')
>>> molecule.generate_conformers()
>>> molecule.compute_wiberg_bond_orders()
```

to_networkx(*self*)

Generate a NetworkX undirected graph from the Molecule.

Nodes are Atoms labeled with particle indices and atomic elements (via the `element` node attribute). Edges denote chemical bonds between Atoms. Virtual sites are not included, since they lack a concept of chemical connectivity.

Returns

graph [networkx.Graph] The resulting graph, with nodes (atoms) labeled with atom indices, elements, stereochemistry and aromaticity flags and bonds with two atom indices, bond order, stereochemistry, and aromaticity flags

Examples

Retrieve the bond graph for imatinib (OpenEye toolkit required)

```
>>> molecule = Molecule.from_iupac('imatinib')
>>> nxgraph = molecule.to_networkx()
```

property partial_charges

Returns the partial charges (if present) on the molecule

Returns

partial_charges [a simtk.unit.Quantity - wrapped numpy array [1 x n_atoms]] The partial charges on this Molecule's atoms.

property n_particles
The number of Particle objects, which corresponds to how many positions must be used.

property n_atoms
The number of Atom objects.

property n_virtual_sites
The number of VirtualSite objects.

property n_bonds
The number of Bond objects.

property n_angles
int: number of angles in the Molecule.

property n_propers
int: number of proper torsions in the Molecule.

property n_impropers
int: number of improper torsions in the Molecule.

property particles
Iterate over all Particle objects.

property atoms
Iterate over all Atom objects.

property conformers
Iterate over all conformers in this molecule.

property n_conformers
Iterate over all Atom objects.

property virtual_sites
Iterate over all VirtualSite objects.

property bonds
Iterate over all Bond objects.

property angles
Get an iterator over all i-j-k angles.

property torsions
Get an iterator over all i-j-k-l torsions. Note that i-j-k-i torsions (cycles) are excluded.

Returns

torsions [iterable of 4-Atom tuples]

property propers
Iterate over all proper torsions in the molecule

property impropers
Iterate over all proper torsions in the molecule

property total_charge
Return the total charge on the molecule

property name
The name (or title) of the molecule

property properties
The properties dictionary of the molecule

chemical_environment_matches(*self*, *query*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*)
Retrieve all matches for a given chemical environment query.

Parameters

query [str or ChemicalEnvironment] SMARTS string (with one or more tagged atoms) or `ChemicalEnvironment` query Query will internally be resolved to SMIRKS using `query.asSMIRKS()` if it has an `.asSMIRKS` method.

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper, optional, default=GLOBAL_TOOLKIT_REGISTRY] `ToolkitRegistry` or `ToolkitWrapper` to use for chemical environment matches

Returns

matches [list of atom index tuples] A list of tuples, containing the indices of the matching atoms.

Examples

Retrieve all the carbon-carbon bond matches in a molecule

```
>>> molecule = Molecule.from_iupac('imatinib')
>>> matches = molecule.chemical_environment_matches('[#6X3:1]~[#6X3:2]')
```

classmethod from_iupac(*iupac_name*, ***kwargs*)
Generate a molecule from IUPAC or common name

Parameters

iupac_name [str] IUPAC name of molecule to be generated

allow_undefined_stereo [bool, default=False] If false, raises an exception if molecule contains undefined stereochemistry.

Returns

molecule [Molecule] The resulting molecule with position

Note: This method requires the OpenEye toolkit to be installed. ..

Examples

Create a molecule from a common name

```
>>> molecule = Molecule.from_iupac('4-[(4-methylpiperazin-1-yl)methyl]-N-(4-methyl-3-{[4-
↪(pyridin-3-yl)pyrimidin-2-yl]amino}phenyl)benzamide')
```

Create a molecule from a common name

```
>>> molecule = Molecule.from_iupac('imatinib')
```

to_iupac(*self*)
Generate IUPAC name from Molecule

Returns

iupac_name [str] IUPAC name of the molecule

Note: This method requires the OpenEye toolkit to be installed. ..

Examples

```
>>> from openforcefield.utils import get_data_file_path
>>> sdf_filepath = get_data_file_path('molecules/ethanol.sdf')
>>> molecule = Molecule(sdf_filepath)
>>> iupac_name = molecule.to_iupac()
```

static from_topology(*topology*)
Return a Molecule representation of an openforcefield Topology containing a single Molecule object.

Parameters

topology [openforcefield.topology.Topology] The `Topology` object containing a single `Molecule` object. Note that OpenMM and MDTraj `Topology` objects are not supported.

Returns

molecule [openforcefield.topology.Molecule] The Molecule object in the topology

Raises

ValueError If the topology does not contain exactly one molecule.

Examples

Create a molecule from a Topology object that contains exactly one molecule

```
>>> molecule = Molecule.from_topology(topology)  # doctest: +SKIP
```

to_topology(*self*)
Return an openforcefield Topology representation containing one copy of this molecule

Returns

topology [openforcefield.topology.Topology] A Topology representation of this molecule

Examples

```
>>> molecule = Molecule.from_iupac('imatinib')
>>> topology = molecule.to_topology()
```

static from_file(*file_path*, *file_format=None*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*, *allow_undefined_stereo=False*)
Create one or more molecules from a file

Parameters

file_path [str or file-like object] The path to the file or file-like object to stream one or more molecules from.

file_format [str, optional, default=None] Format specifier, usually file suffix (eg. 'MOL2', 'SMI') Note that not all toolkits support all formats. Check ToolkitWrapper.toolkit_file_read_formats for your loaded toolkits for details.

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper,]

optional, default=GLOBAL_TOOLKIT_REGISTRY `ToolkitRegistry` or `ToolkitWrapper` to use for file loading. If a Toolkit is passed, only the highest-precedence toolkit is used

allow_undefined_stereo [bool, default=False] If false, raises an exception if oemol contains undefined stereochemistry.

Returns

molecules [Molecule or list of Molecules] If there is a single molecule in the file, a Molecule is returned; otherwise, a list of Molecule objects is returned.

Examples

```
>>> from openforcefield.tests.utils import get_monomer_mol2_file_path
>>> mol2_file_path = get_monomer_mol2_file_path('cyclohexane')
>>> molecule = Molecule.from_file(mol2_file_path)
```

to_file(*self*, *file_path*, *file_format*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*)

Write the current molecule to a file or file-like object

Parameters

file_path [str or file-like object] A file-like object or the path to the file to be written.

file_format [str] Format specifier, one of ['MOL2', 'MOL2H', 'SDF', 'PDB', 'SMI', 'CAN', 'TDT'] Note that not all toolkits support all formats

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper,]

optional, default=GLOBAL_TOOLKIT_REGISTRY `ToolkitRegistry` or `ToolkitWrapper` to use for file writing. If a Toolkit is passed, only the highest-precedence toolkit is used

Raises

ValueError If the requested file_format is not supported by one of the installed cheminformatics toolkits

Examples

```
>>> molecule = Molecule.from_iupac('imatinib')
>>> molecule.to_file('imatinib.mol2', file_format='mol2')  # doctest: +SKIP
>>> molecule.to_file('imatinib.sdf', file_format='sdf')  # doctest: +SKIP
>>> molecule.to_file('imatinib.pdb', file_format='pdb')  # doctest: +SKIP
```

static from_rdkit(*rdmol*, *allow_undefined_stereo=False*)
Create a Molecule from an RDKit molecule.

Requires the RDKit to be installed.

Parameters

rdmol [rkit.RDMol] An RDKit molecule

allow_undefined_stereo [bool, default=False] If false, raises an exception if oemol contains undefined stereochemistry.

Returns

molecule [openforcefield.Molecule] An openforcefield molecule

Examples

Create a molecule from an RDKit molecule

```
>>> from rdkit import Chem
>>> from openforcefield.tests.utils import get_data_file_path
>>> rdmol = Chem.MolFromMolFile(get_data_file_path('systems/monomers/ethanol.sdf'))
>>> molecule = Molecule.from_rdkit(rdmol)
```

to_rdkit(*self*, *aromaticity_model='OEAroModel_MDL'*)
Create an RDKit molecule

Requires the RDKit to be installed.

Parameters

aromaticity_model [str, optional, default=DEFAULT_AROMATICITY_MODEL] The aromaticity model to use

Returns

rdmol [rkit.RDMol] An RDKit molecule

Examples

Convert a molecule to RDKit

```
>>> from openforcefield.utils import get_data_file_path
>>> sdf_filepath = get_data_file_path('molecules/ethanol.sdf')
>>> molecule = Molecule(sdf_filepath)
>>> rdmol = molecule.to_rdkit()
```

static from_openeye(*oemol*, *allow_undefined_stereo=False*)
Create a Molecule from an OpenEye molecule.

Requires the OpenEye toolkit to be installed.

Parameters

oemol [openeye.oechem.OEMol] An OpenEye molecule

allow_undefined_stereo [bool, default=False] If false, raises an exception if oemol contains undefined stereochemistry.

Returns

molecule [openforcefield.topology.Molecule] An openforcefield molecule

Examples

Create a Molecule from an OpenEye OEMol

```
>>> from openeye import oechem
>>> from openforcefield.tests.utils import get_data_file_path
>>> ifs = oechem.oemolistream(get_data_file_path('systems/monomers/ethanol.mol2'))
>>> oemols = list(ifs.GetOEGraphMols())
>>> molecule = Molecule.from_openeye(oemols[0])
```

to_openeye(*self*, *aromaticity_model='OEAroModel_MDL'*)

Create an OpenEye molecule

Requires the OpenEye toolkit to be installed.

Parameters

aromaticity_model [str, optional, default=DEFAULT_AROMATICITY_MODEL] The aromaticity model to use

Returns

oemol [openeye.oechem.OEMol] An OpenEye molecule

Examples

Create an OpenEye molecule from a Molecule

```
>>> molecule = Molecule.from_smiles('CC')
>>> oemol = molecule.to_openeye()
```

get_fractional_bond_orders(*self*, *method='Wiberg'*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*)

Get fractional bond orders.

method [str, optional, default='Wiberg'] The name of the charge method to use. Options are: * 'Wiberg' : Wiberg bond order

toolkit_registry [openforcefield.utils.toolkits ToolkitRegistry] The toolkit registry to use for molecule operations

Examples

Get fractional Wiberg bond orders

```
>>> molecule = Molecule.from_iupac('imatinib')
>>> molecule.generate_conformers()
>>> fractional_bond_orders = molecule.get_fractional_bond_orders(method='Wiberg')
```

classmethod from_bson(*serialized*)

Instantiate an object from a BSON serialized representation.

Specification: http://bsonspec.org/

Parameters

serialized [bytes] A BSON serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_json(*serialized*)
Instantiate an object from a JSON serialized representation.

Specification: https://www.json.org/

Parameters

serialized [str] A JSON serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_messagepack(*serialized*)
Instantiate an object from a MessagePack serialized representation.

Specification: https://msgpack.org/index.html

Parameters

serialized [bytes] A MessagePack-encoded bytes serialized representation

Returns

instance [cls] Instantiated object.

classmethod from_pickle(*serialized*)
Instantiate an object from a pickle serialized representation.

> **Warning:** This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Parameters

serialized [str] A pickled representation of the object

Returns

instance [cls] An instantiated object

classmethod from_toml(*serialized*)
Instantiate an object from a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Parameters

serlialized [str] A TOML serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_xml(*serialized*)
Instantiate an object from an XML serialized representation.

Specification: https://www.w3.org/XML/

Parameters

serialized [bytes] An XML serialized representation

Returns

instance [cls] Instantiated object.

classmethod from_yaml(*serialized*)
Instantiate from a YAML serialized representation.

Specification: http://yaml.org/

Parameters

serialized [str] A YAML serialized representation of the object

Returns

instance [cls] Instantiated object

to_bson(*self*)
Return a BSON serialized representation.

Specification: http://bsonspec.org/

Returns

serialized [bytes] A BSON serialized representation of the objecft

to_json(*self*, *indent=None*)
Return a JSON serialized representation.

Specification: https://www.json.org/

Parameters

indent [int, optional, default=None] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [str] A JSON serialized representation of the object

to_messagepack(*self*)
Return a MessagePack representation.

Specification: https://msgpack.org/index.html

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation of the object

to_pickle(*self*)
Return a pickle serialized representation.

Warning: This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Returns

serialized [str] A pickled representation of the object

to_toml(*self*)
Return a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Returns

serialized [str] A TOML serialized representation of the object

to_xml(*self*, *indent=2*)
Return an XML representation.

Specification: https://www.w3.org/XML/

Parameters

indent [int, optional, default=2] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation.

to_yaml(*self*)
Return a YAML serialized representation.

Specification: http://yaml.org/

Returns

serialized [str] A YAML serialized representation of the object

get_bond_between(*self*, *i*, *j*)
Returns the bond between two atoms

Parameters

i, j [int or Atom] Atoms or atom indices to check

Returns

bond [Bond] The bond between i and j.

openforcefield.topology.Molecule

class openforcefield.topology.**Molecule**(**args*, ***kwargs*)
Mutable chemical representation of a molecule, such as a small molecule or biopolymer.

Examples

Create a molecule from an sdf file

```
>>> from openforcefield.utils import get_data_file_path
>>> sdf_filepath = get_data_file_path('molecules/ethanol.sdf')
>>> molecule = Molecule(sdf_filepath)
```

Convert to OpenEye OEMol object

```
>>> oemol = molecule.to_openeye()
```

Create a molecule from an OpenEye molecule

```
>>> molecule = Molecule.from_openeye(oemol)
```

Convert to RDKit Mol object

```
>>> rdmol = molecule.to_rdkit()
```

Create a molecule from an RDKit molecule

```
>>> molecule = Molecule.from_rdkit(rdmol)
```

Create a molecule from IUPAC name (requires the OpenEye toolkit)

```
>>> molecule = Molecule.from_iupac('imatinib')
```

Create a molecule from SMILES

```
>>> molecule = Molecule.from_smiles('Cc1ccccc1')
```

Warning: This API is experimental and subject to change.

Attributes

angles Get an iterator over all i-j-k angles.

atoms Iterate over all Atom objects.

bonds Iterate over all Bond objects.

conformers Iterate over all conformers in this molecule.

impropers Iterate over all proper torsions in the molecule

n_angles int: number of angles in the Molecule.

n_atoms The number of Atom objects.

n_bonds The number of Bond objects.

n_conformers Iterate over all Atom objects.

n_impropers int: number of improper torsions in the Molecule.

n_particles The number of Particle objects, which corresponds to how many positions must be used.

n_propers int: number of proper torsions in the Molecule.

n_virtual_sites The number of VirtualSite objects.

name The name (or title) of the molecule

partial_charges Returns the partial charges (if present) on the molecule

particles Iterate over all Particle objects.

propers Iterate over all proper torsions in the molecule

properties The properties dictionary of the molecule

torsions Get an iterator over all i-j-k-l torsions.

total_charge Return the total charge on the molecule

virtual_sites	Iterate over all VirtualSite objects.

Methods

add_atom(self, atomic_number, formal_charge, ...)	Add an atom
add_bond(self, atom1, atom2, bond_order, ...)	Add a bond between two specified atom indices
add_bond_charge_virtual_site(self, atoms, ...)	Create a bond charge-type virtual site, in which the location of the charge is specified by the position of two atoms.
add_conformer(self, coordinates)	# TODO: Should this not be public? Adds a conformer of the molecule
add_divalent_lone_pair_virtual_site(self, ...)	Create a divalent lone pair-type virtual site, in which the location of the charge is specified by the position of three atoms.
add_monovalent_lone_pair_virtual_site(self, ...)	Create a bond charge-type virtual site, in which the location of the charge is specified by the position of three atoms.
add_trivalent_lone_pair_virtual_site(self, ...)	Create a trivalent lone pair-type virtual site, in which the location of the charge is specified by the position of four atoms.
chemical_environment_matches(self, query[, ...])	Retrieve all matches for a given chemical environment query.
compute_partial_charges(self[, toolkit_registry])	**Warning! Not Implemented!** Calculate partial atomic charges for this molecule using an underlying toolkit
compute_partial_charges_am1bcc(self[, ...])	Calculate partial atomic charges for this molecule using AM1-BCC run by an underlying toolkit
compute_wiberg_bond_orders(self[, ...])	Calculate wiberg bond orders for this molecule using an underlying toolkit
from_bson(serialized)	Instantiate an object from a BSON serialized representation.
from_dict(molecule_dict)	Create a new Molecule from a dictionary representation
from_file(file_path[, file_format, ...])	Create one or more molecules from a file
from_iupac(iupac_name, **kwargs)	Generate a molecule from IUPAC or common name
from_json(serialized)	Instantiate an object from a JSON serialized representation.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.
from_openeye(oemol[, allow_undefined_stereo])	Create a Molecule from an OpenEye molecule.
from_pickle(serialized)	Instantiate an object from a pickle serialized representation.
from_rdkit(rdmol[, allow_undefined_stereo])	Create a Molecule from an RDKit molecule.
from_smiles(smiles[, ...])	Construct a Molecule from a SMILES representation
from_toml(serialized)	Instantiate an object from a TOML serialized representation.

Continued on next page

Table 5 – continued from previous page

from_topology(topology)	Return a Molecule representation of an openforcefield Topology containing a single Molecule object.
from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
generate_conformers(self[, ...])	Generate conformers for this molecule using an underlying toolkit
get_bond_between(self, i, j)	Returns the bond between two atoms
get_fractional_bond_orders(self[, method, ...])	Get fractional bond orders.
is_isomorphic(self, other[, ...])	Determines whether the molecules are isomorphic by comparing their graphs.
to_bson(self)	Return a BSON serialized representation.
to_dict(self)	Return a dictionary representation of the molecule.
to_file(self, file_path, file_format[, ...])	Write the current molecule to a file or file-like object
to_iupac(self)	Generate IUPAC name from Molecule
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_networkx(self)	Generate a NetworkX undirected graph from the Molecule.
to_openeye(self[, aromaticity_model])	Create an OpenEye molecule
to_pickle(self)	Return a pickle serialized representation.
to_rdkit(self[, aromaticity_model])	Create an RDKit molecule
to_smiles(self[, toolkit_registry])	Return a canonical isomeric SMILES representation of the current molecule
to_toml(self)	Return a TOML serialized representation.
to_topology(self)	Return an openforcefield Topology representation containing one copy of this molecule
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.

__init__(*self*, **args*, ***kwargs*)
Create a new Molecule object

Parameters

other [optional, default=None] If specified, attempt to construct a copy of the Molecule from the specified object. This can be any one of the following:

- a Molecule object
- a file that can be used to construct a Molecule object
- an openeye.oechem.OEMol
- an rdkit.Chem.rdchem.Mol
- a serialized Molecule object

Examples

Create an empty molecule:

```
>>> empty_molecule = Molecule()
```

Create a molecule from a file that can be used to construct a molecule, using either a filename or file-like object:

```
>>> from openforcefield.utils import get_data_file_path
>>> sdf_filepath = get_data_file_path('molecules/ethanol.sdf')
>>> molecule = Molecule(sdf_filepath)
>>> molecule = Molecule(open(sdf_filepath, 'r'), file_format='sdf')
```

```
>>> import gzip
>>> mol2_gz_filepath = get_data_file_path('molecules/toluene.mol2.gz')
>>> molecule = Molecule(gzip.GzipFile(mol2_gz_filepath, 'r'), file_format='mol2')
```

Create a molecule from another molecule:

```
>>> molecule_copy = Molecule(molecule)
```

Convert to OpenEye OEMol object

```
>>> oemol = molecule.to_openeye()
```

Create a molecule from an OpenEye molecule:

```
>>> molecule = Molecule(oemol)
```

Convert to RDKit Mol object

```
>>> rdmol = molecule.to_rdkit()
```

Create a molecule from an RDKit molecule:

```
>>> molecule = Molecule(rdmol)
```

Create a molecule from a serialized molecule object:

```
>>> serialized_molecule = molecule.__getstate__()
>>> molecule_copy = Molecule(serialized_molecule)
```

Methods

__init__(self, *args, **kwargs)	Create a new Molecule object
add_atom(self, atomic_number, formal_charge, ...)	Add an atom
add_bond(self, atom1, atom2, bond_order, ...)	Add a bond between two specified atom indices
add_bond_charge_virtual_site(self, atoms, ...)	Create a bond charge-type virtual site, in which the location of the charge is specified by the position of two atoms.
add_conformer(self, coordinates)	# TODO: Should this not be public? Adds a conformer of the molecule

Continued on next page

Table 6 – continued from previous page

add_divalent_lone_pair_virtual_site(self, ...)	Create a divalent lone pair-type virtual site, in which the location of the charge is specified by the position of three atoms.
add_monovalent_lone_pair_virtual_site(self, ...)	Create a bond charge-type virtual site, in which the location of the charge is specified by the position of three atoms.
add_trivalent_lone_pair_virtual_site(self, ...)	Create a trivalent lone pair-type virtual site, in which the location of the charge is specified by the position of four atoms.
chemical_environment_matches(self, query[, ...])	Retrieve all matches for a given chemical environment query.
compute_partial_charges(self[, toolkit_registry])	**Warning! Not Implemented!** Calculate partial atomic charges for this molecule using an underlying toolkit
compute_partial_charges_am1bcc(self[, ...])	Calculate partial atomic charges for this molecule using AM1-BCC run by an underlying toolkit
compute_wiberg_bond_orders(self[, ...])	Calculate wiberg bond orders for this molecule using an underlying toolkit
from_bson(serialized)	Instantiate an object from a BSON serialized representation.
from_dict(molecule_dict)	Create a new Molecule from a dictionary representation
from_file(file_path[, file_format, ...])	Create one or more molecules from a file
from_iupac(iupac_name, **kwargs)	Generate a molecule from IUPAC or common name
from_json(serialized)	Instantiate an object from a JSON serialized representation.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.
from_openeye(oemol[, allow_undefined_stereo])	Create a Molecule from an OpenEye molecule.
from_pickle(serialized)	Instantiate an object from a pickle serialized representation.
from_rdkit(rdmol[, allow_undefined_stereo])	Create a Molecule from an RDKit molecule.
from_smiles(smiles[, ...])	Construct a Molecule from a SMILES representation
from_toml(serialized)	Instantiate an object from a TOML serialized representation.
from_topology(topology)	Return a Molecule representation of an openforcefield Topology containing a single Molecule object.
from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
generate_conformers(self[, ...])	Generate conformers for this molecule using an underlying toolkit
get_bond_between(self, i, j)	Returns the bond between two atoms
get_fractional_bond_orders(self[, method, ...])	Get fractional bond orders.

Continued on next page

Table 6 – continued from previous page

is_isomorphic(self, other[, ...])	Determines whether the molecules are isomorphic by comparing their graphs.
to_bson(self)	Return a BSON serialized representation.
to_dict(self)	Return a dictionary representation of the molecule.
to_file(self, file_path, file_format[, ...])	Write the current molecule to a file or file-like object
to_iupac(self)	Generate IUPAC name from Molecule
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_networkx(self)	Generate a NetworkX undirected graph from the Molecule.
to_openeye(self[, aromaticity_model])	Create an OpenEye molecule
to_pickle(self)	Return a pickle serialized representation.
to_rdkit(self[, aromaticity_model])	Create an RDKit molecule
to_smiles(self[, toolkit_registry])	Return a canonical isomeric SMILES representation of the current molecule
to_toml(self)	Return a TOML serialized representation.
to_topology(self)	Return an openforcefield Topology representation containing one copy of this molecule
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.

Attributes

angles	Get an iterator over all i-j-k angles.
atoms	Iterate over all Atom objects.
bonds	Iterate over all Bond objects.
conformers	Iterate over all conformers in this molecule.
impropers	Iterate over all proper torsions in the molecule
n_angles	int: number of angles in the Molecule.
n_atoms	The number of Atom objects.
n_bonds	The number of Bond objects.
n_conformers	Iterate over all Atom objects.
n_impropers	int: number of improper torsions in the Molecule.
n_particles	The number of Particle objects, which corresponds to how many positions must be used.
n_propers	int: number of proper torsions in the Molecule.
n_virtual_sites	The number of VirtualSite objects.
name	The name (or title) of the molecule
partial_charges	Returns the partial charges (if present) on the molecule
particles	Iterate over all Particle objects.
propers	Iterate over all proper torsions in the molecule
properties	The properties dictionary of the molecule
torsions	Get an iterator over all i-j-k-l torsions.
total_charge	Return the total charge on the molecule
virtual_sites	Iterate over all VirtualSite objects.

property angles
Get an iterator over all i-j-k angles.

property atoms
Iterate over all Atom objects.

property bonds
Iterate over all Bond objects.

chemical_environment_matches(*self*, *query*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*)
Retrieve all matches for a given chemical environment query.

Parameters

query [str or ChemicalEnvironment] SMARTS string (with one or more tagged atoms) or `ChemicalEnvironment` query Query will internally be resolved to SMIRKS using `query.asSMIRKS()` if it has an `.asSMIRKS` method.

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper, optional, default=GLOBAL_TOOLKIT_REGISTRY] `ToolkitRegistry` or `ToolkitWrapper` to use for chemical environment matches

Returns

matches [list of atom index tuples] A list of tuples, containing the indices of the matching atoms.

Examples

Retrieve all the carbon-carbon bond matches in a molecule

```
>>> molecule = Molecule.from_iupac('imatinib')
>>> matches = molecule.chemical_environment_matches('[#6X3:1]~[#6X3:2]')
```

compute_partial_charges(*self*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*)
Warning! Not Implemented! Calculate partial atomic charges for this molecule using an underlying toolkit

Parameters

quantum_chemical_method [string, default='AM1-BCC'] The quantum chemical method to use for partial charge calculation.

partial_charge_method [string, default='None'] The partial charge calculation method to use for partial charge calculation.

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper, optional, default=None] `ToolkitRegistry` or `ToolkitWrapper` to use for SMILES-to-molecule conversion

Raises

InvalidToolkitError If an invalid object is passed as the toolkit_registry parameter

Examples

```
>>> molecule = Molecule.from_smiles('CCCCCC')
>>> molecule.generate_conformers()
```

compute_partial_charges_am1bcc(*self*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*)

Calculate partial atomic charges for this molecule using AM1-BCC run by an underlying toolkit

Parameters

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper, optional, default=None] `ToolkitRegistry` or `ToolkitWrapper` to use for the calculation

Raises

InvalidToolkitError If an invalid object is passed as the toolkit_registry parameter

Examples

```
>>> molecule = Molecule.from_smiles('CCCCCC')
>>> molecule.generate_conformers()
>>> molecule.compute_partial_charges_am1bcc()
```

compute_wiberg_bond_orders(*self*, *charge_model=None*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*)

Calculate wiberg bond orders for this molecule using an underlying toolkit

Parameters

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper, optional, default=None] `ToolkitRegistry` or `ToolkitWrapper` to use for SMILES-to-molecule conversion

charge_model [string, optional] The charge model to use for partial charge calculation

Raises

InvalidToolkitError If an invalid object is passed as the toolkit_registry parameter

Examples

```
>>> molecule = Molecule.from_smiles('CCCCCC')
>>> molecule.generate_conformers()
>>> molecule.compute_wiberg_bond_orders()
```

property conformers

Iterate over all conformers in this molecule.

classmethod from_bson(*serialized*)

Instantiate an object from a BSON serialized representation.

Specification: http://bsonspec.org/

Parameters

serialized [bytes] A BSON serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_dict(*molecule_dict*)

Create a new Molecule from a dictionary representation

Parameters

molecule_dict [OrderedDict] A dictionary representation of the molecule.

Returns

molecule [Molecule] A Molecule created from the dictionary representation

static from_file(*file_path*, *file_format=None*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*, *allow_undefined_stereo=False*)

Create one or more molecules from a file

Parameters

file_path [str or file-like object] The path to the file or file-like object to stream one or more molecules from.

file_format [str, optional, default=None] Format specifier, usually file suffix (eg. 'MOL2', 'SMI') Note that not all toolkits support all formats. Check ToolkitWrapper.toolkit_file_read_formats for your loaded toolkits for details.

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper,]

optional, default=GLOBAL_TOOLKIT_REGISTRY `ToolkitRegistry` or `ToolkitWrapper` to use for file loading. If a Toolkit is passed, only the highest-precedence toolkit is used

allow_undefined_stereo [bool, default=False] If false, raises an exception if oemol contains undefined stereochemistry.

Returns

molecules [Molecule or list of Molecules] If there is a single molecule in the file, a Molecule is returned; otherwise, a list of Molecule objects is returned.

Examples

```
>>> from openforcefield.tests.utils import get_monomer_mol2_file_path
>>> mol2_file_path = get_monomer_mol2_file_path('cyclohexane')
>>> molecule = Molecule.from_file(mol2_file_path)
```

classmethod from_iupac(*iupac_name*, ***kwargs*)

Generate a molecule from IUPAC or common name

Parameters

iupac_name [str] IUPAC name of molecule to be generated

allow_undefined_stereo [bool, default=False] If false, raises an exception if molecule contains undefined stereochemistry.

Returns

molecule [Molecule] The resulting molecule with position

Note: This method requires the OpenEye toolkit to be installed. ..

Examples

Create a molecule from a common name

```
>>> molecule = Molecule.from_iupac('4-[(4-methylpiperazin-1-yl)methyl]-N-(4-methyl-3-{[4-
↪(pyridin-3-yl)pyrimidin-2-yl]amino}phenyl)benzamide')
```

Create a molecule from a common name

```
>>> molecule = Molecule.from_iupac('imatinib')
```

classmethod from_json(*serialized*)
Instantiate an object from a JSON serialized representation.

Specification: https://www.json.org/

Parameters

serialized [str] A JSON serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_messagepack(*serialized*)
Instantiate an object from a MessagePack serialized representation.

Specification: https://msgpack.org/index.html

Parameters

serialized [bytes] A MessagePack-encoded bytes serialized representation

Returns

instance [cls] Instantiated object.

static from_openeye(*oemol*, *allow_undefined_stereo=False*)
Create a Molecule from an OpenEye molecule.

Requires the OpenEye toolkit to be installed.

Parameters

oemol [openeye.oechem.OEMol] An OpenEye molecule

allow_undefined_stereo [bool, default=False] If false, raises an exception if oemol contains undefined stereochemistry.

Returns

molecule [openforcefield.topology.Molecule] An openforcefield molecule

Examples

Create a Molecule from an OpenEye OEMol

```
>>> from openeye import oechem
>>> from openforcefield.tests.utils import get_data_file_path
>>> ifs = oechem.oemolistream(get_data_file_path('systems/monomers/ethanol.mol2'))
>>> oemols = list(ifs.GetOEGraphMols())
>>> molecule = Molecule.from_openeye(oemols[0])
```

classmethod from_pickle(*serialized*)
Instantiate an object from a pickle serialized representation.

Warning: This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Parameters

serialized [str] A pickled representation of the object

Returns

instance [cls] An instantiated object

static from_rdkit(*rdmol*, *allow_undefined_stereo=False*)
Create a Molecule from an RDKit molecule.

Requires the RDKit to be installed.

Parameters

rdmol [rkit.RDMol] An RDKit molecule

allow_undefined_stereo [bool, default=False] If false, raises an exception if oemol contains undefined stereochemistry.

Returns

molecule [openforcefield.Molecule] An openforcefield molecule

Examples

Create a molecule from an RDKit molecule

```
>>> from rdkit import Chem
>>> from openforcefield.tests.utils import get_data_file_path
>>> rdmol = Chem.MolFromMolFile(get_data_file_path('systems/monomers/ethanol.sdf'))
>>> molecule = Molecule.from_rdkit(rdmol)
```

static from_smiles(*smiles*, *hydrogens_are_explicit=False*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*, *allow_undefined_stereo=False*)
Construct a Molecule from a SMILES representation

Parameters

smiles [str] The SMILES representation of the molecule.

hydrogens_are_explicit [bool, default = False] If False, the cheminformatics toolkit will perform hydrogen addition

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper, optional, default=None] `ToolkitRegistry` or `ToolkitWrapper` to use for SMILES-to-molecule conversion

allow_undefined_stereo [bool, default=False] Whether to accept SMILES with undefined stereochemistry. If False, an exception will be raised if a SMILES with undefined stereochemistry is passed into this function.

Returns

molecule [openforcefield.topology.Molecule]

Examples

```
>>> molecule = Molecule.from_smiles('Cc1ccccc1')
```

classmethod from_toml(*serialized*)

Instantiate an object from a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Parameters

serlialized [str] A TOML serialized representation of the object

Returns

instance [cls] An instantiated object

static from_topology(*topology*)

Return a Molecule representation of an openforcefield Topology containing a single Molecule object.

Parameters

topology [openforcefield.topology.Topology] The `Topology` object containing a single `Molecule` object. Note that OpenMM and MDTraj `Topology` objects are not supported.

Returns

molecule [openforcefield.topology.Molecule] The Molecule object in the topology

Raises

ValueError If the topology does not contain exactly one molecule.

Examples

Create a molecule from a Topology object that contains exactly one molecule

```
>>> molecule = Molecule.from_topology(topology)  # doctest: +SKIP
```

classmethod from_xml(*serialized*)

Instantiate an object from an XML serialized representation.

Specification: https://www.w3.org/XML/

Parameters

serialized [bytes] An XML serialized representation

Returns

instance [cls] Instantiated object.

classmethod from_yaml(*serialized*)
Instantiate from a YAML serialized representation.

Specification: http://yaml.org/

Parameters

serialized [str] A YAML serialized representation of the object

Returns

instance [cls] Instantiated object

generate_conformers(*self*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*, *n_conformers=10*, *clear_existing=True*)
Generate conformers for this molecule using an underlying toolkit

Parameters

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper, optional, default=None] `ToolkitRegistry` or `ToolkitWrapper` to use for SMILES-to-molecule conversion

n_conformers [int, default=1] The maximum number of conformers to produce

clear_existing [bool, default=True] Whether to overwrite existing conformers for the molecule

Raises

InvalidToolkitError If an invalid object is passed as the toolkit_registry parameter

Examples

```
>>> molecule = Molecule.from_smiles('CCCCCC')
>>> molecule.generate_conformers()
```

get_bond_between(*self*, *i*, *j*)
Returns the bond between two atoms

Parameters

i, j [int or Atom] Atoms or atom indices to check

Returns

bond [Bond] The bond between i and j.

get_fractional_bond_orders(*self*, *method='Wiberg'*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*)
Get fractional bond orders.

method [str, optional, default='Wiberg'] The name of the charge method to use. Options are: * 'Wiberg' : Wiberg bond order

toolkit_registry [openforcefield.utils.toolkits ToolkitRegistry] The toolkit registry to use for molecule operations

Examples

Get fractional Wiberg bond orders

```
>>> molecule = Molecule.from_iupac('imatinib')
>>> molecule.generate_conformers()
>>> fractional_bond_orders = molecule.get_fractional_bond_orders(method='Wiberg')
```

property impropers
Iterate over all proper torsions in the molecule

is_isomorphic(*self*, *other*, *compare_atom_stereochemistry=True*, *compare_bond_stereochemistry=True*)
Determines whether the molecules are isomorphic by comparing their graphs.

Parameters

other [an openforcefield.topology.molecule.FrozenMolecule] The molecule to test for isomorphism.

compare_atom_stereochemistry [bool, optional] If `False`, atoms' stereochemistry is ignored for the purpose of determining equality. Default is `True`.

compare_bond_stereochemistry [bool, optional] If `False`, bonds' stereochemistry is ignored for the purpose of determining equality. Default is `True`.

Returns

molecules_are_isomorphic [bool]

property n_angles
int: number of angles in the Molecule.

property n_atoms
The number of Atom objects.

property n_bonds
The number of Bond objects.

property n_conformers
Iterate over all Atom objects.

property n_impropers
int: number of improper torsions in the Molecule.

property n_particles
The number of Particle objects, which corresponds to how many positions must be used.

property n_propers
int: number of proper torsions in the Molecule.

property n_virtual_sites
The number of VirtualSite objects.

property name
The name (or title) of the molecule

property partial_charges
Returns the partial charges (if present) on the molecule

Returns

partial_charges [a simtk.unit.Quantity - wrapped numpy array [1 x n_atoms]] The partial charges on this Molecule's atoms.

property particles
Iterate over all Particle objects.

property propers
Iterate over all proper torsions in the molecule

property properties
The properties dictionary of the molecule

to_bson(*self*)
Return a BSON serialized representation.

Specification: http://bsonspec.org/

Returns

serialized [bytes] A BSON serialized representation of the objecft

to_dict(*self*)
Return a dictionary representation of the molecule.

Returns

molecule_dict [OrderedDict] A dictionary representation of the molecule.

to_file(*self*, *file_path*, *file_format*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*)
Write the current molecule to a file or file-like object

Parameters

file_path [str or file-like object] A file-like object or the path to the file to be written.

file_format [str] Format specifier, one of ['MOL2', 'MOL2H', 'SDF', 'PDB', 'SMI', 'CAN', 'TDT'] Note that not all toolkits support all formats

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper,]

optional, default=GLOBAL_TOOLKIT_REGISTRY `ToolkitRegistry` or `ToolkitWrapper` to use for file writing. If a Toolkit is passed, only the highest-precedence toolkit is used

Raises

ValueError If the requested file_format is not supported by one of the installed chemInformatics toolkits

Examples

```
>>> molecule = Molecule.from_iupac('imatinib')
>>> molecule.to_file('imatinib.mol2', file_format='mol2')  # doctest: +SKIP
>>> molecule.to_file('imatinib.sdf', file_format='sdf')  # doctest: +SKIP
>>> molecule.to_file('imatinib.pdb', file_format='pdb')  # doctest: +SKIP
```

to_iupac(*self*)
Generate IUPAC name from Molecule

Returns

iupac_name [str] IUPAC name of the molecule

Note: This method requires the OpenEye toolkit to be installed. ..

Examples

```
>>> from openforcefield.utils import get_data_file_path
>>> sdf_filepath = get_data_file_path('molecules/ethanol.sdf')
>>> molecule = Molecule(sdf_filepath)
>>> iupac_name = molecule.to_iupac()
```

to_json(*self*, *indent=None*)
Return a JSON serialized representation.

Specification: https://www.json.org/

Parameters

indent [int, optional, default=None] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [str] A JSON serialized representation of the object

to_messagepack(*self*)
Return a MessagePack representation.

Specification: https://msgpack.org/index.html

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation of the object

to_networkx(*self*)
Generate a NetworkX undirected graph from the Molecule.

Nodes are Atoms labeled with particle indices and atomic elements (via the `element` node attribute). Edges denote chemical bonds between Atoms. Virtual sites are not included, since they lack a concept of chemical connectivity.

Returns

graph [networkx.Graph] The resulting graph, with nodes (atoms) labeled with atom indices, elements, stereochemistry and aromaticity flags and bonds with two atom indices, bond order, stereochemistry, and aromaticity flags

Examples

Retrieve the bond graph for imatinib (OpenEye toolkit required)

```
>>> molecule = Molecule.from_iupac('imatinib')
>>> nxgraph = molecule.to_networkx()
```

to_openeye(*self*, *aromaticity_model='OEAroModel_MDL'*)
Create an OpenEye molecule

Requires the OpenEye toolkit to be installed.

Parameters

aromaticity_model [str, optional, default=DEFAULT_AROMATICITY_MODEL] The aromaticity model to use

Returns

oemol [openeye.oechem.OEMol] An OpenEye molecule

Examples

Create an OpenEye molecule from a Molecule

```
>>> molecule = Molecule.from_smiles('CC')
>>> oemol = molecule.to_openeye()
```

to_pickle(*self*)
Return a pickle serialized representation.

Warning: This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Returns

serialized [str] A pickled representation of the object

to_rdkit(*self*, *aromaticity_model='OEAroModel_MDL'*)
Create an RDKit molecule

Requires the RDKit to be installed.

Parameters

aromaticity_model [str, optional, default=DEFAULT_AROMATICITY_MODEL] The aromaticity model to use

Returns

rdmol [rkit.RDMol] An RDKit molecule

Examples

Convert a molecule to RDKit

```
>>> from openforcefield.utils import get_data_file_path
>>> sdf_filepath = get_data_file_path('molecules/ethanol.sdf')
>>> molecule = Molecule(sdf_filepath)
>>> rdmol = molecule.to_rdkit()
```

to_smiles(*self*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*)
Return a canonical isomeric SMILES representation of the current molecule

Note: RDKit and OpenEye versions will not necessarily return the same representation.

Parameters

toolkit_registry [openforcefield.utils.toolkits.ToolRegistry or openforcefield.utils.toolkits.ToolkitWrapper, optional, default=None] `ToolkitRegistry` or `ToolkitWrapper` to use for SMILES conversion

Returns

smiles [str] Canonical isomeric explicit-hydrogen SMILES

Examples

```
>>> from openforcefield.utils import get_data_file_path
>>> sdf_filepath = get_data_file_path('molecules/ethanol.sdf')
>>> molecule = Molecule(sdf_filepath)
>>> smiles = molecule.to_smiles()
```

to_toml(*self*)
Return a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Returns

serialized [str] A TOML serialized representation of the object

to_topology(*self*)
Return an openforcefield Topology representation containing one copy of this molecule

Returns

topology [openforcefield.topology.Topology] A Topology representation of this molecule

Examples

```
>>> molecule = Molecule.from_iupac('imatinib')
>>> topology = molecule.to_topology()
```

to_xml(*self*, *indent=2*)
Return an XML representation.

Specification: https://www.w3.org/XML/

Parameters

indent [int, optional, default=2] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation.

to_yaml(*self*)
Return a YAML serialized representation.

Specification: http://yaml.org/

Returns

serialized [str] A YAML serialized representation of the object

property torsions
Get an iterator over all i-j-k-l torsions. Note that i-j-k-i torsions (cycles) are excluded.

Returns

torsions [iterable of 4-Atom tuples]

property total_charge
Return the total charge on the molecule

property virtual_sites
Iterate over all VirtualSite objects.

add_atom(*self*, *atomic_number*, *formal_charge*, *is_aromatic*, *stereochemistry=None*, *name=None*)
Add an atom

Parameters

atomic_number [int] Atomic number of the atom

formal_charge [int] Formal charge of the atom

is_aromatic [bool] If True, atom is aromatic; if False, not aromatic

stereochemistry [str, optional, default=None] Either 'R' or 'S' for specified stereochemistry, or None if stereochemistry is irrelevant

name [str, optional, default=None] An optional name for the atom

Returns

index [int] The index of the atom in the molecule

Examples

Define a methane molecule

```
>>> molecule = Molecule()
>>> molecule.name = 'methane'
>>> C = molecule.add_atom(6, 0, False)
>>> H1 = molecule.add_atom(1, 0, False)
>>> H2 = molecule.add_atom(1, 0, False)
>>> H3 = molecule.add_atom(1, 0, False)
>>> H4 = molecule.add_atom(1, 0, False)
>>> bond_idx = molecule.add_bond(C, H1, False, 1)
>>> bond_idx = molecule.add_bond(C, H2, False, 1)
>>> bond_idx = molecule.add_bond(C, H3, False, 1)
>>> bond_idx = molecule.add_bond(C, H4, False, 1)
```

add_bond_charge_virtual_site(*self*, *atoms*, *distance*, *charge_increments=None*, *weights=None*, *epsilon=None*, *sigma=None*, *rmin_half=None*, *name=''*)
Create a bond charge-type virtual site, in which the location of the charge is specified by the position of two atoms. This supports placement of a virtual site S along a vector between two specified atoms, e.g. to allow for a sigma hole for halogens or similar contexts. With positive values of the distance, the virtual site lies outside the first indexed atom. Parameters ———- atoms : list of openforcefield.topology.molecule.Atom objects or ints of shape [N

The atoms defining the virtual site's position or their indices

distance : float

weights [list of floats of shape [N] or None, optional, default=None] weights[index] is the weight of particles[index] contributing to the position of the virtual site. Default is None

charge_increments [list of floats of shape [N], optional, default=None] The amount of charge to remove from the VirtualSite's atoms and put in the VirtualSite. Indexing in this list should match the ordering in the atoms list. Default is None.

epsilon [float] Epsilon term for VdW properties of virtual site. Default is None.

sigma [float, default=None] Sigma term for VdW properties of virtual site. Default is None.

rmin_half [float] Rmin_half term for VdW properties of virtual site. Default is None.

name [string or None, default=''] The name of this virtual site. Default is ''.

Returns

index [int] The index of the newly-added virtual site in the molecule

add_monovalent_lone_pair_virtual_site(*self*, *atoms*, *distance*, *out_of_plane_angle*, *in_plane_angle*, ***kwargs*)

Create a bond charge-type virtual site, in which the location of the charge is specified by the position of three atoms.

TODO : Do "weights" have any meaning here?

Parameters

atoms [list of three openforcefield.topology.molecule.Atom objects or ints] The three atoms defining the virtual site's position or their molecule atom indices

distance [float]

out_of_plane_angle [float]

in_plane_angle [float]

epsilon [float] Epsilon term for VdW properties of virtual site. Default is None.

sigma [float, default=None] Sigma term for VdW properties of virtual site. Default is None.

rmin_half [float] Rmin_half term for VdW properties of virtual site. Default is None.

name [string or None, default=''] The name of this virtual site. Default is ''.

Returns

index [int] The index of the newly-added virtual site in the molecule

add_divalent_lone_pair_virtual_site(*self*, *atoms*, *distance*, *out_of_plane_angle*, *in_plane_angle*, ***kwargs*)

Create a divalent lone pair-type virtual site, in which the location of the charge is specified by the position of three atoms.

TODO : Do "weights" have any meaning here?

Parameters

atoms [list of 3 openforcefield.topology.molecule.Atom objects or ints] The three atoms defining the virtual site's position or their molecule atom indices

distance [float]

out_of_plane_angle [float]

in_plane_angle [float]

epsilon [float] Epsilon term for VdW properties of virtual site. Default is None.

sigma [float, default=None] Sigma term for VdW properties of virtual site. Default is None.

rmin_half [float] Rmin_half term for VdW properties of virtual site. Default is None.

name [string or None, default=''] The name of this virtual site. Default is ''.

Returns

index [int] The index of the newly-added virtual site in the molecule

add_trivalent_lone_pair_virtual_site(*self*, *atoms*, *distance*, *out_of_plane_angle*, *in_plane_angle*, ***kwargs*)

Create a trivalent lone pair-type virtual site, in which the location of the charge is specified by the position of four atoms.

TODO : Do "weights" have any meaning here?

Parameters

atoms [list of 4 openforcefield.topology.molecule.Atom objects or ints] The three atoms defining the virtual site's position or their molecule atom indices

distance [float]

out_of_plane_angle [float]

in_plane_angle [float]

epsilon [float] Epsilon term for VdW properties of virtual site. Default is None.

sigma [float, default=None] Sigma term for VdW properties of virtual site. Default is None.

rmin_half [float] Rmin_half term for VdW properties of virtual site. Default is None.

name [string or None, default='] The name of this virtual site. Default is ''.

Returns

index [int] The index of the newly-added virtual site in the molecule

add_bond(*self*, *atom1*, *atom2*, *bond_order*, *is_aromatic*, *stereochemistry=None*, *fractional_bond_order=None*)

Add a bond between two specified atom indices

Parameters

atom1 [int or openforcefield.topology.molecule.Atom] Index of first atom

atom2 [int or openforcefield.topology.molecule.Atom] Index of second atom

bond_order [int] Integral bond order of Kekulized form

is_aromatic [bool] True if this bond is aromatic, False otherwise

stereochemistry [str, optional, default=None] Either 'E' or 'Z' for specified stereochemistry, or None if stereochemistry is irrelevant

fractional_bond_order [float, optional, default=None] The fractional (eg. Wiberg) bond order

Returns

index: int Index of the bond in this molecule

add_conformer(*self*, *coordinates*)

TODO: Should this not be public? Adds a conformer of the molecule

Parameters

coordinates: simtk.unit.Quantity(np.array) with shape (n_atoms, 3)
Coordinates of the new conformer, with the first dimension of the array corresponding to the atom index in the Molecule's indexing system.

Returns

———-

index: int Index of the conformer in the Molecule

openforcefield.topology.Topology

class openforcefield.topology.**Topology**(*other=None*)

A Topology is a chemical representation of a system containing one or more molecules appearing in a specified order.

Warning: This API is experimental and subject to change.

Examples

Import some utilities

```
>>> from simtk.openmm import app
>>> from openforcefield.tests.utils import get_data_file_path, get_packmol_pdb_file_path
>>> pdb_filepath = get_packmol_pdb_file_path('cyclohexane_ethanol_0.4_0.6')
>>> monomer_names = ('cyclohexane', 'ethanol')
```

Create a Topology object from a PDB file and sdf files defining the molecular contents

```
>>> from openforcefield.topology import Molecule, Topology
>>> pdbfile = app.PDBFile(pdb_filepath)
>>> sdf_filepaths = [get_data_file_path(f'systems/monomers/{name}.sdf') for name in monomer_names]
>>> unique_molecules = [Molecule.from_file(sdf_filepath) for sdf_filepath in sdf_filepaths]
>>> topology = Topology.from_openmm(pdbfile.topology, unique_molecules=unique_molecules)
```

Create a Topology object from a PDB file and IUPAC names of the molecular contents

```
>>> pdbfile = app.PDBFile(pdb_filepath)
>>> unique_molecules = [Molecule.from_iupac(name) for name in monomer_names]
>>> topology = Topology.from_openmm(pdbfile.topology, unique_molecules=unique_molecules)
```

Create an empty Topology object and add a few copies of a single benzene molecule

```
>>> topology = Topology()
>>> molecule = Molecule.from_iupac('benzene')
>>> molecule_topology_indices = [topology.add_molecule(molecule) for index in range(10)]
```

Attributes

angles Iterable of Tuple[TopologyAtom]: iterator over the angles in this Topology.

aromaticity_model Get the aromaticity model applied to all molecules in the topology.

box_vectors Return the box vectors of the topology, if specified

charge_model Get the partial charge model applied to all molecules in the topology.

constrained_atom_pairs Returns the constrained atom pairs of the Topology

fractional_bond_order_model Get the fractional bond order model for the Topology.

impropers Iterable of Tuple[TopologyAtom]: iterator over the improper torsions in this Topology.

n_angles int: number of angles in this Topology.

n_impropers int: number of improper torsions in this Topology.

n_propers int: number of proper torsions in this Topology.

n_reference_molecules Returns the number of reference (unique) molecules in in this Topology.

n_topology_atoms Returns the number of topology atoms in in this Topology.

n_topology_bonds Returns the number of TopologyBonds in in this Topology.

n_topology_molecules Returns the number of topology molecules in in this Topology.

n_topology_particles Returns the number of topology particles (TopologyAtoms and TopologyVirtualSites) in in this Topology.

n_topology_virtual_sites Returns the number of TopologyVirtualSites in in this Topology.

propers Iterable of Tuple[TopologyAtom]: iterator over the proper torsions in this Topology.

reference_molecules Get an iterator of reference molecules in this Topology.

topology_atoms Returns an iterator over the atoms in this Topology.

topology_bonds Returns an iterator over the bonds in this Topology

topology_molecules Returns an iterator over all the TopologyMolecules in this Topology

topology_particles Returns an iterator over the particles (TopologyAtoms and TopologyVirtualSites) in this Topology.

topology_virtual_sites Get an iterator over the virtual sites in this Topology

Methods

add_constraint(self, iatom, jatom[, distance])	Mark a pair of atoms as constrained.
add_molecule(self, molecule[, ...])	Add a Molecule to the Topology.
add_particle(self, particle)	Add a Particle to the Topology.
assert_bonded(self, atom1, atom2)	Raise an exception if the specified atoms are not bonded in the topology.
atom(self, atom_topology_index)	Get the TopologyAtom at a given Topology atom index.
bond(self, bond_topology_index)	Get the TopologyBond at a given Topology bond index.
chemical_environment_matches(self, query[, ...])	Retrieve all matches for a given chemical environment query.
from_bson(serialized)	Instantiate an object from a BSON serialized representation.
from_dict(d)	Static constructor from dictionary representation.
from_json(serialized)	Instantiate an object from a JSON serialized representation.

Continued on next page

Table 8 – continued from previous page

from_mdtraj(mdtraj_topology[, unique_molecules])	Construct an openforcefield Topology object from an MDTraj Topology object.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.
from_molecules(molecules)	Create a new Topology object containing one copy of each of the specified molecule(s).
from_openmm(openmm_topology[, unique_molecules])	Construct an openforcefield Topology object from an OpenMM Topology object.
from_parmed(parmed_structure[, unique_molecules])	**Warning:** This functionality will be implemented in a future toolkit release.
from_pickle(serialized)	Instantiate an object from a pickle serialized representation.
from_toml(serialized)	Instantiate an object from a TOML serialized representation.
from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
get_bond_between(self, i, j)	Returns the bond between two atoms
get_fractional_bond_order(self, iatom, jatom)	Retrieve the fractional bond order for a bond.
is_bonded(self, i, j)	Returns True if the two atoms are bonded
is_constrained(self, iatom, jatom)	Check if a pair of atoms are marked as constrained.
to_bson(self)	Return a BSON serialized representation.
to_dict(self)	Convert to dictionary representation.
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_openmm(self)	Create an OpenMM Topology object.

Continued on next page

Table 8 – continued from previous page

to_parmed(self)	**Warning:** This functionality will be implemented in a future toolkit release.
to_pickle(self)	Return a pickle serialized representation.
to_toml(self)	Return a TOML serialized representation.
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.
virtual_site(self, vsite_topology_index)	Get the TopologyAtom at a given Topology atom index.

__init__(*self*, *other=None*)
Create a new Topology.

Parameters

other [optional, default=None] If specified, attempt to construct a copy of the Topology from the specified object. This might be a Topology object, or a file that can be used to construct a Topology object or serialized Topology object.

Methods

__init__(self[, other])	Create a new Topology.
add_constraint(self, iatom, jatom[, distance])	Mark a pair of atoms as constrained.
add_molecule(self, molecule[, ...])	Add a Molecule to the Topology.
add_particle(self, particle)	Add a Particle to the Topology.
assert_bonded(self, atom1, atom2)	Raise an exception if the specified atoms are not bonded in the topology.
atom(self, atom_topology_index)	Get the TopologyAtom at a given Topology atom index.
bond(self, bond_topology_index)	Get the TopologyBond at a given Topology bond index.

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Table 9 – continued from previous page

chemical_environment_matches(self, query[, ...])	Retrieve all matches for a given chemical environment query.
from_bson(serialized)	Instantiate an object from a BSON serialized representation.
from_dict(d)	Static constructor from dictionary representation.
from_json(serialized)	Instantiate an object from a JSON serialized representation.
from_mdtraj(mdtraj_topology[, unique_molecules])	Construct an openforcefield Topology object from an MDTraj Topology object.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.
from_molecules(molecules)	Create a new Topology object containing one copy of each of the specified molecule(s).
from_openmm(openmm_topology[, unique_molecules])	Construct an openforcefield Topology object from an OpenMM Topology object.
from_parmed(parmed_structure[, unique_molecules])	**Warning:** This functionality will be implemented in a future toolkit release.
from_pickle(serialized)	Instantiate an object from a pickle serialized representation.
from_toml(serialized)	Instantiate an object from a TOML serialized representation.
from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
get_bond_between(self, i, j)	Returns the bond between two atoms
get_fractional_bond_order(self, iatom, jatom)	Retrieve the fractional bond order for a bond.
is_bonded(self, i, j)	Returns True if the two atoms are bonded
is_constrained(self, iatom, jatom)	Check if a pair of atoms are marked as constrained.
to_bson(self)	Return a BSON serialized representation.

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Table 9 – continued from previous page

to_dict(self)	Convert to dictionary representation.
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_openmm(self)	Create an OpenMM Topology object.
to_parmed(self)	

Warning: This functionality will be implemented in a future toolkit release.

to_pickle(self)	Return a pickle serialized representation.
to_toml(self)	Return a TOML serialized representation.
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.
virtual_site(self, vsite_topology_index)	Get the TopologyAtom at a given Topology atom index.

Attributes

angles	Iterable of Tuple[TopologyAtom]: iterator over the angles in this Topology.
aromaticity_model	Get the aromaticity model applied to all molecules in the topology.
box_vectors	Return the box vectors of the topology, if specified Returns ——- box_vectors : simtk.unit.Quantity wrapped numpy array The unit-wrapped box vectors of this topology
charge_model	Get the partial charge model applied to all molecules in the topology.
constrained_atom_pairs	Returns the constrained atom pairs of the Topology
fractional_bond_order_model	Get the fractional bond order model for the Topology.
impropers	Iterable of Tuple[TopologyAtom]: iterator over the improper torsions in this Topology.

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Table 10 – continued from previous page

n_angles	int: number of angles in this Topology.
n_impropers	int: number of improper torsions in this Topology.
n_propers	int: number of proper torsions in this Topology.
n_reference_molecules	Returns the number of reference (unique) molecules in in this Topology.
n_topology_atoms	Returns the number of topology atoms in in this Topology.
n_topology_bonds	Returns the number of TopologyBonds in in this Topology.
n_topology_molecules	Returns the number of topology molecules in in this Topology.
n_topology_particles	Returns the number of topology particles (TopologyAtoms and TopologyVirtualSites) in in this Topology.
n_topology_virtual_sites	Returns the number of TopologyVirtualSites in in this Topology.
propers	Iterable of Tuple[TopologyAtom]: iterator over the proper torsions in this Topology.
reference_molecules	Get an iterator of reference molecules in this Topology.
topology_atoms	Returns an iterator over the atoms in this Topology.
topology_bonds	Returns an iterator over the bonds in this Topology
topology_molecules	Returns an iterator over all the TopologyMolecules in this Topology
topology_particles	Returns an iterator over the particles (TopologyAtoms and TopologyVirtualSites) in this Topology.
topology_virtual_sites	Get an iterator over the virtual sites in this Topology

property reference_molecules
Get an iterator of reference molecules in this Topology.

Returns

iterable of openforcefield.topology.Molecule

classmethod from_molecules(*molecules*)
Create a new Topology object containing one copy of each of the specified molecule(s).

Parameters

molecules [Molecule or iterable of Molecules] One or more molecules to be added to the Topology

Returns

topology [Topology] The Topology created from the specified molecule(s)

assert_bonded(*self*, *atom1*, *atom2*)
Raise an exception if the specified atoms are not bonded in the topology.

Parameters

atom1, atom2 [openforcefield.topology.Atom or int] The atoms or atom topology indices to check to ensure they are bonded

property aromaticity_model

Get the aromaticity model applied to all molecules in the topology.

Returns

aromaticity_model [str] Aromaticity model in use.

property box_vectors

Return the box vectors of the topology, if specified Returns ——- box_vectors : simtk.unit.Quantity wrapped numpy array

The unit-wrapped box vectors of this topology

property charge_model

Get the partial charge model applied to all molecules in the topology.

Returns

charge_model [str] Charge model used for all molecules in the Topology.

property constrained_atom_pairs

Returns the constrained atom pairs of the Topology

Returns

constrained_atom_pairs [dict] dictionary of the form d[(atom1_topology_index, atom2_topology_index)] = distance (float)

property fractional_bond_order_model

Get the fractional bond order model for the Topology.

Returns

fractional_bond_order_model [str] Fractional bond order model in use.

property n_reference_molecules

Returns the number of reference (unique) molecules in in this Topology.

Returns

n_reference_molecules [int]

property n_topology_molecules

Returns the number of topology molecules in in this Topology.

Returns

n_topology_molecules [int]

property topology_molecules

Returns an iterator over all the TopologyMolecules in this Topology

Returns

topology_molecules [Iterable of TopologyMolecule]

property n_topology_atoms

Returns the number of topology atoms in in this Topology.

Returns

n_topology_atoms [int]

property topology_atoms
Returns an iterator over the atoms in this Topology. These will be in ascending order of topology index (Note that this is not necessarily the same as the reference molecule index)

Returns

topology_atoms [Iterable of TopologyAtom]

property n_topology_bonds
Returns the number of TopologyBonds in in this Topology.

Returns

n_bonds [int]

property topology_bonds
Returns an iterator over the bonds in this Topology

Returns

topology_bonds [Iterable of TopologyBond]

property n_topology_particles
Returns the number of topology particles (TopologyAtoms and TopologyVirtualSites) in in this Topology.

Returns

n_topology_particles [int]

property topology_particles
Returns an iterator over the particles (TopologyAtoms and TopologyVirtualSites) in this Topology. The TopologyAtoms will be in order of ascending Topology index (Note that this may differ from the order of atoms in the reference molecule index).

Returns

topology_particles [Iterable of TopologyAtom and TopologyVirtualSite]

property n_topology_virtual_sites
Returns the number of TopologyVirtualSites in in this Topology.

Returns

n_virtual_sites [iterable of TopologyVirtualSites]

property topology_virtual_sites
Get an iterator over the virtual sites in this Topology

Returns

topology_virtual_sites [Iterable of TopologyVirtualSite]

property n_angles
int: number of angles in this Topology.

property angles
Iterable of Tuple[TopologyAtom]: iterator over the angles in this Topology.

property n_propers
int: number of proper torsions in this Topology.

property propers
Iterable of Tuple[TopologyAtom]: iterator over the proper torsions in this Topology.

property n_impropers
int: number of improper torsions in this Topology.

property impropers
Iterable of Tuple[TopologyAtom]: iterator over the improper torsions in this Topology.

chemical_environment_matches(*self*, *query*, *aromaticity_model='MDL'*, *toolkit_registry=<openforcefield.utils.toolkits.ToolkitRegistry object at 0x7f4fe4886b70>*)
Retrieve all matches for a given chemical environment query.

TODO: * Do we want to generalize this to other kinds of queries too, like mdtraj DSL, pymol selections, atom index slices, etc?

We could just call it topology.matches(query)

Parameters

query [str or ChemicalEnvironment] SMARTS string (with one or more tagged atoms) or `ChemicalEnvironment` query Query will internally be resolved to SMARTS using `query.as_smarts()` if it has an `.as_smarts` method.

aromaticity_model [str] Override the default aromaticity model for this topology and use the specified aromaticity model instead. Allowed values: ['MDL']

Returns

matches [list of Topology._ChemicalEnvironmentMatch] A list of tuples, containing the topology indices of the matching atoms.

to_dict(*self*)
Convert to dictionary representation.

classmethod from_dict(*d*)
Static constructor from dictionary representation.

classmethod from_openmm(*openmm_topology*, *unique_molecules=None*)
Construct an openforcefield Topology object from an OpenMM Topology object.

Parameters

openmm_topology [simtk.openmm.app.Topology] An OpenMM Topology object

unique_molecules [iterable of objects that can be used to construct unique Molecule objects] All unique molecules must be provided, in any order, though multiple copies of each molecule are allowed. The atomic elements and bond connectivity will be used to match the reference molecules to molecule graphs appearing in the OpenMM `Topology`. If bond orders are present in the OpenMM `Topology`, these will be used in matching as well. If all bonds have bond orders assigned in `mdtraj_topology`, these bond orders will be used to attempt to construct the list of unique Molecules if the `unique_molecules` argument is omitted.

Returns

topology [openforcefield.topology.Topology] An openforcefield Topology object

to_openmm(*self*)
Create an OpenMM Topology object.

The OpenMM `Topology` object will have one residue per topology molecule. Currently, the number of chains depends on how many copies of the same molecule are in the `Topology`. Molecules with

more than 5 copies are all assigned to a single chain, otherwise one chain is created for each molecule. This behavior may change in the future.

Parameters

openmm_topology [simtk.openmm.app.Topology] An OpenMM Topology object

static from_mdtraj(*mdtraj_topology*, *unique_molecules=None*)

Construct an openforcefield Topology object from an MDTraj Topology object.

Parameters

mdtraj_topology [mdtraj.Topology] An MDTraj Topology object

unique_molecules [iterable of objects that can be used to construct unique Molecule objects] All unique molecules mult be provided, in any order, though multiple copies of each molecule are allowed. The atomic elements and bond connectivity will be used to match the reference molecules to molecule graphs appearing in the MDTraj `Topology`. If bond orders are present in the MDTraj `Topology`, these will be used in matching as well. If all bonds have bond orders assigned in `mdtraj_topology`, these bond orders will be used to attempt to construct the list of unique Molecules if the `unique_molecules` argument is omitted.

Returns

topology [openforcefield.Topology] An openforcefield Topology object

static from_parmed(*parmed_structure*, *unique_molecules=None*)

> **Warning:** This functionality will be implemented in a future toolkit release.

Construct an openforcefield Topology object from a ParmEd Structure object.

Parameters

parmed_structure [parmed.Structure] A ParmEd structure object

unique_molecules [iterable of objects that can be used to construct unique Molecule objects] All unique molecules mult be provided, in any order, though multiple copies of each molecule are allowed. The atomic elements and bond connectivity will be used to match the reference molecules to molecule graphs appearing in the structure's `topology` object. If bond orders are present in the structure's `topology` object, these will be used in matching as well. If all bonds have bond orders assigned in the structure's `topology` object, these bond orders will be used to attempt to construct the list of unique Molecules if the `unique_molecules` argument is omitted.

Returns

topology [openforcefield.Topology] An openforcefield Topology object

to_parmed(*self*)

> **Warning:** This functionality will be implemented in a future toolkit release.

Create a ParmEd Structure object.

Returns

parmed_structure [parmed.Structure] A ParmEd Structure objecft

`get_bond_between`(*self*, *i*, *j*)
Returns the bond between two atoms

Parameters

i, j [int or TopologyAtom] Atoms or atom indices to check

Returns

bond [TopologyBond] The bond between i and j.

`is_bonded`(*self*, *i*, *j*)
Returns True if the two atoms are bonded

Parameters

i, j [int or TopologyAtom] Atoms or atom indices to check

Returns

is_bonded [bool] True if atoms are bonded, False otherwise.

`atom`(*self*, *atom_topology_index*)
Get the TopologyAtom at a given Topology atom index.

Parameters

atom_topology_index [int] The index of the TopologyAtom in this Topology

Returns

An openforcefield.topology.TopologyAtom

`virtual_site`(*self*, *vsite_topology_index*)
Get the TopologyAtom at a given Topology atom index.

Parameters

vsite_topology_index [int] The index of the TopologyVirtualSite in this Topology

Returns

An openforcefield.topology.TopologyVirtualSite

`bond`(*self*, *bond_topology_index*)
Get the TopologyBond at a given Topology bond index.

Parameters

bond_topology_index [int] The index of the TopologyBond in this Topology

Returns

An openforcefield.topology.TopologyBond

`add_particle`(*self*, *particle*)
Add a Particle to the Topology.

Parameters

particle [Particle] The Particle to be added. The Topology will take ownership of the Particle.

`add_molecule`(*self*, *molecule*, *local_topology_to_reference_index=None*)
Add a Molecule to the Topology.

Parameters

molecule [Molecule] The Molecule to be added.

local_topology_to_reference_index: dict, optional, default = None Dictionary of {TopologyMolecule_atom_index : Molecule_atom_index} for the TopologyMolecule that will be built

Returns

index [int] The index of this molecule in the topology

classmethod from_bson(*serialized*)
Instantiate an object from a BSON serialized representation.

Specification: http://bsonspec.org/

Parameters

serialized [bytes] A BSON serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_json(*serialized*)
Instantiate an object from a JSON serialized representation.

Specification: https://www.json.org/

Parameters

serialized [str] A JSON serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_messagepack(*serialized*)
Instantiate an object from a MessagePack serialized representation.

Specification: https://msgpack.org/index.html

Parameters

serialized [bytes] A MessagePack-encoded bytes serialized representation

Returns

instance [cls] Instantiated object.

classmethod from_pickle(*serialized*)
Instantiate an object from a pickle serialized representation.

> **Warning:** This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Parameters

serialized [str] A pickled representation of the object

Returns

instance [cls] An instantiated object

classmethod from_toml(*serialized*)
Instantiate an object from a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Parameters

serlialized [str] A TOML serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_xml(*serialized*)
Instantiate an object from an XML serialized representation.

Specification: https://www.w3.org/XML/

Parameters

serialized [bytes] An XML serialized representation

Returns

instance [cls] Instantiated object.

classmethod from_yaml(*serialized*)
Instantiate from a YAML serialized representation.

Specification: http://yaml.org/

Parameters

serialized [str] A YAML serialized representation of the object

Returns

instance [cls] Instantiated object

to_bson(*self*)
Return a BSON serialized representation.

Specification: http://bsonspec.org/

Returns

serialized [bytes] A BSON serialized representation of the objecft

to_json(*self*, *indent=None*)
Return a JSON serialized representation.

Specification: https://www.json.org/

Parameters

indent [int, optional, default=None] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [str] A JSON serialized representation of the object

to_messagepack(*self*)
Return a MessagePack representation.

Specification: https://msgpack.org/index.html

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation of the object

to_pickle(*self*)
Return a pickle serialized representation.

> **Warning:** This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Returns

serialized [str] A pickled representation of the object

to_toml(*self*)
Return a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Returns

serialized [str] A TOML serialized representation of the object

to_xml(*self*, *indent=2*)
Return an XML representation.

Specification: https://www.w3.org/XML/

Parameters

indent [int, optional, default=2] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation.

to_yaml(*self*)
Return a YAML serialized representation.

Specification: http://yaml.org/

Returns

serialized [str] A YAML serialized representation of the object

add_constraint(*self*, *iatom*, *jatom*, *distance=True*)
Mark a pair of atoms as constrained.

Constraints between atoms that are not bonded (e.g., rigid waters) are permissible.

Parameters

iatom, jatom [Atom] Atoms to mark as constrained These atoms may be bonded or not in the Topology

distance [simtk.unit.Quantity, optional, default=True] Constraint distance `True` if distance has yet to be determined `False` if constraint is to be removed

is_constrained(*self*, *iatom*, *jatom*)
Check if a pair of atoms are marked as constrained.

Parameters

iatom, jatom [int] Indices of atoms to mark as constrained.

Returns

distance [simtk.unit.Quantity or bool] True if constrained but constraints have not yet been applied Distance if constraint has already been added to System

get_fractional_bond_order(*self*, *iatom*, *jatom*)
Retrieve the fractional bond order for a bond.

An Exception is raised if it cannot be determined.

Parameters

iatom, jatom [Atom] Atoms for which a fractional bond order is to be retrieved.

Returns

order [float] Fractional bond order between the two specified atoms.

2.1.2 Secondary objects

Particle	Base class for all particles in a molecule.
Atom	A particle representing a chemical atom.
Bond	Chemical bond representation.
VirtualSite	A particle representing a virtual site whose position is defined in terms of Atom positions.

openforcefield.topology.Particle

class openforcefield.topology.**Particle**
Base class for all particles in a molecule.

A particle object could be an Atom or a VirtualSite.

> **Warning:** This API is experimental and subject to change.

Attributes

molecule The Molecule this atom is part of.

molecule_particle_index Returns the index of this particle in its molecule

name The name of the particle

Methods

from_bson(serialized)	Instantiate an object from a BSON serialized representation.
from_dict(d)	Static constructor from dictionary representation.
from_json(serialized)	Instantiate an object from a JSON serialized representation.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.

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Table 12 – continued from previous page

from_pickle(serialized)	Instantiate an object from a pickle serialized representation.
from_toml(serialized)	Instantiate an object from a TOML serialized representation.
from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
to_bson(self)	Return a BSON serialized representation.
to_dict(self)	Convert to dictionary representation.
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_pickle(self)	Return a pickle serialized representation.
to_toml(self)	Return a TOML serialized representation.
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.

__init__(*self*, */*, **args*, ***kwargs*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(self, /, *args, **kwargs)	Initialize self.
from_bson(serialized)	Instantiate an object from a BSON serialized representation.
from_dict(d)	Static constructor from dictionary representation.
from_json(serialized)	Instantiate an object from a JSON serialized representation.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.
from_pickle(serialized)	Instantiate an object from a pickle serialized representation.
from_toml(serialized)	Instantiate an object from a TOML serialized representation.
from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
to_bson(self)	Return a BSON serialized representation.
to_dict(self)	Convert to dictionary representation.
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_pickle(self)	Return a pickle serialized representation.
to_toml(self)	Return a TOML serialized representation.
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.

Attributes

molecule	The Molecule this atom is part of.
molecule_particle_index	Returns the index of this particle in its molecule
name	The name of the particle

property molecule
The Molecule this atom is part of.

property molecule_particle_index
Returns the index of this particle in its molecule

property name
The name of the particle

to_dict(*self*)
Convert to dictionary representation.

classmethod from_dict(*d*)
Static constructor from dictionary representation.

classmethod from_bson(*serialized*)
Instantiate an object from a BSON serialized representation.

Specification: http://bsonspec.org/

Parameters

serialized [bytes] A BSON serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_json(*serialized*)
Instantiate an object from a JSON serialized representation.

Specification: https://www.json.org/

Parameters

serialized [str] A JSON serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_messagepack(*serialized*)
Instantiate an object from a MessagePack serialized representation.

Specification: https://msgpack.org/index.html

Parameters

serialized [bytes] A MessagePack-encoded bytes serialized representation

Returns

instance [cls] Instantiated object.

classmethod from_pickle(*serialized*)
Instantiate an object from a pickle serialized representation.

> **Warning:** This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Parameters

serialized [str] A pickled representation of the object

Returns

instance [cls] An instantiated object

classmethod from_toml(*serialized*)
Instantiate an object from a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Parameters

serlialized [str] A TOML serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_xml(*serialized*)
Instantiate an object from an XML serialized representation.

Specification: https://www.w3.org/XML/

Parameters

serialized [bytes] An XML serialized representation

Returns

instance [cls] Instantiated object.

classmethod from_yaml(*serialized*)
Instantiate from a YAML serialized representation.

Specification: http://yaml.org/

Parameters

serialized [str] A YAML serialized representation of the object

Returns

instance [cls] Instantiated object

to_bson(*self*)
Return a BSON serialized representation.

Specification: http://bsonspec.org/

Returns

serialized [bytes] A BSON serialized representation of the objecft

to_json(*self*, *indent=None*)
Return a JSON serialized representation.

Specification: https://www.json.org/

Parameters

indent [int, optional, default=None] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [str] A JSON serialized representation of the object

to_messagepack(*self*)
Return a MessagePack representation.

Specification: https://msgpack.org/index.html

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation of the object

to_pickle(*self*)
Return a pickle serialized representation.

Warning: This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Returns

serialized [str] A pickled representation of the object

to_toml(*self*)
Return a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Returns

serialized [str] A TOML serialized representation of the object

to_xml(*self*, *indent=2*)
Return an XML representation.

Specification: https://www.w3.org/XML/

Parameters

indent [int, optional, default=2] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation.

to_yaml(*self*)
Return a YAML serialized representation.

Specification: http://yaml.org/

Returns

serialized [str] A YAML serialized representation of the object

openforcefield.topology.Atom

class openforcefield.topology.**Atom**(*atomic_number*, *formal_charge*, *is_aromatic*, *name=None*, *molecule=None*, *stereochemistry=None*)

A particle representing a chemical atom.

Note that non-chemical virtual sites are represented by the `VirtualSite` object.

Warning: This API is experimental and subject to change.

Attributes

atomic_number The integer atomic number of the atom.

bonded_atoms The list of `Atom` objects this atom is involved in bonds with

bonds The list of `Bond` objects this atom is involved in.

element The element name

formal_charge The atom's formal charge

is_aromatic The atom's is_aromatic flag

mass The standard atomic weight (abundance-weighted isotopic mass) of the atomic site.

molecule The `Molecule` this atom is part of.

molecule_atom_index The index of this Atom within the the list of atoms in `Molecules`.

molecule_particle_index The index of this Atom within the the list of particles in the parent `Molecule`.

name The name of this atom, if any

partial_charge The partial charge of the atom, if any.

stereochemistry The atom's stereochemistry (if defined, otherwise None)

virtual_sites The list of `VirtualSite` objects this atom is involved in.

Methods

add_bond(self, bond)	Adds a bond that this atom is involved in ..
add_virtual_site(self, vsite)	Adds a bond that this atom is involved in ..
from_bson(serialized)	Instantiate an object from a BSON serialized representation.
from_dict(atom_dict)	Create an Atom from a dict representation.
from_json(serialized)	Instantiate an object from a JSON serialized representation.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.
from_pickle(serialized)	Instantiate an object from a pickle serialized representation.
from_toml(serialized)	Instantiate an object from a TOML serialized representation.

Continued on next page

Table 15 – continued from previous page

from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
is_bonded_to(self, atom2)	Determine whether this atom is bound to another atom
to_bson(self)	Return a BSON serialized representation.
to_dict(self)	Return a dict representation of the atom.
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_pickle(self)	Return a pickle serialized representation.
to_toml(self)	Return a TOML serialized representation.
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.

__init__(*self*, *atomic_number*, *formal_charge*, *is_aromatic*, *name=None*, *molecule=None*, *stereochemistry=None*)

Create an immutable Atom object.

Object is serializable and immutable.

Parameters

atomic_number [int] Atomic number of the atom

formal_charge [int] Formal charge of the atom

is_aromatic [bool] If True, atom is aromatic; if False, not aromatic

stereochemistry [str, optional, default=None] Either 'R' or 'S' for specified stereochemistry, or None for ambiguous stereochemistry

name [str, optional, default=None] An optional name to be associated with the atom

Examples

Create a non-aromatic carbon atom

```
>>> atom = Atom(6, 0, False)
```

Create a chiral carbon atom

```
>>> atom = Atom(6, 0, False, stereochemistry='R', name='CT')
```

Methods

__init__(self, atomic_number, formal_charge, ...)	Create an immutable Atom object.
add_bond(self, bond)	Adds a bond that this atom is involved in ..
add_virtual_site(self, vsite)	Adds a bond that this atom is involved in ..
from_bson(serialized)	Instantiate an object from a BSON serialized representation.
from_dict(atom_dict)	Create an Atom from a dict representation.

Continued on next page

Table 16 – continued from previous page

from_json(serialized)	Instantiate an object from a JSON serialized representation.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.
from_pickle(serialized)	Instantiate an object from a pickle serialized representation.
from_toml(serialized)	Instantiate an object from a TOML serialized representation.
from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
is_bonded_to(self, atom2)	Determine whether this atom is bound to another atom
to_bson(self)	Return a BSON serialized representation.
to_dict(self)	Return a dict representation of the atom.
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_pickle(self)	Return a pickle serialized representation.
to_toml(self)	Return a TOML serialized representation.
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.

Attributes

atomic_number	The integer atomic number of the atom.
bonded_atoms	The list of Atom objects this atom is involved in bonds with
bonds	The list of Bond objects this atom is involved in.
element	The element name
formal_charge	The atom's formal charge
is_aromatic	The atom's is_aromatic flag
mass	The standard atomic weight (abundance-weighted isotopic mass) of the atomic site.
molecule	The Molecule this atom is part of.
molecule_atom_index	The index of this Atom within the the list of atoms in Molecules.
molecule_particle_index	The index of this Atom within the the list of particles in the parent Molecule.
name	The name of this atom, if any
partial_charge	The partial charge of the atom, if any.
stereochemistry	The atom's stereochemistry (if defined, otherwise None)
virtual_sites	The list of VirtualSite objects this atom is involved in.

add_bond(*self*, *bond*)

Adds a bond that this atom is involved in .. todo :: Is this how we want to keep records?

Parameters

bond: an openforcefield.topology.molecule.Bond A bond involving this atom

add_virtual_site(*self*, *vsite*)
Adds a bond that this atom is involved in .. todo :: Is this how we want to keep records?

Parameters

bond: an openforcefield.topology.molecule.Bond A bond involving this atom

to_dict(*self*)
Return a dict representation of the atom.

classmethod from_dict(*atom_dict*)
Create an Atom from a dict representation.

property formal_charge
The atom's formal charge

property partial_charge
The partial charge of the atom, if any.

Returns

float or None

property is_aromatic
The atom's is_aromatic flag

property stereochemistry
The atom's stereochemistry (if defined, otherwise None)

property element
The element name

property atomic_number
The integer atomic number of the atom.

property mass
The standard atomic weight (abundance-weighted isotopic mass) of the atomic site.

TODO (from jeff): Are there atoms that have different chemical properties based on their isotopes?

property name
The name of this atom, if any

property bonds
The list of `Bond` objects this atom is involved in.

property bonded_atoms
The list of `Atom` objects this atom is involved in bonds with

is_bonded_to(*self*, *atom2*)
Determine whether this atom is bound to another atom

Parameters

atom2: openforcefield.topology.molecule.Atom a different atom in the same molecule

Returns

bool Whether this atom is bound to atom2

property virtual_sites
The list of `VirtualSite` objects this atom is involved in.

property molecule_atom_index
The index of this Atom within the the list of atoms in `Molecules`. Note that this can be different from `molecule_particle_index`.

property molecule_particle_index
The index of this Atom within the the list of particles in the parent `Molecule`. Note that this can be different from `molecule_atom_index`.

classmethod from_bson(*serialized*)
Instantiate an object from a BSON serialized representation.

Specification: http://bsonspec.org/

Parameters

serialized [bytes] A BSON serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_json(*serialized*)
Instantiate an object from a JSON serialized representation.

Specification: https://www.json.org/

Parameters

serialized [str] A JSON serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_messagepack(*serialized*)
Instantiate an object from a MessagePack serialized representation.

Specification: https://msgpack.org/index.html

Parameters

serialized [bytes] A MessagePack-encoded bytes serialized representation

Returns

instance [cls] Instantiated object.

classmethod from_pickle(*serialized*)
Instantiate an object from a pickle serialized representation.

> **Warning:** This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Parameters

serialized [str] A pickled representation of the object

Returns

instance [cls] An instantiated object

classmethod from_toml(*serialized*)
Instantiate an object from a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Parameters

serlialized [str] A TOML serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_xml(*serialized*)
Instantiate an object from an XML serialized representation.

Specification: https://www.w3.org/XML/

Parameters

serialized [bytes] An XML serialized representation

Returns

instance [cls] Instantiated object.

classmethod from_yaml(*serialized*)
Instantiate from a YAML serialized representation.

Specification: http://yaml.org/

Parameters

serialized [str] A YAML serialized representation of the object

Returns

instance [cls] Instantiated object

property molecule
The `Molecule` this atom is part of.

to_bson(*self*)
Return a BSON serialized representation.

Specification: http://bsonspec.org/

Returns

serialized [bytes] A BSON serialized representation of the objecft

to_json(*self*, *indent=None*)
Return a JSON serialized representation.

Specification: https://www.json.org/

Parameters

indent [int, optional, default=None] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [str] A JSON serialized representation of the object

to_messagepack(*self*)
Return a MessagePack representation.

Specification: https://msgpack.org/index.html

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation of the object

to_pickle(*self*)
Return a pickle serialized representation.

> **Warning:** This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Returns

serialized [str] A pickled representation of the object

to_toml(*self*)
Return a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Returns

serialized [str] A TOML serialized representation of the object

to_xml(*self*, *indent=2*)
Return an XML representation.

Specification: https://www.w3.org/XML/

Parameters

indent [int, optional, default=2] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation.

to_yaml(*self*)
Return a YAML serialized representation.

Specification: http://yaml.org/

Returns

serialized [str] A YAML serialized representation of the object

openforcefield.topology.Bond

class openforcefield.topology.**Bond**(*atom1*, *atom2*, *bond_order*, *is_aromatic*, *fractional_bond_order=None*, *stereochemistry=None*)
Chemical bond representation.

> **Warning:** This API is experimental and subject to change.

Attributes

atom1, atom2 [openforcefield.topology.Atom] Atoms involved in the bond

bondtype [int] Discrete bond type representation for the Open Forcefield aromaticity model TODO: Do we want to pin ourselves to a single standard aromaticity model?

type [str] String based bond type

order [int] Integral bond order

fractional_bond_order [float, optional] Fractional bond order, or None.

.. warning :: This API is experimental and subject to change.

Methods

from_bson(serialized)	Instantiate an object from a BSON serialized representation.
from_dict(molecule, d)	Create a Bond from a dict representation.
from_json(serialized)	Instantiate an object from a JSON serialized representation.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.
from_pickle(serialized)	Instantiate an object from a pickle serialized representation.
from_toml(serialized)	Instantiate an object from a TOML serialized representation.
from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
to_bson(self)	Return a BSON serialized representation.
to_dict(self)	Return a dict representation of the bond.
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_pickle(self)	Return a pickle serialized representation.
to_toml(self)	Return a TOML serialized representation.
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.

__init__(*self*, *atom1*, *atom2*, *bond_order*, *is_aromatic*, *fractional_bond_order=None*, *stereochemistry=None*)
Create a new chemical bond.

Methods

__init__(self, atom1, atom2, bond_order, ...)	Create a new chemical bond.
from_bson(serialized)	Instantiate an object from a BSON serialized representation.
from_dict(molecule, d)	Create a Bond from a dict representation.
from_json(serialized)	Instantiate an object from a JSON serialized representation.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.
from_pickle(serialized)	Instantiate an object from a pickle serialized representation.

Continued on next page

Table 19 – continued from previous page

from_toml(serialized)	Instantiate an object from a TOML serialized representation.
from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
to_bson(self)	Return a BSON serialized representation.
to_dict(self)	Return a dict representation of the bond.
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_pickle(self)	Return a pickle serialized representation.
to_toml(self)	Return a TOML serialized representation.
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.

Attributes

atom1	
atom1_index	
atom2	
atom2_index	
atoms	
bond_order	
fractional_bond_order	
is_aromatic	
molecule	
molecule_bond_index	The index of this Bond within the the list of bonds in Molecules.
stereochemistry	

to_dict(*self*)
Return a dict representation of the bond.

classmethod from_dict(*molecule*, *d*)
Create a Bond from a dict representation.

property molecule_bond_index
The index of this Bond within the the list of bonds in Molecules.

classmethod from_bson(*serialized*)
Instantiate an object from a BSON serialized representation.

Specification: http://bsonspec.org/

Parameters

serialized [bytes] A BSON serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_json(*serialized*)
Instantiate an object from a JSON serialized representation.

Specification: https://www.json.org/

Parameters

serialized [str] A JSON serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_messagepack(*serialized*)
Instantiate an object from a MessagePack serialized representation.

Specification: https://msgpack.org/index.html

Parameters

serialized [bytes] A MessagePack-encoded bytes serialized representation

Returns

instance [cls] Instantiated object.

classmethod from_pickle(*serialized*)
Instantiate an object from a pickle serialized representation.

> **Warning:** This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Parameters

serialized [str] A pickled representation of the object

Returns

instance [cls] An instantiated object

classmethod from_toml(*serialized*)
Instantiate an object from a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Parameters

serlialized [str] A TOML serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_xml(*serialized*)
Instantiate an object from an XML serialized representation.

Specification: https://www.w3.org/XML/

Parameters

serialized [bytes] An XML serialized representation

Returns

instance [cls] Instantiated object.

classmethod from_yaml(*serialized*)
Instantiate from a YAML serialized representation.

Specification: http://yaml.org/

Parameters

serialized [str] A YAML serialized representation of the object

Returns

instance [cls] Instantiated object

to_bson(*self*)
Return a BSON serialized representation.

Specification: http://bsonspec.org/

Returns

serialized [bytes] A BSON serialized representation of the objecft

to_json(*self*, *indent=None*)
Return a JSON serialized representation.

Specification: https://www.json.org/

Parameters

indent [int, optional, default=None] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [str] A JSON serialized representation of the object

to_messagepack(*self*)
Return a MessagePack representation.

Specification: https://msgpack.org/index.html

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation of the object

to_pickle(*self*)
Return a pickle serialized representation.

Warning: This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Returns

serialized [str] A pickled representation of the object

to_toml(*self*)
Return a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Returns

serialized [str] A TOML serialized representation of the object

to_xml(*self*, *indent=2*)
Return an XML representation.

Specification: https://www.w3.org/XML/

Parameters

indent [int, optional, default=2] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation.

to_yaml(*self*)

Return a YAML serialized representation.

Specification: http://yaml.org/

Returns

serialized [str] A YAML serialized representation of the object

openforcefield.topology.VirtualSite

class openforcefield.topology.**VirtualSite**(*atoms*, *charge_increments=None*, *epsilon=None*, *sigma=None*, *rmin_half=None*, *name=None*)

A particle representing a virtual site whose position is defined in terms of `Atom` positions.

Note that chemical atoms are represented by the `Atom`.

Warning: This API is experimental and subject to change.

Attributes

atoms Atoms on whose position this VirtualSite depends.

charge_increments Charges taken from this VirtualSite's atoms and given to the VirtualSite

epsilon The VdW epsilon term of this VirtualSite

molecule The `Molecule` this atom is part of.

molecule_particle_index The index of this VirtualSite within the the list of particles in the parent `Molecule`.

molecule_virtual_site_index The index of this VirtualSite within the list of virtual sites within `Molecule` Note that this can be different from `particle_index`.

name The name of this VirtualSite

rmin_half The VdW rmin_half term of this VirtualSite

sigma The VdW sigma term of this VirtualSite

type The type of this VirtualSite (returns the class name as string)

Methods

from_bson(serialized)	Instantiate an object from a BSON serialized representation.
from_dict(vsite_dict)	Create a virtual site from a dict representation.

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Table 21 – continued from previous page

from_json(serialized)	Instantiate an object from a JSON serialized representation.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.
from_pickle(serialized)	Instantiate an object from a pickle serialized representation.
from_toml(serialized)	Instantiate an object from a TOML serialized representation.
from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
to_bson(self)	Return a BSON serialized representation.
to_dict(self)	Return a dict representation of the virtual site.
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_pickle(self)	Return a pickle serialized representation.
to_toml(self)	Return a TOML serialized representation.
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.

__init__(*self*, *atoms*, *charge_increments=None*, *epsilon=None*, *sigma=None*, *rmin_half=None*, *name=None*)
Base class for VirtualSites

Parameters

atoms [list of Atom of shape [N]] atoms[index] is the corresponding Atom for weights[index]

charge_increments [list of floats of shape [N], optional, default=None] The amount of charge to remove from the VirtualSite's atoms and put in the VirtualSite. Indexing in this list should match the ordering in the atoms list. Default is None.

sigma [float, default=None] Sigma term for VdW properties of virtual site. Default is None.

epsilon [float] Epsilon term for VdW properties of virtual site. Default is None.

rmin_half [float] Rmin_half term for VdW properties of virtual site. Default is None.

name [string or None, default=None] The name of this virtual site. Default is None.

virtual_site_type [str] Virtual site type.

name [str or None, default=None] The name of this virtual site. Default is None

Methods

__init__(self, atoms[, charge_increments, ...])	Base class for VirtualSites
from_bson(serialized)	Instantiate an object from a BSON serialized representation.
from_dict(vsite_dict)	Create a virtual site from a dict representation.

Continued on next page

Table 22 – continued from previous page

from_json(serialized)	Instantiate an object from a JSON serialized representation.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.
from_pickle(serialized)	Instantiate an object from a pickle serialized representation.
from_toml(serialized)	Instantiate an object from a TOML serialized representation.
from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
to_bson(self)	Return a BSON serialized representation.
to_dict(self)	Return a dict representation of the virtual site.
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_pickle(self)	Return a pickle serialized representation.
to_toml(self)	Return a TOML serialized representation.
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.

Attributes

atoms	Atoms on whose position this VirtualSite depends.
charge_increments	Charges taken from this VirtualSite's atoms and given to the VirtualSite
epsilon	The VdW epsilon term of this VirtualSite
molecule	The Molecule this atom is part of.
molecule_particle_index	The index of this VirtualSite within the the list of particles in the parent Molecule.
molecule_virtual_site_index	The index of this VirtualSite within the list of virtual sites within Molecule Note that this can be different from particle_index.
name	The name of this VirtualSite
rmin_half	The VdW rmin_half term of this VirtualSite
sigma	The VdW sigma term of this VirtualSite
type	The type of this VirtualSite (returns the class name as string)

to_dict(*self*)
Return a dict representation of the virtual site.

classmethod from_dict(*vsite_dict*)
Create a virtual site from a dict representation.

property molecule_virtual_site_index
The index of this VirtualSite within the list of virtual sites within Molecule Note that this can be different from particle_index.

property molecule_particle_index
The index of this VirtualSite within the the list of particles in the parent Molecule. Note that this

can be different from `molecule_virtual_site_index`.

property atoms
Atoms on whose position this VirtualSite depends.

property charge_increments
Charges taken from this VirtualSite's atoms and given to the VirtualSite

property epsilon
The VdW epsilon term of this VirtualSite

property sigma
The VdW sigma term of this VirtualSite

property rmin_half
The VdW rmin_half term of this VirtualSite

property name
The name of this VirtualSite

property type
The type of this VirtualSite (returns the class name as string)

classmethod from_bson(*serialized*)
Instantiate an object from a BSON serialized representation.

Specification: http://bsonspec.org/

Parameters

serialized [bytes] A BSON serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_json(*serialized*)
Instantiate an object from a JSON serialized representation.

Specification: https://www.json.org/

Parameters

serialized [str] A JSON serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_messagepack(*serialized*)
Instantiate an object from a MessagePack serialized representation.

Specification: https://msgpack.org/index.html

Parameters

serialized [bytes] A MessagePack-encoded bytes serialized representation

Returns

instance [cls] Instantiated object.

classmethod from_pickle(*serialized*)
Instantiate an object from a pickle serialized representation.

> **Warning:** This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Parameters

serialized [str] A pickled representation of the object

Returns

instance [cls] An instantiated object

classmethod from_toml(*serialized*)
Instantiate an object from a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Parameters

serlialized [str] A TOML serialized representation of the object

Returns

instance [cls] An instantiated object

classmethod from_xml(*serialized*)
Instantiate an object from an XML serialized representation.

Specification: https://www.w3.org/XML/

Parameters

serialized [bytes] An XML serialized representation

Returns

instance [cls] Instantiated object.

classmethod from_yaml(*serialized*)
Instantiate from a YAML serialized representation.

Specification: http://yaml.org/

Parameters

serialized [str] A YAML serialized representation of the object

Returns

instance [cls] Instantiated object

property molecule
The `Molecule` this atom is part of.

to_bson(*self*)
Return a BSON serialized representation.

Specification: http://bsonspec.org/

Returns

serialized [bytes] A BSON serialized representation of the objecft

to_json(*self*, *indent=None*)
Return a JSON serialized representation.

Specification: https://www.json.org/

Parameters

indent [int, optional, default=None] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [str] A JSON serialized representation of the object

to_messagepack(*self*)
Return a MessagePack representation.

Specification: https://msgpack.org/index.html

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation of the object

to_pickle(*self*)
Return a pickle serialized representation.

> **Warning:** This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Returns

serialized [str] A pickled representation of the object

to_toml(*self*)
Return a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Returns

serialized [str] A TOML serialized representation of the object

to_xml(*self*, *indent=2*)
Return an XML representation.

Specification: https://www.w3.org/XML/

Parameters

indent [int, optional, default=2] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation.

to_yaml(*self*)
Return a YAML serialized representation.

Specification: http://yaml.org/

Returns

serialized [str] A YAML serialized representation of the object

2.2 Forcefield typing tools

2.2.1 Chemical environments

Tools for representing and operating on chemical environments

> **Warning:** This class is largely redundant with the same one in the Chemper package, and will likely be removed.

ChemicalEnvironment	Chemical environment abstract base class that matches an atom, bond, angle, etc.

openforcefield.typing.chemistry.ChemicalEnvironment

class openforcefield.typing.chemistry.**ChemicalEnvironment**(*smirks=None*, *label=None*, *replacements=None*, *toolkit='openeye'*)

Chemical environment abstract base class that matches an atom, bond, angle, etc.

> **Warning:** This class is largely redundant with the same one in the Chemper package, and will likely be removed.

Methods

Atom([ORtypes, ANDtypes, index, ring])	Atom representation, which may have some ORtypes and ANDtypes properties.
Bond([ORtypes, ANDtypes])	Bond representation, which may have ORtype and ANDtype descriptors.
addAtom(self, bondToAtom[, bondORtypes, ...])	Add an atom to the specified target atom.
asSMIRKS(self[, smarts])	Returns a SMIRKS representation of the chemical environment
getAlphaAtoms(self)	Returns a list of atoms alpha to any indexed atom
getAlphaBonds(self)	Returns a list of Bond objects that connect
getAtoms(self)	**Returns**
getBetaAtoms(self)	Returns a list of atoms beta to any indexed atom
getBetaBonds(self)	Returns a list of Bond objects that connect
getBond(self, atom1, atom2)	Get bond betwen two atoms
getBondOrder(self, atom)	Returns minimum bond order around a given atom 0 if atom has no neighbors aromatic bonds count as 1.5 any bond counts as 1.0
getBonds(self[, atom])	**Parameters**

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Table 25 – continued from previous page

getComponentList(self, component_type[, ...])	Returns a list of atoms or bonds matching the descriptor
getIndexedAtoms(self)	returns the list of Atom objects with an index
getIndexedBonds(self)	Returns a list of Bond objects that connect two indexed atoms
getNeighbors(self, atom)	Returns atoms that are bound to the given atom in the form of a list of Atom objects
getType(self)	Uses number of indexed atoms and bond connectivity to determine the type of chemical environment
getUnindexedAtoms(self)	returns a list of Atom objects that are not indexed
getUnindexedBonds(self)	Returns a list of Bond objects that connect
getValence(self, atom)	Returns the valence (number of neighboring atoms) around the given atom
isAlpha(self, component)	Takes an atom or bond are returns True if it is alpha to an indexed atom
isBeta(self, component)	Takes an atom or bond are returns True if it is beta to an indexed atom
isIndexed(self, component)	returns True if the atom or bond is indexed
isUnindexed(self, component)	returns True if the atom or bond is not indexed
isValid(self[, smirks])	Returns if the environment is valid, that is if it creates a parseable SMIRKS string.
removeAtom(self, atom[, onlyEmpty])	Remove the specified atom from the chemical environment.
selectAtom(self[, descriptor])	Select a random atom fitting the descriptor.
selectBond(self[, descriptor])	Select a random bond fitting the descriptor.
validate(smirks[, ensure_valence_type, toolkit])	Validate the provided SMIRKS string is valid, and if requested, tags atoms appropriate to the specified valence type.

__init__(*self*, *smirks=None*, *label=None*, *replacements=None*, *toolkit='openeye'*)
Initialize a chemical environment abstract base class.

smirks = string, optional if smirks is not None, a chemical environment is built from the provided SMIRKS string

label = anything, optional intended to be used to label this chemical environment could be a string, int, or float, or anything

replacements = list of lists, optional, [substitution, smarts] form for parsing SMIRKS

Methods

__init__(self[, smirks, label, ...])	Initialize a chemical environment abstract base class.
addAtom(self, bondToAtom[, bondORtypes, ...])	Add an atom to the specified target atom.
asSMIRKS(self[, smarts])	Returns a SMIRKS representation of the chemical environment
getAlphaAtoms(self)	Returns a list of atoms alpha to any indexed atom

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Table 26 – continued from previous page

getAlphaBonds(self)	Returns a list of Bond objects that connect
getAtoms(self)	**Returns**
getBetaAtoms(self)	Returns a list of atoms beta to any indexed atom
getBetaBonds(self)	Returns a list of Bond objects that connect
getBond(self, atom1, atom2)	Get bond betwen two atoms
getBondOrder(self, atom)	Returns minimum bond order around a given atom 0 if atom has no neighbors aromatic bonds count as 1.5 any bond counts as 1.0
getBonds(self[, atom])	**Parameters**
getComponentList(self, component_type[, ...])	Returns a list of atoms or bonds matching the descriptor
getIndexedAtoms(self)	returns the list of Atom objects with an index
getIndexedBonds(self)	Returns a list of Bond objects that connect two indexed atoms
getNeighbors(self, atom)	Returns atoms that are bound to the given atom in the form of a list of Atom objects
getType(self)	Uses number of indexed atoms and bond connectivity to determine the type of chemical environment
getUnindexedAtoms(self)	returns a list of Atom objects that are not indexed
getUnindexedBonds(self)	Returns a list of Bond objects that connect
getValence(self, atom)	Returns the valence (number of neighboring atoms) around the given atom
isAlpha(self, component)	Takes an atom or bond are returns True if it is alpha to an indexed atom
isBeta(self, component)	Takes an atom or bond are returns True if it is beta to an indexed atom
isIndexed(self, component)	returns True if the atom or bond is indexed
isUnindexed(self, component)	returns True if the atom or bond is not indexed
isValid(self[, smirks])	Returns if the environment is valid, that is if it creates a parseable SMIRKS string.
removeAtom(self, atom[, onlyEmpty])	Remove the specified atom from the chemical environment.
selectAtom(self[, descriptor])	Select a random atom fitting the descriptor.
selectBond(self[, descriptor])	Select a random bond fitting the descriptor.
validate(smirks[, ensure_valence_type, toolkit])	Validate the provided SMIRKS string is valid, and if requested, tags atoms appropriate to the specified valence type.

class Atom(*ORtypes=None*, *ANDtypes=None*, *index=None*, *ring=None*)

Atom representation, which may have some ORtypes and ANDtypes properties.

Attributes

ORtypes [list of tuples in the form (base, [list of decorators])] where bases and decorators are both strings The descriptor types that will be combined with logical OR

ANDtypes [list of string] The descriptor types that will be combined with logical

AND

Methods

addANDtype(self, ANDtype)	Adds ANDtype to the set for this atom.
addORtype(self, ORbase, ORdecorators)	Adds ORtype to the set for this atom.
asSMARTS(self)	Return the atom representation as SMARTS.
asSMIRKS(self)	Return the atom representation as SMIRKS.
getANDtypes(self)	returns a copy of the list of ANDtypes for this atom
getORtypes(self)	returns a copy of the dictionary of ORtypes for this atom
setANDtypes(self, newANDtypes)	sets new ANDtypes for this atom
setORtypes(self, newORtypes)	sets new ORtypes for this atom

asSMARTS(*self*)
Return the atom representation as SMARTS.
Returns
smarts [str]
The SMARTS string for this atom

asSMIRKS(*self*)
Return the atom representation as SMIRKS.
Returns
smirks [str]
The SMIRKS string for this atom

addORtype(*self*, *ORbase*, *ORdecorators*)
Adds ORtype to the set for this atom.
Parameters
ORbase: string, such as '#6'
ORdecorators: list of strings, such as ['X4','+0']

addANDtype(*self*, *ANDtype*)
Adds ANDtype to the set for this atom.
Parameters
ANDtype: string added to the list of ANDtypes for this atom

getORtypes(*self*)
returns a copy of the dictionary of ORtypes for this atom

setORtypes(*self*, *newORtypes*)
sets new ORtypes for this atom
Parameters
newORtypes: list of tuples in the form (base, [ORdecorators]) for example: ('#6', ['X4','H0','+0']) –> '#6X4H0+0'

getANDtypes(*self*)
returns a copy of the list of ANDtypes for this atom

setANDtypes(*self*, *newANDtypes*)
sets new ANDtypes for this atom
Parameters
newANDtypes: list of strings strings that will be AND'd together in a SMARTS

class Bond(*ORtypes=None*, *ANDtypes=None*)

Bond representation, which may have ORtype and ANDtype descriptors.

Attributes

ORtypes [list of tuples of ORbases and ORdecorators] in form (base: [list of decorators]) The ORtype types that will be combined with logical OR

ANDtypes [list of string] The ANDtypes that will be combined with logical AND

Methods

addANDtype(self, ANDtype)	Adds ANDtype to the set for this atom.
addORtype(self, ORbase, ORdecorators)	Adds ORtype to the set for this atom.
asSMARTS(self)	Return the atom representation as SMARTS.
asSMIRKS(self)	

Returns

getANDtypes(self)	returns a copy of the list of ANDtypes for this atom
getORtypes(self)	returns a copy of the dictionary of ORtypes for this atom
getOrder(self)	Returns a float for the order of this bond for multiple ORtypes or ~ it returns the minimum possible order the intended application is for checking valence around a given atom
setANDtypes(self, newANDtypes)	sets new ANDtypes for this atom
setORtypes(self, newORtypes)	sets new ORtypes for this atom

asSMARTS(*self*)

Return the atom representation as SMARTS.

Returns

smarts [str] The SMARTS string for just this atom

asSMIRKS(*self*)

Returns

smarts [str] The SMIRKS string for just this bond

getOrder(*self*)

Returns a float for the order of this bond for multiple ORtypes or ~ it returns the minimum possible order the intended application is for checking valence around a given atom

addANDtype(*self*, *ANDtype*)

Adds ANDtype to the set for this atom.

Parameters

ANDtype: string added to the list of ANDtypes for this atom

addORtype(*self*, *ORbase*, *ORdecorators*)

Adds ORtype to the set for this atom.

Parameters

ORbase: string, such as '#6'

ORdecorators: list of strings, such as ['X4','+0']

getANDtypes(*self*)

returns a copy of the list of ANDtypes for this atom

getORtypes(*self*)
returns a copy of the dictionary of ORtypes for this atom

setANDtypes(*self*, *newANDtypes*)
sets new ANDtypes for this atom

Parameters

newANDtypes: list of strings strings that will be AND'd together in a SMARTS

setORtypes(*self*, *newORtypes*)
sets new ORtypes for this atom

Parameters

newORtypes: list of tuples in the form (base, [ORdecorators]) for example: ('#6', ['X4','H0','+0']) –> '#6X4H0+0'

static validate(*smirks*, *ensure_valence_type=None*, *toolkit='openeye'*)
Validate the provided SMIRKS string is valid, and if requested, tags atoms appropriate to the specified valence type.

Parameters

smirks [str] The SMIRKS expression to validate

ensure_valence_type [str, optional, default=None] If specified, ensure the tagged atoms are appropriate to the specified valence type

This method will raise a :class:'SMIRKSParsingError' if the provided SMIRKS string is not valid.

isValid(*self*, *smirks=None*)
Returns if the environment is valid, that is if it creates a parseable SMIRKS string.

asSMIRKS(*self*, *smarts=False*)
Returns a SMIRKS representation of the chemical environment

Parameters

smarts: optional, boolean if True, returns a SMARTS instead of SMIRKS without index labels

selectAtom(*self*, *descriptor=None*)
Select a random atom fitting the descriptor.

Parameters

descriptor: optional, None None - returns any atom with equal probability int - will return an atom with that index 'Indexed' - returns a random indexed atom 'Unindexed' - returns a random unindexed atom 'Alpha' - returns a random alpha atom 'Beta' - returns a random beta atom

Returns

a single Atom object fitting the description

or None if no such atom exists

getComponentList(*self*, *component_type*, *descriptor=None*)
Returns a list of atoms or bonds matching the descriptor

Parameters

component_type: string: 'atom' or 'bond'

descriptor: string, optional 'all', 'Indexed', 'Unindexed', 'Alpha', 'Beta'

selectBond(*self*, *descriptor=None*)
Select a random bond fitting the descriptor.

Parameters

descriptor: optional, None None - returns any bond with equal probability int - will return an bond with that index 'Indexed' - returns a random indexed bond 'Unindexed' - returns a random unindexed bond 'Alpha' - returns a random alpha bond 'Beta' - returns a random beta bond

Returns

a single Bond object fitting the description

or None if no such atom exists

addAtom(*self*, *bondToAtom*, *bondORtypes=None*, *bondANDtypes=None*, *newORtypes=None*, *newANDtypes=None*, *newAtomIndex=None*, *newAtomRing=None*, *beyondBeta=False*)
Add an atom to the specified target atom.

Parameters

bondToAtom: atom object, required atom the new atom will be bound to

bondORtypes: list of tuples, optional strings that will be used for the ORtypes for the new bond

bondANDtypes: list of strings, optional strings that will be used for the ANDtypes for the new bond

newORtypes: list of strings, optional strings that will be used for the ORtypes for the new atom

newANDtypes: list of strings, optional strings that will be used for the ANDtypes for the new atom

newAtomIndex: int, optional integer label that could be used to index the atom in a SMIRKS string

beyondBeta: boolean, optional if True, allows bonding beyond beta position

Returns

newAtom: atom object for the newly created atom

removeAtom(*self*, *atom*, *onlyEmpty=False*)
Remove the specified atom from the chemical environment. if the atom is not indexed for the SMIRKS string or used to connect two other atoms.

Parameters

atom: atom object, required atom to be removed if it meets the conditions.

onlyEmpty: boolean, optional True only an atom with no ANDtypes and 1 ORtype can be removed

Returns

Boolean True: atom was removed, False: atom was not removed

getAtoms(*self*)

Returns

list of atoms in the environment

getBonds(*self*, *atom=None*)

Parameters

atom: Atom object, optional, returns bonds connected to atom

returns all bonds in fragment if atom is None

Returns

a complete list of bonds in the fragment

getBond(*self*, *atom1*, *atom2*)
Get bond betwen two atoms

Parameters

atom1 and atom2: atom objects

Returns

bond object between the atoms or None if no bond there

getIndexedAtoms(*self*)
returns the list of Atom objects with an index

getUnindexedAtoms(*self*)
returns a list of Atom objects that are not indexed

getAlphaAtoms(*self*)

Returns a list of atoms alpha to any indexed atom that are not also indexed

getBetaAtoms(*self*)

Returns a list of atoms beta to any indexed atom that are not alpha or indexed atoms

getIndexedBonds(*self*)
Returns a list of Bond objects that connect two indexed atoms

getUnindexedBonds(*self*)

Returns a list of Bond objects that connect an indexed atom to an unindexed atom two unindexed atoms

getAlphaBonds(*self*)

Returns a list of Bond objects that connect an indexed atom to alpha atoms

getBetaBonds(*self*)

Returns a list of Bond objects that connect alpha atoms to beta atoms

isAlpha(*self*, *component*)
Takes an atom or bond are returns True if it is alpha to an indexed atom

isUnindexed(*self*, *component*)
returns True if the atom or bond is not indexed

isIndexed(*self*, *component*)
returns True if the atom or bond is indexed

isBeta(*self*, *component*)
Takes an atom or bond are returns True if it is beta to an indexed atom

getType(*self*)
Uses number of indexed atoms and bond connectivity to determine the type of chemical environment

Returns

chemical environemnt type: 'Atom', 'Bond', 'Angle', 'ProperTorsion', 'ImproperTorsion' None if number of indexed atoms is 0 or > 4

getNeighbors(*self*, *atom*)
Returns atoms that are bound to the given atom in the form of a list of Atom objects

getValence(*self*, *atom*)
Returns the valence (number of neighboring atoms) around the given atom

getBondOrder(*self*, *atom*)
Returns minimum bond order around a given atom 0 if atom has no neighbors aromatic bonds count as 1.5 any bond counts as 1.0

2.2.2 Forcefield typing engines

Engines for applying parameters to chemical systems

The SMIRks-Native Open Force Field (SMIRNOFF)

A reference implementation of the SMIRNOFF specification for parameterizing biomolecular systems

ForceField

The `ForceField` class is a primary part of the top-level toolkit API. `ForceField` objects are initialized from SMIRNOFF data sources (e.g. an `OFFXML` file). For a basic example of system creation using a `ForceField`, see `examples/SMIRNOFF_simulation`.

`ForceField`	A factory that assigns SMIRNOFF parameters to a molecular system

openforcefield.typing.engines.smirnoff.forcefield.ForceField

class openforcefield.typing.engines.smirnoff.forcefield.**ForceField**(**sources*, *parameter_handler_classes=None*, *parameter_io_handler_classes=None*, *disable_version_check=False*, *allow_cosmetic_attributes=False*)

A factory that assigns SMIRNOFF parameters to a molecular system

`ForceField` is a factory that constructs an OpenMM `simtk.openmm.System` object from a `openforcefield.topology.Topology` object defining a (bio)molecular system containing one or more molecules.

When a `ForceField` object is created from one or more specified SMIRNOFF serialized representations, all `ParameterHandler` subclasses currently imported are identified and registered to handle different sections of the SMIRNOFF force field definition file(s).

All `ParameterIOHandler` subclasses currently imported are identified and registered to handle different serialization formats (such as XML).

The force field definition is processed by these handlers to populate the `ForceField` object model data structures that can easily be manipulated via the API:

Processing a `Topology` object defining a chemical system will then call all :class‘ParameterHandler‘ objects in an order guaranteed to satisfy the declared processing order constraints of each :class‘ParameterHandler‘.

Examples

Create a new ForceField containing the smirnoff99Frosst parameter set:

```
>>> from openforcefield.typing.engines.smirnoff import ForceField
>>> forcefield = ForceField('test_forcefields/smirnoff99Frosst.offxml')
```

Create an OpenMM system from a `openforcefield.topology.Topology` object:

```
>>> from openforcefield.topology import Molecule, Topology
>>> ethanol = Molecule.from_smiles('CCO')
>>> topology = Topology.from_molecules(molecules=[ethanol])
>>> system = forcefield.create_openmm_system(topology)
```

Modify the long-range electrostatics method:

```
>>> forcefield.get_parameter_handler('Electrostatics').method = 'PME'
```

Inspect the first few vdW parameters:

```
>>> low_precedence_parameters = forcefield.get_parameter_handler('vdW').parameters[0:3]
```

Retrieve the vdW parameters by SMIRKS string and manipulate it:

```
>>> parameter = forcefield.get_parameter_handler('vdW').parameters['[#1:1]-[#7]']
>>> parameter.rmin_half += 0.1 * unit.angstroms
>>> parameter.epsilon *= 1.02
```

Make a child vdW type more specific (checking modified SMIRKS for validity):

```
>>> forcefield.get_parameter_handler('vdW').parameters[-1].smirks += '~[#53]'
```

Warning: While we check whether the modified SMIRKS is still valid and has the appropriate valence type, we currently don’t check whether the typing remains hierarchical, which could result in some types no longer being assignable because more general types now come *below* them and preferentially match.

Delete a parameter:

```
>>> del forcefield.get_parameter_handler('vdW').parameters['[#1:1]-[#6X4]']
```

Insert a parameter at a specific point in the parameter tree:

```
>>> from openforcefield.typing.engines.smirnoff import vdWHandler
>>> new_parameter = vdWHandler.vdWType(smirks='[*:1]', epsilon=0.0157*unit.kilocalories_per_mole,␣
↪rmin_half=0.6000*unit.angstroms)
>>> forcefield.get_parameter_handler('vdW').parameters.insert(0, new_parameter)
```

Warning: We currently don't check whether removing a parameter could accidentally remove the root type, so it's possible to no longer type all molecules this way.

Attributes

parameters [dict of str] `parameters[tagname]` is the instantiated `ParameterHandler` class that handles parameters associated with the force `tagname`. This is the primary means of retrieving and modifying parameters, such as `parameters['vdW'][0].sigma *= 1.1`

parameter_object_handlers [dict of str] Registered list of `ParameterHandler` classes that will handle different forcefield tags to create the parameter object model. `parameter_object_handlers[tagname]` is the `ParameterHandler` that will be instantiated to process the force field definition section `tagname`. `ParameterHandler` classes are registered when the ForceField object is created, but can be manipulated afterwards.

parameter_io_handlers [dict of str] Registered list of `ParameterIOHandler` classes that will handle serializing/deserializing the parameter object model to string or file representations, such as XML. `parameter_io_handlers[iotype]` is the `ParameterHandler` that will be instantiated to process the serialization scheme `iotype`. `ParameterIOHandler` classes are registered when the ForceField object is created, but can be manipulated afterwards.

Methods

`create_openmm_system`(self, topology, **kwargs)	Create an OpenMM System representing the interactions for the specified Topology with the current force field
`create_parmed_structure`(self, topology, ...)	Create a ParmEd Structure object representing the interactions for the specified Topology with the current force field
`get_parameter_handler`(self, tagname[, ...])	Retrieve the parameter handlers associated with the provided tagname.
`get_parameter_io_handler`(self, io_format)	Retrieve the parameter handlers associated with the provided tagname.
`label_molecules`(self, topology)	Return labels for a list of molecules corresponding to parameters from this force field.
`parse_smirnoff_from_source`(self, source)	Reads a SMIRNOFF data structure from a source, which can be one of many types.
`parse_sources`(self, sources[, ...])	Parse a SMIRNOFF force field definition.
`register_parameter_handler`(self, ...)	Register a new ParameterHandler for a specific tag, making it available for lookup in the ForceField.
`register_parameter_io_handler`(self, ...)	Register a new ParameterIOHandler, making it available for lookup in the ForceField.
`to_file`(self, filename[, io_format, ...])	Write this Forcefield and all its associated parameters to a string in a given format which complies with the SMIRNOFF spec.

Continued on next page

Table 30 – continued from previous page

to_string(self[, io_format, ...])	Write this Forcefield and all its associated parameters to a string in a given format which complies with the SMIRNOFF spec.

__init__(*self*, **sources*, *parameter_handler_classes=None*, *parameter_io_handler_classes=None*, *disable_version_check=False*, *allow_cosmetic_attributes=False*)

Create a new ForceField object from one or more SMIRNOFF parameter definition files.

Parameters

sources [string or file-like object or open file handle or URL (or iterable of these)] A list of files defining the SMIRNOFF force field to be loaded. Currently, only the SMIRNOFF XML format is supported. Each entry may be an absolute file path, a path relative to the current working directory, a path relative to this module's data subdirectory (for built in force fields), or an open file-like object with a `read()` method from which the forcefield XML data can be loaded. If multiple files are specified, any top-level tags that are repeated will be merged if they are compatible, with files appearing later in the sequence resulting in parameters that have higher precedence. Support for multiple files is primarily intended to allow solvent parameters to be specified by listing them last in the sequence.

parameter_handler_classes [iterable of ParameterHandler classes, optional, default=None] If not None, the specified set of ParameterHandler classes will be instantiated to create the parameter object model. By default, all imported subclasses of ParameterHandler are automatically registered.

parameter_io_handler_classes [iterable of ParameterIOHandler classes] If not None, the specified set of ParameterIOHandler classes will be used to parse/generate serialized parameter sets. By default, all imported subclasses of ParameterIOHandler are automatically registered.

disable_version_check [bool, optional, default=False] If True, will disable checks against the current highest supported forcefield version. This option is primarily intended for forcefield development.

allow_cosmetic_attributes [bool, optional. Default = False] Whether to retain non-spec kwargs from data sources.

Examples

Load one SMIRNOFF parameter set in XML format (searching the package data directory by default, which includes some standard parameter sets):

```
>>> forcefield = ForceField('test_forcefields/smirnoff99Frosst.offxml')
```

Load multiple SMIRNOFF parameter sets:

forcefield = ForceField('test_forcefields/smirnoff99Frosst.offxml', 'test_forcefields/tip3p.offxml')

Load a parameter set from a string:

```
>>> offxml = '<SMIRNOFF version="0.2" aromaticity_model="OEAroModel_MDL"/>'
>>> forcefield = ForceField(offxml)
```

Methods

`__init__`(self, *sources[, ...])	Create a new `ForceField` object from one or more SMIRNOFF parameter definition files.
`create_openmm_system`(self, topology, **kwargs)	Create an OpenMM System representing the interactions for the specified Topology with the current force field
`create_parmed_structure`(self, topology, ...)	Create a ParmEd Structure object representing the interactions for the specified Topology with the current force field
`get_parameter_handler`(self, tagname[, ...])	Retrieve the parameter handlers associated with the provided tagname.
`get_parameter_io_handler`(self, io_format)	Retrieve the parameter handlers associated with the provided tagname.
`label_molecules`(self, topology)	Return labels for a list of molecules corresponding to parameters from this force field.
`parse_smirnoff_from_source`(self, source)	Reads a SMIRNOFF data structure from a source, which can be one of many types.
`parse_sources`(self, sources[, ...])	Parse a SMIRNOFF force field definition.
`register_parameter_handler`(self, ...)	Register a new ParameterHandler for a specific tag, making it available for lookup in the ForceField.
`register_parameter_io_handler`(self, ...)	Register a new ParameterIOHandler, making it available for lookup in the ForceField.
`to_file`(self, filename[, io_format, ...])	Write this Forcefield and all its associated parameters to a string in a given format which complies with the SMIRNOFF spec.
`to_string`(self[, io_format, ...])	Write this Forcefield and all its associated parameters to a string in a given format which complies with the SMIRNOFF spec.

Attributes

`author`	Returns the author data for this ForceField object.
`date`	Returns the date data for this ForceField object.

property author
Returns the author data for this ForceField object. If not defined in any loaded files, this will be None.

Returns

author [str] The author data for this forcefield.

property date
Returns the date data for this ForceField object. If not defined in any loaded files, this will be None.

Returns

date [str] The date data for this forcefield.

register_parameter_handler(*self*, *parameter_handler*)

Register a new ParameterHandler for a specific tag, making it available for lookup in the ForceField.

> **Warning:** This API is experimental and subject to change.

Parameters

parameter_handler [A ParameterHandler object] The ParameterHandler to register. The TAGNAME attribute of this object will be used as the key for registration.

register_parameter_io_handler(*self*, *parameter_io_handler*)

Register a new ParameterIOHandler, making it available for lookup in the ForceField.

> **Warning:** This API is experimental and subject to change.

Parameters

parameter_io_handler [A ParameterIOHandler object] The ParameterIOHandler to register. The FORMAT attribute of this object will be used to associate it to a file format/suffix.

get_parameter_handler(*self*, *tagname*, *handler_kwargs=None*, *allow_cosmetic_attributes=False*)

Retrieve the parameter handlers associated with the provided tagname.

If the parameter handler has not yet been instantiated, it will be created and returned. If a parameter handler object already exists, it will be checked for compatibility and an Exception raised if it is incompatible with the provided kwargs. If compatible, the existing ParameterHandler will be returned.

Parameters

tagname [str] The name of the parameter to be handled.

handler_kwargs [dict, optional. Default = None] Dict to be passed to the handler for construction or checking compatibility. If this is None and no existing ParameterHandler exists for the desired tag, a handler will be initialized with all default values. If this is None and a handler for the desired tag exists, the existing ParameterHandler will be returned.

allow_cosmetic_attributes [bool, optional. Default = False] Whether to permit non-spec kwargs in smirnoff_data.

Returns

handler [An openforcefield.engines.typing.smirnoff.ParameterHandler]

Raises

KeyError if there is no ParameterHandler for the given tagname

get_parameter_io_handler(*self*, *io_format*)

Retrieve the parameter handlers associated with the provided tagname. If the parameter IO handler has not yet been instantiated, it will be created.

Parameters

io_format [str] The name of the io format to be handled.

Returns

io_handler [An openforcefield.engines.typing.smirnoff.ParameterIOHandler]

Raises

KeyError if there is no ParameterIOHandler for the given tagname

parse_sources(*self*, *sources*, *allow_cosmetic_attributes=True*)

Parse a SMIRNOFF force field definition.

Parameters

sources [string or file-like object or open file handle or URL (or iterable of these)] A list of files defining the SMIRNOFF force field to be loaded. Currently, only the SMIRNOFF XML format is supported. Each entry may be an absolute file path, a path relative to the current working directory, a path relative to this module's data subdirectory (for built in force fields), or an open file-like object with a `read()` method from which the forcefield XML data can be loaded. If multiple files are specified, any top-level tags that are repeated will be merged if they are compatible, with files appearing later in the sequence resulting in parameters that have higher precedence. Support for multiple files is primarily intended to allow solvent parameters to be specified by listing them last in the sequence.

allow_cosmetic_attributes [bool, optional. Default = False] Whether to permit non-spec kwargs present in the source.

.. notes ::

- New SMIRNOFF sections are handled independently, as if they were specified in the same file.
- If a SMIRNOFF section that has already been read appears again, its definitions are appended to the end of the previously-read definitions if the sections are configured with compatible attributes; otherwise, an `IncompatibleTagException` is raised.

parse_smirnoff_from_source(*self*, *source*)

Reads a SMIRNOFF data structure from a source, which can be one of many types.

Parameters

source [str or bytes] sources : string or file-like object or open file handle or URL (or iterable of these) A list of files defining the SMIRNOFF force field to be loaded Currently, only the SMIRNOFF XML format is supported. Each entry may be an absolute file path, a path relative to the current working directory, a path relative to this module's data subdirectory (for built in force fields), or an open file-like object with a `read()` method from which the forcefield XML data can be loaded.

Returns

smirnoff_data [OrderedDict] A representation of a SMIRNOFF-format data structure. Begins at top-level 'SMIRNOFF' key.

to_string(*self*, *io_format='XML'*, *discard_cosmetic_attributes=False*)

Write this Forcefield and all its associated parameters to a string in a given format which complies with the SMIRNOFF spec.

Parameters

io_format [str or ParameterIOHandler, optional. Default='XML'] The serialization format to write to

discard_cosmetic_attributes [bool, default=False] Whether to discard any non-spec attributes stored in the ForceField.

Returns

forcefield_string [str] The string representation of the serialized forcefield

to_file(*self*, *filename*, *io_format=None*, *discard_cosmetic_attributes=False*)

Write this Forcefield and all its associated parameters to a string in a given format which complies with the SMIRNOFF spec.

Parameters

filename [str] The filename to write to

io_format [str or ParameterIOHandler, optional. Default=None] The serialization format to write out. If None, will attempt to be inferred from the filename.

discard_cosmetic_attributes [bool, default=False] Whether to discard any non-spec attributes stored in the ForceField.

Returns

forcefield_string [str] The string representation of the serialized forcefield

create_openmm_system(*self*, *topology*, ***kwargs*)

Create an OpenMM System representing the interactions for the specified Topology with the current force field

Parameters

topology [openforcefield.topology.Topology] The `Topology` corresponding to the system to be parameterized

charge_from_molecules [List[openforcefield.molecule.Molecule], optional] If specified, partial charges will be taken from the given molecules instead of being determined by the force field.

Returns

system [simtk.openmm.System] The newly created OpenMM System corresponding to the specified `topology`

create_parmed_structure(*self*, *topology*, *positions*, ***kwargs*)

Create a ParmEd Structure object representing the interactions for the specified Topology with the current force field

This method creates a ParmEd `Structure` object containing a topology, positions, and parameters.

Parameters

topology [openforcefield.topology.Topology] The `Topology` corresponding to the `System` object to be created.

positions [simtk.unit.Quantity of dimension (natoms,3) with units compatible with angstroms] The positions corresponding to the `System` object to be created

Returns

structure [parmed.Structure] The newly created `parmed.Structure` object

label_molecules(*self*, *topology*)

Return labels for a list of molecules corresponding to parameters from this force field. For each molecule, a dictionary of force types is returned, and for each force type, each force term is provided with the atoms involved, the parameter id assigned, and the corresponding SMIRKS.

Parameters

topology [openforcefield.topology.Topology] A Topology object containing one or more unique molecules to be labeled

Returns

molecule_labels [list] List of labels for unique molecules. Each entry in the list corresponds to one unique molecule in the Topology and is a dictionary keyed by force type, i.e., `molecule_labels[0]['HarmonicBondForce']` gives details for the harmonic bond parameters for the first molecule. Each element is a list of the form: `[ ( [ atom1, ..., atomN], parameter_id, SMIRKS), ... ]`.

Parameter Type

`ParameterType` objects are representations of individual SMIRKS-based SMIRNOFF parameters. These are usually initialized during `ForceField` creation, and can be inspected and modified by users via the Python API. For more information, see `examples/forcefield_modification`.

`ParameterType`	Base class for SMIRNOFF parameter types.
`BondHandler.BondType`	A SMIRNOFF bond type
`AngleHandler.AngleType`	A SMIRNOFF angle type.
`ProperTorsionHandler.ProperTorsionType`	A SMIRNOFF torsion type for proper torsions.
`ImproperTorsionHandler.ImproperTorsionType`	A SMIRNOFF torsion type for improper torsions.
`vdWHandler.vdWType`	A SMIRNOFF vdWForce type.

openforcefield.typing.engines.smirnoff.parameters.ParameterType

class openforcefield.typing.engines.smirnoff.parameters.**ParameterType**(*smirks*, *allow_cosmetic_attributes=False*, ***kwargs*)

Base class for SMIRNOFF parameter types.

This base class provides utilities to create new parameter types. See the below for examples of how to do this.

> **Warning:** This API is experimental and subject to change.

See also:

ParameterAttribute

IndexedParameterAttribute

Examples

This class allows to define new parameter types by just listing its attributes. In the example below, `_VALENCE_TYPE` AND `_ELEMENT_NAME` are used for the validation of the SMIRKS pattern associated to the parameter and the automatic serialization/deserialization into a `dict`.

```
>>> class MyBondParameter(ParameterType):
...     _VALENCE_TYPE = 'Bond'
...     _ELEMENT_NAME = 'Bond'
...     length = ParameterAttribute(unit=unit.angstrom)
...     k = ParameterAttribute(unit=unit.kilocalorie_per_mole / unit.angstrom**2)
...
```

The parameter automatically inherits the required smirks attribute from `ParameterType`. Associating a `unit` to a `ParameterAttribute` cause the attribute to accept only values in compatible units and to parse string expressions.

```
>>> my_par = MyBondParameter(
...     smirks='[*:1]-[*:2]',
...     length='1.01 * angstrom',
...     k=5 * unit.kilocalorie_per_mole / unit.angstrom**2
... )
>>> my_par.length
Quantity(value=1.01, unit=angstrom)
>>> my_par.k = 3.0 * unit.gram
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: k=3.0 g should have units of kilocalorie/
↪(angstrom**2*mole)
```

Each attribute can be made optional by specifying a default value, and you can attach a converter function by passing a callable as an argument or through the decorator syntax.

```
>>> class MyParameterType(ParameterType):
...     _VALENCE_TYPE = 'Atom'
...     _ELEMENT_NAME = 'Atom'
...
...     attr_optional = ParameterAttribute(default=2)
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to floats
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameterType(smirks='[*:1]', attr_all_to_float='3.0', attr_int_to_float=1)
>>> my_par.attr_optional
2
>>> my_par.attr_all_to_float
3.0
>>> my_par.attr_int_to_float
1.0
```

The float() function can convert strings to integers, but our custom converter forbids it

```
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_int_to_float = '4.0'
```

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```
Traceback (most recent call last):
...
TypeError: Cannot convert '4.0' to float
```

Parameter attributes that can be indexed can be handled with the `IndexedParameterAttribute`. These support unit validation and converters exactly as "ParameterAttribute"s, but the validation/conversion is performed for each indexed attribute.

```
>>> class MyTorsionType(ParameterType):
...     _VALENCE_TYPE = 'ProperTorsion'
...     _ELEMENT_NAME = 'Proper'
...     periodicity = IndexedParameterAttribute(converter=int)
...     k = IndexedParameterAttribute(unit=unit.kilocalorie_per_mole)
...
>>> my_par = MyTorsionType(
...     smirks='[*:1]-[*:2]-[*:3]-[*:4]',
...     periodicity1=2,
...     k1=5 * unit.kilocalorie_per_mole,
...     periodicity2='3',
...     k2=6 * unit.kilocalorie_per_mole,
... )
>>> my_par.periodicity
[2, 3]
```

Attributes

smirks [str] The SMIRKS pattern that this parameter matches.

id [str or None] An optional identifier for the parameter.

parent_id [str or None] Optionally, the identifier of the parameter of which this parameter is a specialization.

Methods

`add_cosmetic_attribute`(self, attr_name, ...)	Add a cosmetic attribute to this object.
`delete_cosmetic_attribute`(self, attr_name)	Delete a cosmetic attribute from this object.
`to_dict`(self[, discard_cosmetic_attributes])	Convert this object to dict format.

__init__(*self*, *smirks*, *allow_cosmetic_attributes=False*, ***kwargs*)

Create a ParameterType.

Parameters

smirks [str] The SMIRKS match for the provided parameter type.

allow_cosmetic_attributes [bool optional. Default = False] Whether to permit non-spec kwargs ("cosmetic attributes"). If True, non-spec kwargs will be stored as an attribute of this parameter which can be accessed and written out. Otherwise an exception will be raised.

Methods

`__init__`(self, smirks[, ...])	Create a ParameterType.
`add_cosmetic_attribute`(self, attr_name, ...)	Add a cosmetic attribute to this object.
`delete_cosmetic_attribute`(self, attr_name)	Delete a cosmetic attribute from this object.
`to_dict`(self[, discard_cosmetic_attributes])	Convert this object to dict format.

Attributes

`id`	A descriptor for `ParameterType` attributes.
`parent_id`	A descriptor for `ParameterType` attributes.
`smirks`	A descriptor for `ParameterType` attributes.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)
Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

to_dict(*self*, *discard_cosmetic_attributes=False*)
Convert this object to dict format.

The returning dictionary contains all the `ParameterAttribute` and `IndexedParameterAttribute` as well as cosmetic attributes if `discard_cosmetic_attributes` is `False`.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False] Whether to discard non-spec attributes of this object

Returns

smirnoff_dict [dict] The SMIRNOFF-compliant dict representation of this object.

openforcefield.typing.engines.smirnoff.parameters.BondHandler.BondType

class openforcefield.typing.engines.smirnoff.parameters.BondHandler.**BondType**(*smirks*, *allow_cosmetic_attributes=False*, ***kwargs*)

A SMIRNOFF bond type

Warning: This API is experimental and subject to change.

Attributes

id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

k A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
```

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```
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

length A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
```

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```
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

parent_id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

smirks A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
```

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```
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
to_dict(self[, discard_cosmetic_attributes])	Convert this object to dict format.

__init__(*self*, *smirks*, *allow_cosmetic_attributes=False*, ***kwargs*)
Create a ParameterType.

Parameters

smirks [str] The SMIRKS match for the provided parameter type.

allow_cosmetic_attributes [bool optional. Default = False] Whether to permit non-spec kwargs ("cosmetic attributes"). If True, non-spec kwargs will be stored as an attribute of this parameter which can be accessed and written out. Otherwise an exception will be raised.

Methods

__init__(self, smirks[, ...])	Create a ParameterType.
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
to_dict(self[, discard_cosmetic_attributes])	Convert this object to dict format.

Attributes

id	A descriptor for ParameterType attributes.
k	A descriptor for ParameterType attributes.
length	A descriptor for ParameterType attributes.
parent_id	A descriptor for ParameterType attributes.
smirks	A descriptor for ParameterType attributes.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)
Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

to_dict(*self*, *discard_cosmetic_attributes=False*)
Convert this object to dict format.

The returning dictionary contains all the ParameterAttribute and IndexedParameterAttribute as well as cosmetic attributes if discard_cosmetic_attributes is False.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False] Whether to discard non-spec attributes of this object

Returns

smirnoff_dict [dict] The SMIRNOFF-compliant dict representation of this object.

openforcefield.typing.engines.smirnoff.parameters.AngleHandler.AngleType

class openforcefield.typing.engines.smirnoff.parameters.AngleHandler.**AngleType**(*smirks*, *allow_cosmetic_attributes=False*, ***kwargs*)

A SMIRNOFF angle type.

Warning: This API is experimental and subject to change.

Attributes

angle A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
```

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```
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
```

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```
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

k A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

parent_id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
```

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```
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

smirks A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
to_dict(self[, discard_cosmetic_attributes])	Convert this object to dict format.

__init__(*self*, *smirks*, *allow_cosmetic_attributes=False*, ***kwargs*)
Create a ParameterType.

Parameters

smirks [str] The SMIRKS match for the provided parameter type.

allow_cosmetic_attributes [bool optional. Default = False] Whether to permit non-spec kwargs ("cosmetic attributes"). If True, non-spec kwargs will be stored as an attribute of this parameter which can be accessed and written out. Otherwise an exception will be raised.

Methods

__init__(self, smirks[, ...])	Create a ParameterType.
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
to_dict(self[, discard_cosmetic_attributes])	Convert this object to dict format.

Attributes

angle	A descriptor for ParameterType attributes.
id	A descriptor for ParameterType attributes.
k	A descriptor for ParameterType attributes.
parent_id	A descriptor for ParameterType attributes.
smirks	A descriptor for ParameterType attributes.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)
Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

to_dict(*self*, *discard_cosmetic_attributes=False*)
Convert this object to dict format.

The returning dictionary contains all the `ParameterAttribute` and `IndexedParameterAttribute` as well as cosmetic attributes if `discard_cosmetic_attributes` is `False`.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False] Whether to discard non-spec attributes of this object

Returns

smirnoff_dict [dict] The SMIRNOFF-compliant dict representation of this object.

openforcefield.typing.engines.smirnoff.parameters.ProperTorsionHandler.ProperTorsionType

class openforcefield.typing.engines.smirnoff.parameters.ProperTorsionHandler.**ProperTorsionType**(*smirks*, *allow_cosmetic_at*, ***kwargs*)

A SMIRNOFF torsion type for proper torsions.

> **Warning:** This API is experimental and subject to change.

Attributes

id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

idivf The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

k The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

parent_id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

periodicity The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

phase The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

smirks A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
to_dict(self[, discard_cosmetic_attributes])	Convert this object to dict format.

__init__(*self*, *smirks*, *allow_cosmetic_attributes=False*, ***kwargs*)
Create a ParameterType.

Parameters

smirks [str] The SMIRKS match for the provided parameter type.

allow_cosmetic_attributes [bool optional. Default = False] Whether to permit non-spec kwargs ("cosmetic attributes"). If True, non-spec kwargs will be stored as an attribute of this parameter which can be accessed and written out. Otherwise an exception will be raised.

Methods

__init__(self, smirks[, ...])	Create a ParameterType.
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
to_dict(self[, discard_cosmetic_attributes])	Convert this object to dict format.

Attributes

id	A descriptor for ParameterType attributes.
idivf	The attribute of a parameter with an unspecified number of terms.
k	The attribute of a parameter with an unspecified number of terms.
parent_id	A descriptor for ParameterType attributes.
periodicity	The attribute of a parameter with an unspecified number of terms.
phase	The attribute of a parameter with an unspecified number of terms.

Continued on next page

Table 45 – continued from previous page

`smirks`	A descriptor for `ParameterType` attributes.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)
Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

to_dict(*self*, *discard_cosmetic_attributes=False*)
Convert this object to dict format.

The returning dictionary contains all the `ParameterAttribute` and `IndexedParameterAttribute` as well as cosmetic attributes if `discard_cosmetic_attributes` is `False`.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False] Whether to discard non-spec attributes of this object

Returns

smirnoff_dict [dict] The SMIRNOFF-compliant dict representation of this object.

openforcefield.typing.engines.smirnoff.parameters.ImproperTorsionHandler.ImproperTorsionType

class openforcefield.typing.engines.smirnoff.parameters.ImproperTorsionHandler.**ImproperTorsionType**(*smirks*, *allow_cosmet* ***kwargs*)

A SMIRNOFF torsion type for improper torsions.

> **Warning:** This API is experimental and subject to change.

Attributes

id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
```

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```
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

idivf The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

k The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

parent_id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
```

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```
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

periodicity The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

phase The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

smirks A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
```

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```
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
to_dict(self[, discard_cosmetic_attributes])	Convert this object to dict format.

__init__(*self*, *smirks*, *allow_cosmetic_attributes=False*, ***kwargs*)
Create a ParameterType.

Parameters

smirks [str] The SMIRKS match for the provided parameter type.

allow_cosmetic_attributes [bool optional. Default = False] Whether to permit non-spec kwargs ("cosmetic attributes"). If True, non-spec kwargs will be stored as an attribute of this parameter which can be accessed and written out. Otherwise an exception will be raised.

Methods

__init__(self, smirks[, ...])	Create a ParameterType.
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
to_dict(self[, discard_cosmetic_attributes])	Convert this object to dict format.

Attributes

`id`	A descriptor for `ParameterType` attributes.
`idivf`	The attribute of a parameter with an unspecified number of terms.
`k`	The attribute of a parameter with an unspecified number of terms.
`parent_id`	A descriptor for `ParameterType` attributes.
`periodicity`	The attribute of a parameter with an unspecified number of terms.
`phase`	The attribute of a parameter with an unspecified number of terms.
`smirks`	A descriptor for `ParameterType` attributes.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)
Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

to_dict(*self*, *discard_cosmetic_attributes=False*)
Convert this object to dict format.

The returning dictionary contains all the `ParameterAttribute` and `IndexedParameterAttribute` as well as cosmetic attributes if `discard_cosmetic_attributes` is `False`.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False] Whether to discard non-spec attributes of this object

Returns

smirnoff_dict [dict] The SMIRNOFF-compliant dict representation of this object.

openforcefield.typing.engines.smirnoff.parameters.vdWHandler.vdWType

class openforcefield.typing.engines.smirnoff.parameters.vdWHandler.**vdWType**(***kwargs*)

A SMIRNOFF vdWForce type.

> **Warning:** This API is experimental and subject to change.

Attributes

epsilon A descriptor for ParameterType attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have None as a default value, required attributes have the default set to the special type UNDEFINED.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a Quantity.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
```

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```
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

parent_id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

rmin_half A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
```

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```
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

sigma A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

smirks A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
```

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```
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
to_dict(self[, discard_cosmetic_attributes])	Convert this object to dict format.

__init__(*self*, ***kwargs*)
Create a ParameterType.

Parameters

smirks [str] The SMIRKS match for the provided parameter type.

allow_cosmetic_attributes [bool optional. Default = False] Whether to permit non-spec kwargs ("cosmetic attributes"). If True, non-spec kwargs will be stored as an attribute of this parameter which can be accessed and written out. Otherwise an exception will be raised.

Methods

__init__(self, **kwargs)	Create a ParameterType.
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
to_dict(self[, discard_cosmetic_attributes])	Convert this object to dict format.

Attributes

epsilon	A descriptor for ParameterType attributes.
id	A descriptor for ParameterType attributes.
parent_id	A descriptor for ParameterType attributes.
rmin_half	A descriptor for ParameterType attributes.
sigma	A descriptor for ParameterType attributes.
smirks	A descriptor for ParameterType attributes.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)
Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

to_dict(*self*, *discard_cosmetic_attributes=False*)
Convert this object to dict format.

The returning dictionary contains all the `ParameterAttribute` and `IndexedParameterAttribute` as well as cosmetic attributes if `discard_cosmetic_attributes` is `False`.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False] Whether to discard non-spec attributes of this object

Returns

smirnoff_dict [dict] The SMIRNOFF-compliant dict representation of this object.

Parameter Handlers

Each `ForceField` primarily consists of several `ParameterHandler` objects, which each contain the machinery to add one energy component to a system. During system creation, each `ParameterHandler` registered to a `ForceField` has its `assign_parameters()` function called..

ParameterList	Parameter list that also supports accessing items by SMARTS string.
ParameterHandler	Base class for parameter handlers.
BondHandler	Handle SMIRNOFF <Bonds> tags
AngleHandler	Handle SMIRNOFF <AngleForce> tags
ProperTorsionHandler	Handle SMIRNOFF <ProperTorsionForce> tags
ImproperTorsionHandler	Handle SMIRNOFF <ImproperTorsionForce> tags
vdWHandler	Handle SMIRNOFF <vdW> tags
ElectrostaticsHandler	Handles SMIRNOFF <Electrostatics> tags.
ToolkitAM1BCCHandler	Handle SMIRNOFF <ToolkitAM1BCC> tags

openforcefield.typing.engines.smirnoff.parameters.ParameterList

class openforcefield.typing.engines.smirnoff.parameters.**ParameterList**(*input_parameter_list=None*)
Parameter list that also supports accessing items by SMARTS string.

> **Warning:** This API is experimental and subject to change.

Methods

append(self, parameter)	Add a ParameterType object to the end of the ParameterList
clear(self, /)	Remove all items from list.
copy(self, /)	Return a shallow copy of the list.
count(self, value, /)	Return number of occurrences of value.
extend(self, other)	Add a ParameterList object to the end of the ParameterList
index(self, item)	Get the numerical index of a ParameterType object or SMIRKS in this ParameterList.
insert(self, index, parameter)	Add a ParameterType object as if this were a list
pop(self[, index])	Remove and return item at index (default last).
remove(self, value, /)	Remove first occurrence of value.
reverse(self, /)	Reverse *IN PLACE*.
sort(self, /, *[, key, reverse])	Stable sort *IN PLACE*.
to_list(self[, discard_cosmetic_attributes])	Render this ParameterList to a normal list, serializing each ParameterType object in it to dict.

__init__(*self*, *input_parameter_list=None*)

Initialize a new ParameterList, optionally providing a list of ParameterType objects to initially populate it.

Parameters

input_parameter_list: list[ParameterType], default=None A pre-existing list of ParameterType-based objects. If None, this ParameterList will be initialized empty.

Methods

__init__(self[, input_parameter_list])	Initialize a new ParameterList, optionally providing a list of ParameterType objects to initially populate it.
append(self, parameter)	Add a ParameterType object to the end of the ParameterList
clear(self, /)	Remove all items from list.
copy(self, /)	Return a shallow copy of the list.
count(self, value, /)	Return number of occurrences of value.
extend(self, other)	Add a ParameterList object to the end of the ParameterList
index(self, item)	Get the numerical index of a ParameterType object or SMIRKS in this ParameterList.
insert(self, index, parameter)	Add a ParameterType object as if this were a list
pop(self[, index])	Remove and return item at index (default last).
remove(self, value, /)	Remove first occurrence of value.
reverse(self, /)	Reverse *IN PLACE*.
sort(self, /, *[, key, reverse])	Stable sort *IN PLACE*.
to_list(self[, discard_cosmetic_attributes])	Render this ParameterList to a normal list, serializing each ParameterType object in it to dict.

append(*self*, *parameter*)

Add a ParameterType object to the end of the ParameterList

Parameters

parameter [a ParameterType object]

extend(*self*, *other*)
Add a ParameterList object to the end of the ParameterList

Parameters

other [a ParameterList]

index(*self*, *item*)
Get the numerical index of a ParameterType object or SMIRKS in this ParameterList. Raises ValueError if the item is not found.

Parameters

item [ParameterType object or str] The parameter or SMIRKS to look up in this ParameterList

Returns

index [int] The index of the found item

insert(*self*, *index*, *parameter*)
Add a ParameterType object as if this were a list

Parameters

index [int] The numerical position to insert the parameter at

parameter [a ParameterType object] The parameter to insert

to_list(*self*, *discard_cosmetic_attributes=True*)
Render this ParameterList to a normal list, serializing each ParameterType object in it to dict.

Parameters

discard_cosmetic_attributes [bool, optional. Default = True] Whether to discard non-spec attributes of each ParameterType object.

Returns

parameter_list [List[dict]] A serialized representation of a ParameterList, with each ParameterType it contains converted to dict.

clear(*self*, */*)
Remove all items from list.

copy(*self*, */*)
Return a shallow copy of the list.

count(*self*, *value*, */*)
Return number of occurrences of value.

pop(*self*, *index=-1*, */*)
Remove and return item at index (default last).

Raises IndexError if list is empty or index is out of range.

remove(*self*, *value*, */*)
Remove first occurrence of value.

Raises ValueError if the value is not present.

reverse(*self*, */*)
Reverse *IN PLACE*.

sort(*self*, */*, ***, *key=None*, *reverse=False*)
Stable sort *IN PLACE*.

openforcefield.typing.engines.smirnoff.parameters.ParameterHandler

class openforcefield.typing.engines.smirnoff.parameters.**ParameterHandler**(*allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)

Base class for parameter handlers.

Parameter handlers are configured with some global parameters for a given section. They may also contain a `ParameterList` populated with `ParameterType` objects if they are responsible for assigning SMIRKS-based parameters.

Warning: This API is experimental and subject to change.

Attributes

known_kwargs List of kwargs that can be parsed by the function.

parameters The ParameterList that holds this ParameterHandler's parameter objects

version A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.
check_handler_compatibility(self, handler_kwargs)	Checks if a set of kwargs used to create a ParameterHandler are compatible with this ParameterHandler.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the elements of the topology/molecule matched by a parameter type.
get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument
postprocess_system(self, topology, system, ...)	Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

__init__(*self*, *allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)
Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.

Parameters

allow_cosmetic_attributes [bool, optional. Default = False] Whether to permit non-spec kwargs. If True, non-spec kwargs will be stored as attributes of this object and can be accessed and modified. Otherwise an exception will be raised if a non-spec kwarg is encountered.

skip_version_check: bool, optional. Default = False If False, the SMIRNOFF section version will not be checked, and the ParameterHandler will be initialized with version set to _MAX_SUPPORTED_SECTION_VERSION.

****kwargs** [dict] The dict representation of the SMIRNOFF data source

Methods

__init__(self[, allow_cosmetic_attributes, ...])	Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.
check_handler_compatibility(self, handler_kwargs)	Checks if a set of kwargs used to create a ParameterHandler are compatible with this ParameterHandler.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the elements of the topology/molecule matched by a parameter type.

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Table 56 – continued from previous page

get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument
postprocess_system(self, topology, system, ...)	Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Attributes

known_kwargs	List of kwargs that can be parsed by the function.
parameters	The ParameterList that holds this ParameterHandler's parameter objects
version	A descriptor for ParameterType attributes.

property parameters
The ParameterList that holds this ParameterHandler's parameter objects

property known_kwargs
List of kwargs that can be parsed by the function.

check_handler_compatibility(*self*, *handler_kwargs*)
Checks if a set of kwargs used to create a ParameterHandler are compatible with this ParameterHandler. This is called if a second handler is attempted to be initialized for the same tag.

Parameters

handler_kwargs [dict] The kwargs that would be used to construct

Raises

IncompatibleParameterError if handler_kwargs are incompatible with existing parameters.

add_parameter(*self*, *parameter_kwargs*)
Add a parameter to the forcefield, ensuring all parameters are valid.

Parameters

parameter_kwargs [dict] The kwargs to pass to the ParameterHandler.INFOTYPE (a ParameterType) constructor

get_parameter(*self*, *parameter_attrs*)
Return the parameters in this ParameterHandler that match the parameter_attrs argument

Parameters

parameter_attrs [dict of {attr: value}] The attrs mapped to desired values (for example {"smirks": "[*:1]~[#16:2]=,:[#6:3]~[*:4]", "id": "t105"})

Returns

list of ParameterType objects A list of matching ParameterType objects

find_matches(*self*, *entity*)
Find the elements of the topology/molecule matched by a parameter type.

Parameters

entity [openforcefield.topology.Topology] Topology to search.

Returns

matches [ValenceDict[Tuple[int], ParameterHandler._Match]] `matches[particle_indices]` is the `ParameterType` object matching the tuple of particle indices in `entity`.

assign_parameters(*self*, *topology*, *system*)
Assign parameters for the given Topology to the specified System object.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

postprocess_system(*self*, *topology*, *system*, ***kwargs*)
Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

to_dict(*self*, *discard_cosmetic_attributes=False*)
Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False.] Whether to discard non-spec parameter and header attributes in this ParameterHandler.

Returns

smirnoff_data [OrderedDict] SMIRNOFF-spec compliant representation of this ParameterHandler and its internal ParameterList.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)
Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

openforcefield.typing.engines.smirnoff.parameters.BondHandler

class openforcefield.typing.engines.smirnoff.parameters.**BondHandler**(*allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)

Handle SMIRNOFF <Bonds> tags

> **Warning:** This API is experimental and subject to change.

Attributes

fractional_bondorder_interpolation A descriptor for ParameterType attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have None as a default value, required attributes have the default set to the special type UNDEFINED.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a Quantity.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

fractional_bondorder_method A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
```

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```
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

known_kwargs List of kwargs that can be parsed by the function.

parameters The ParameterList that holds this ParameterHandler's parameter objects

potential A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
```

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```
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

version A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

BondType(smirks[, allow_cosmetic_attributes])	A SMIRNOFF bond type
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.
check_handler_compatibility(self, other_handler)	Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the elements of the topology/molecule matched by a parameter type.
get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument
postprocess_system(self, topology, system, ...)	Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

create_force

__init__(*self*, *allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)
Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.

Parameters

allow_cosmetic_attributes [bool, optional. Default = False] Whether to permit non-spec kwargs. If True, non-spec kwargs will be stored as attributes of this object and can be accessed and modified. Otherwise an exception will be raised if a non-spec kwarg is encountered.

skip_version_check: bool, optional. Default = False If False, the SMIRNOFF section version will not be checked, and the ParameterHandler will be initialized with version set to _MAX_SUPPORTED_SECTION_VERSION.

****kwargs** [dict] The dict representation of the SMIRNOFF data source

Methods

__init__(self[, allow_cosmetic_attributes, ...])	Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.

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check_handler_compatibility(self, other_handler)	Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler.
create_force(self, system, topology, **kwargs)	
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the elements of the topology/molecule matched by a parameter type.
get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument
postprocess_system(self, topology, system, ...)	Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Attributes

fractional_bondorder_interpolation	A descriptor for ParameterType attributes.
fractional_bondorder_method	A descriptor for ParameterType attributes.
known_kwargs	List of kwargs that can be parsed by the function.
parameters	The ParameterList that holds this ParameterHandler's parameter objects
potential	A descriptor for ParameterType attributes.
version	A descriptor for ParameterType attributes.

class BondType(*smirks*, *allow_cosmetic_attributes=False*, ***kwargs*)

A SMIRNOFF bond type

> **Warning:** This API is experimental and subject to change.

Attributes

id A descriptor for ParameterType attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have None as a default value, required attributes have the default set to the special type UNDEFINED.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
```

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```
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

k A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

length A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

parent_id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
```

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```
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

smirks A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
to_dict(self[, discard_cosmetic_attributes])	Convert this object to dict format.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)
Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

delete_cosmetic_attribute(*self*, *attr_name*)

Delete a cosmetic attribute from this object.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

to_dict(*self*, *discard_cosmetic_attributes=False*)

Convert this object to dict format.

The returning dictionary contains all the `ParameterAttribute` and `IndexedParameterAttribute` as well as cosmetic attributes if `discard_cosmetic_attributes` is `False`.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False] Whether to discard non-spec attributes of this object

Returns

smirnoff_dict [dict] The SMIRNOFF-compliant dict representation of this object.

check_handler_compatibility(*self*, *other_handler*)

Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler. This is called if a second handler is attempted to be initialized for the same tag.

Parameters

other_handler [a ParameterHandler object] The handler to compare to.

Raises

IncompatibleParameterError if handler_kwargs are incompatible with existing parameters.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)

Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

add_parameter(*self*, *parameter_kwargs*)
Add a parameter to the forcefield, ensuring all parameters are valid.

Parameters

parameter_kwargs [dict] The kwargs to pass to the ParameterHandler.INFOTYPE (a ParameterType) constructor

assign_parameters(*self*, *topology*, *system*)
Assign parameters for the given Topology to the specified System object.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

Warning: The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

find_matches(*self*, *entity*)
Find the elements of the topology/molecule matched by a parameter type.

Parameters

entity [openforcefield.topology.Topology] Topology to search.

Returns

matches [ValenceDict[Tuple[int], ParameterHandler._Match]] `matches[particle_indices]` is the `ParameterType` object matching the tuple of particle indices in `entity`.

get_parameter(*self*, *parameter_attrs*)
Return the parameters in this ParameterHandler that match the parameter_attrs argument

Parameters

parameter_attrs [dict of {attr: value}] The attrs mapped to desired values (for example {"smirks": "[*:1]~[#16:2]=,:[#6:3]~[*:4]", "id": "t105"})

Returns

list of ParameterType objects A list of matching ParameterType objects

property known_kwargs
List of kwargs that can be parsed by the function.

property parameters
The ParameterList that holds this ParameterHandler's parameter objects

postprocess_system(*self*, *topology*, *system*, ***kwargs*)
Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

to_dict(*self*, *discard_cosmetic_attributes=False*)
Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False.] Whether to discard non-spec parameter and header attributes in this ParameterHandler.

Returns

smirnoff_data [OrderedDict] SMIRNOFF-spec compliant representation of this ParameterHandler and its internal ParameterList.

openforcefield.typing.engines.smirnoff.parameters.AngleHandler

class openforcefield.typing.engines.smirnoff.parameters.**AngleHandler**(*allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)

Handle SMIRNOFF `<AngleForce>` tags

Warning: This API is experimental and subject to change.

Attributes

known_kwargs List of kwargs that can be parsed by the function.

parameters The ParameterList that holds this ParameterHandler's parameter objects

potential A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
```

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```
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

version A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

AngleType(smirks[, allow_cosmetic_attributes])	A SMIRNOFF angle type.
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.
check_handler_compatibility(self, other_handler)	Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the elements of the topology/molecule matched by a parameter type.
get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument
postprocess_system(self, topology, system, ...)	Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

create_force

__init__(*self*, *allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)
Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.

Parameters

allow_cosmetic_attributes [bool, optional. Default = False] Whether to permit non-spec kwargs. If True, non-spec kwargs will be stored as attributes of this object and can be accessed and modified. Otherwise an exception will be raised if a non-spec kwarg is encountered.

skip_version_check: bool, optional. Default = False If False, the SMIRNOFF section version will not be checked, and the ParameterHandler will be initialized with version set to _MAX_SUPPORTED_SECTION_VERSION.

****kwargs** [dict] The dict representation of the SMIRNOFF data source

Methods

__init__(self[, allow_cosmetic_attributes, ...])	Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.

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check_handler_compatibility(self, other_handler)	Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler.
create_force(self, system, topology, **kwargs)	
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the elements of the topology/molecule matched by a parameter type.
get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument
postprocess_system(self, topology, system, ...)	Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Attributes

known_kwargs	List of kwargs that can be parsed by the function.
parameters	The ParameterList that holds this ParameterHandler's parameter objects
potential	A descriptor for ParameterType attributes.
version	A descriptor for ParameterType attributes.

class AngleType(*smirks*, *allow_cosmetic_attributes=False*, ***kwargs*)

A SMIRNOFF angle type.

> **Warning:** This API is experimental and subject to change.

Attributes

angle A descriptor for ParameterType attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have None as a default value, required attributes have the default set to the special type UNDEFINED.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a Quantity.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
```

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```
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

k A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

parent_id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
```

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```
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

smirks A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
to_dict(self[, discard_cosmetic_attributes])	Convert this object to dict format.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)
Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

delete_cosmetic_attribute(*self*, *attr_name*)

Delete a cosmetic attribute from this object.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

to_dict(*self*, *discard_cosmetic_attributes=False*)

Convert this object to dict format.

The returning dictionary contains all the `ParameterAttribute` and `IndexedParameterAttribute` as well as cosmetic attributes if `discard_cosmetic_attributes` is `False`.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False] Whether to discard non-spec attributes of this object

Returns

smirnoff_dict [dict] The SMIRNOFF-compliant dict representation of this object.

check_handler_compatibility(*self*, *other_handler*)

Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler. This is called if a second handler is attempted to be initialized for the same tag.

Parameters

other_handler [a ParameterHandler object] The handler to compare to.

Raises

IncompatibleParameterError if handler_kwargs are incompatible with existing parameters.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)

Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

add_parameter(*self*, *parameter_kwargs*)
Add a parameter to the forcefield, ensuring all parameters are valid.

Parameters

parameter_kwargs [dict] The kwargs to pass to the ParameterHandler.INFOTYPE (a ParameterType) constructor

assign_parameters(*self*, *topology*, *system*)
Assign parameters for the given Topology to the specified System object.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

Warning: The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

find_matches(*self*, *entity*)
Find the elements of the topology/molecule matched by a parameter type.

Parameters

entity [openforcefield.topology.Topology] Topology to search.

Returns

matches [ValenceDict[Tuple[int], ParameterHandler._Match]] `matches[particle_indices]` is the `ParameterType` object matching the tuple of particle indices in `entity`.

get_parameter(*self*, *parameter_attrs*)
Return the parameters in this ParameterHandler that match the parameter_attrs argument

Parameters

parameter_attrs [dict of {attr: value}] The attrs mapped to desired values (for example {"smirks": "[*:1]~[#16:2]=,:[#6:3]~[*:4]", "id": "t105"})

Returns

list of ParameterType objects A list of matching ParameterType objects

property known_kwargs
List of kwargs that can be parsed by the function.

property parameters
The ParameterList that holds this ParameterHandler's parameter objects

postprocess_system(*self*, *topology*, *system*, ***kwargs*)
Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

to_dict(*self*, *discard_cosmetic_attributes=False*)
Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False.] Whether to discard non-spec parameter and header attributes in this ParameterHandler.

Returns

smirnoff_data [OrderedDict] SMIRNOFF-spec compliant representation of this ParameterHandler and its internal ParameterList.

openforcefield.typing.engines.smirnoff.parameters.ProperTorsionHandler

class openforcefield.typing.engines.smirnoff.parameters.**ProperTorsionHandler**(*allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)

Handle SMIRNOFF `<ProperTorsionForce>` tags

> **Warning:** This API is experimental and subject to change.

Attributes

default_idivf A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
```

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```
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

known_kwargs List of kwargs that can be parsed by the function.

parameters The ParameterList that holds this ParameterHandler's parameter objects

potential A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

version A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
```

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```
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

ProperTorsionType(smirks[, ...])	A SMIRNOFF torsion type for proper torsions.
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.
check_handler_compatibility(self, other_handler)	Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the elements of the topology/molecule matched by a parameter type.
get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument

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Table 66 – continued from previous page

postprocess_system(self, topology, system, . . .)	Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

create_force

__init__(*self*, *allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)
Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.

Parameters

allow_cosmetic_attributes [bool, optional. Default = False] Whether to permit non-spec kwargs. If True, non-spec kwargs will be stored as attributes of this object and can be accessed and modified. Otherwise an exception will be raised if a non-spec kwarg is encountered.

skip_version_check: bool, optional. Default = False If False, the SMIRNOFF section version will not be checked, and the ParameterHandler will be initialized with version set to _MAX_SUPPORTED_SECTION_VERSION.

****kwargs** [dict] The dict representation of the SMIRNOFF data source

Methods

__init__(self[, allow_cosmetic_attributes, . . .])	Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.
add_cosmetic_attribute(self, attr_name, . . .)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.
check_handler_compatibility(self, other_handler)	Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler.
create_force(self, system, topology, **kwargs)	
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the elements of the topology/molecule matched by a parameter type.
get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument
postprocess_system(self, topology, system, . . .)	Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Attributes

default_idivf	A descriptor for ParameterType attributes.
known_kwargs	List of kwargs that can be parsed by the function.
parameters	The ParameterList that holds this ParameterHandler's parameter objects
potential	A descriptor for ParameterType attributes.
version	A descriptor for ParameterType attributes.

class ProperTorsionType(*smirks*, *allow_cosmetic_attributes=False*, ***kwargs*)

A SMIRNOFF torsion type for proper torsions.

Warning: This API is experimental and subject to change.

Attributes

id A descriptor for ParameterType attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have None as a default value, required attributes have the default set to the special type UNDEFINED.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a Quantity.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

idivf The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

k The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

parent_id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

periodicity The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

phase The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

smirks A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
```

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```
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
to_dict(self[, discard_cosmetic_attributes])	Convert this object to dict format.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)

Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters
attr_name [str] Name of the attribute to define for this object.
attr_value [str] The value of the attribute to define for this object.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters
attr_name [str] Name of the cosmetic attribute to delete.

to_dict(*self*, *discard_cosmetic_attributes=False*)
Convert this object to dict format.

The returning dictionary contains all the `ParameterAttribute` and `IndexedParameterAttribute` as well as cosmetic attributes if `discard_cosmetic_attributes` is `False`.

Parameters
discard_cosmetic_attributes [bool, optional. Default = False] Whether to discard non-spec attributes of this object
Returns
smirnoff_dict [dict] The SMIRNOFF-compliant dict representation of this object.

check_handler_compatibility(*self*, *other_handler*)
Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler. This is called if a second handler is attempted to be initialized for the same tag.

Parameters

other_handler [a ParameterHandler object] The handler to compare to.

Raises

IncompatibleParameterError if handler_kwargs are incompatible with existing parameters.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)
Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

add_parameter(*self*, *parameter_kwargs*)
Add a parameter to the forcefield, ensuring all parameters are valid.

Parameters

parameter_kwargs [dict] The kwargs to pass to the ParameterHandler.INFOTYPE (a ParameterType) constructor

assign_parameters(*self*, *topology*, *system*)
Assign parameters for the given Topology to the specified System object.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

Warning: The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

find_matches(*self*, *entity*)
Find the elements of the topology/molecule matched by a parameter type.

Parameters

entity [openforcefield.topology.Topology] Topology to search.

Returns

matches [ValenceDict[Tuple[int], ParameterHandler._Match]] `matches[particle_indices]` is the `ParameterType` object matching the tuple of particle indices in `entity`.

get_parameter(*self*, *parameter_attrs*)
Return the parameters in this ParameterHandler that match the parameter_attrs argument

Parameters

parameter_attrs [dict of {attr: value}] The attrs mapped to desired values (for example {"smirks": "[*:1]~[#16:2]=,:[#6:3]~[*:4]", "id": "t105"})

Returns

list of ParameterType objects A list of matching ParameterType objects

property known_kwargs
List of kwargs that can be parsed by the function.

property parameters
The ParameterList that holds this ParameterHandler's parameter objects

postprocess_system(*self*, *topology*, *system*, ***kwargs*)
Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

to_dict(*self*, *discard_cosmetic_attributes=False*)

Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False.] Whether to discard non-spec parameter and header attributes in this ParameterHandler.

Returns

smirnoff_data [OrderedDict] SMIRNOFF-spec compliant representation of this ParameterHandler and its internal ParameterList.

openforcefield.typing.engines.smirnoff.parameters.ImproperTorsionHandler

class openforcefield.typing.engines.smirnoff.parameters.**ImproperTorsionHandler**(*allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)

Handle SMIRNOFF <ImproperTorsionForce> tags

Warning: This API is experimental and subject to change.

Attributes

default_idivf A descriptor for ParameterType attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have None as a default value, required attributes have the default set to the special type UNDEFINED.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a Quantity.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
```

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```
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

known_kwargs List of kwargs that can be parsed by the function.

parameters The ParameterList that holds this ParameterHandler's parameter objects

potential A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

version A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have None as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

ImproperTorsionType(smirks[, ...])	A SMIRNOFF torsion type for improper torsions.
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.
check_handler_compatibility(self, other_handler)	Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the improper torsions in the topology/molecule matched by a parameter type.
get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument
postprocess_system(self, topology, system, ...)	Allow the force to perform a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

create_force	

__init__(*self*, *allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)
Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.

Parameters

allow_cosmetic_attributes [bool, optional. Default = False] Whether to permit non-spec kwargs. If True, non-spec kwargs will be stored as attributes of this object and can be accessed and modified. Otherwise an exception will be raised if a non-spec kwarg is encountered.

skip_version_check: bool, optional. Default = False If False, the SMIRNOFF section version will not be checked, and the ParameterHandler will be initialized with version set to _MAX_SUPPORTED_SECTION_VERSION.

****kwargs** [dict] The dict representation of the SMIRNOFF data source

Methods

__init__(self[, allow_cosmetic_attributes, ...])	Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.
check_handler_compatibility(self, other_handler)	Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler.
create_force(self, system, topology, **kwargs)	
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the improper torsions in the topology/molecule matched by a parameter type.
get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument
postprocess_system(self, topology, system, ...)	Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Attributes

default_idivf	A descriptor for ParameterType attributes.
known_kwargs	List of kwargs that can be parsed by the function.
parameters	The ParameterList that holds this ParameterHandler's parameter objects
potential	A descriptor for ParameterType attributes.
version	A descriptor for ParameterType attributes.

class ImproperTorsionType(*smirks*, *allow_cosmetic_attributes=False*, ***kwargs*)
A SMIRNOFF torsion type for improper torsions.

> **Warning:** This API is experimental and subject to change.

Attributes

id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

idivf The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

k The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

parent_id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
```

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```
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

periodicity The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
```

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```
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

phase The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

ParameterAttribute A simple parameter attribute.

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

smirks A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
```

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```
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
to_dict(self[, discard_cosmetic_attributes])	Convert this object to dict format.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)

Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters
attr_name [str] Name of the attribute to define for this object.
attr_value [str] The value of the attribute to define for this object.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).
Parameters
attr_name [str] Name of the cosmetic attribute to delete.

to_dict(*self*, *discard_cosmetic_attributes=False*)
Convert this object to dict format.

The returning dictionary contains all the `ParameterAttribute` and `IndexedParameterAttribute` as well as cosmetic attributes if `discard_cosmetic_attributes` is `False`.
Parameters
discard_cosmetic_attributes [bool, optional. Default = False] Whether to discard non-spec attributes of this object
Returns
smirnoff_dict [dict] The SMIRNOFF-compliant dict representation of this object.

check_handler_compatibility(*self*, *other_handler*)
Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler. This is called if a second handler is attempted to be initialized for the same tag.

Parameters

other_handler [a ParameterHandler object] The handler to compare to.

Raises

IncompatibleParameterError if handler_kwargs are incompatible with existing parameters.

find_matches(*self*, *entity*)
Find the improper torsions in the topology/molecule matched by a parameter type.

Parameters

entity [openforcefield.topology.Topology] Topology to search.

Returns

matches [ImproperDict[Tuple[int], ParameterHandler._Match]]
`matches[atom_indices]` is the `ParameterType` object matching the 4-tuple of atom indices in `entity`.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)
Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

add_parameter(*self*, *parameter_kwargs*)
Add a parameter to the forcefield, ensuring all parameters are valid.

Parameters

parameter_kwargs [dict] The kwargs to pass to the ParameterHandler.INFOTYPE (a ParameterType) constructor

assign_parameters(*self*, *topology*, *system*)
Assign parameters for the given Topology to the specified System object.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

get_parameter(*self*, *parameter_attrs*)
Return the parameters in this ParameterHandler that match the parameter_attrs argument

Parameters

parameter_attrs [dict of {attr: value}] The attrs mapped to desired values (for example {"smirks": "[*:1]~[#16:2]=,:[#6:3]~[*:4]", "id": "t105"})

Returns

list of ParameterType objects A list of matching ParameterType objects

property known_kwargs
List of kwargs that can be parsed by the function.

property parameters
The ParameterList that holds this ParameterHandler's parameter objects

postprocess_system(*self*, *topology*, *system*, ***kwargs*)
Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

to_dict(*self*, *discard_cosmetic_attributes=False*)

Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False.] Whether to discard non-spec parameter and header attributes in this ParameterHandler.

Returns

smirnoff_data [OrderedDict] SMIRNOFF-spec compliant representation of this ParameterHandler and its internal ParameterList.

openforcefield.typing.engines.smirnoff.parameters.vdWHandler

class openforcefield.typing.engines.smirnoff.parameters.**vdWHandler**(*allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)

Handle SMIRNOFF <vdW> tags

Warning: This API is experimental and subject to change.

Attributes

combining_rules A descriptor for ParameterType attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have None as a default value, required attributes have the default set to the special type UNDEFINED.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a Quantity.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
```

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```
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

cutoff A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

known_kwargs List of kwargs that can be parsed by the function.

method A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
```

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```
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

parameters The ParameterList that holds this ParameterHandler's parameter objects

potential A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
```

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```
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

scale12 A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

scale13 A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
```

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```
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

scale14 A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

scale15 A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
```

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```
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

switch_width A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

version A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
```

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```
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.
check_handler_compatibility(self, other_handler)	Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the elements of the topology/molecule matched by a parameter type.
get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument
postprocess_system(self, system, topology, ...)	Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.
vdWType(**kwargs)	A SMIRNOFF vdWForce type.

create_force

__init__(*self*, *allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)
Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.

Parameters

allow_cosmetic_attributes [bool, optional. Default = False] Whether to permit non-spec kwargs. If True, non-spec kwargs will be stored as attributes of this object and can be accessed and modified. Otherwise an exception will be raised if a non-spec kwarg is encountered.

skip_version_check: bool, optional. Default = False If False, the SMIRNOFF section version will not be checked, and the ParameterHandler will be initialized with version set to _MAX_SUPPORTED_SECTION_VERSION.

****kwargs** [dict] The dict representation of the SMIRNOFF data source

Methods

__init__(self[, allow_cosmetic_attributes, ...])	Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.
check_handler_compatibility(self, other_handler)	Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler.

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create_force(self, system, topology, **kwargs)	
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the elements of the topology/molecule matched by a parameter type.
get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument
postprocess_system(self, system, topology, ...)	Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Attributes

combining_rules	A descriptor for ParameterType attributes.
cutoff	A descriptor for ParameterType attributes.
known_kwargs	List of kwargs that can be parsed by the function.
method	A descriptor for ParameterType attributes.
parameters	The ParameterList that holds this ParameterHandler's parameter objects
potential	A descriptor for ParameterType attributes.
scale12	A descriptor for ParameterType attributes.
scale13	A descriptor for ParameterType attributes.
scale14	A descriptor for ParameterType attributes.
scale15	A descriptor for ParameterType attributes.
switch_width	A descriptor for ParameterType attributes.
version	A descriptor for ParameterType attributes.

class vdWType(***kwargs*)

A SMIRNOFF vdWForce type.

> **Warning:** This API is experimental and subject to change.

Attributes

epsilon A descriptor for ParameterType attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have None as a default value, required attributes have the default set to the special type UNDEFINED.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
```

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```
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

parent_id A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
```

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```
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

rmin_half A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

sigma A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
```

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```
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

smirks A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
to_dict(self[, discard_cosmetic_attributes])	Convert this object to dict format.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)

Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

delete_cosmetic_attribute(*self*, *attr_name*)

Delete a cosmetic attribute from this object.

Warning: The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

to_dict(*self*, *discard_cosmetic_attributes=False*)

Convert this object to dict format.

The returning dictionary contains all the `ParameterAttribute` and `IndexedParameterAttribute` as well as cosmetic attributes if `discard_cosmetic_attributes` is `False`.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False] Whether to discard non-spec attributes of this object

Returns

smirnoff_dict [dict] The SMIRNOFF-compliant dict representation of this object.

check_handler_compatibility(*self*, *other_handler*)

Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler. This is called if a second handler is attempted to be initialized for the same tag.

Parameters

other_handler [a ParameterHandler object] The handler to compare to.

Raises

IncompatibleParameterError if handler_kwargs are incompatible with existing parameters.

postprocess_system(*self*, *system*, *topology*, ***kwargs*)

Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)

Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

Warning: The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

add_parameter(*self*, *parameter_kwargs*)
Add a parameter to the forcefield, ensuring all parameters are valid.

Parameters

parameter_kwargs [dict] The kwargs to pass to the ParameterHandler.INFOTYPE (a ParameterType) constructor

assign_parameters(*self*, *topology*, *system*)
Assign parameters for the given Topology to the specified System object.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

Warning: The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

find_matches(*self*, *entity*)
Find the elements of the topology/molecule matched by a parameter type.

Parameters

entity [openforcefield.topology.Topology] Topology to search.

Returns

matches [ValenceDict[Tuple[int], ParameterHandler._Match]] `matches[particle_indices]` is the `ParameterType` object matching the tuple of particle indices in `entity`.

get_parameter(*self*, *parameter_attrs*)
Return the parameters in this ParameterHandler that match the parameter_attrs argument

Parameters

parameter_attrs [dict of {attr: value}] The attrs mapped to desired values (for example {"smirks": "[*:1]~[#16:2]=,:[#6:3]~[*:4]", "id": "t105"})

Returns

list of ParameterType objects A list of matching ParameterType objects

property known_kwargs
List of kwargs that can be parsed by the function.

property parameters
The ParameterList that holds this ParameterHandler's parameter objects

to_dict(*self*, *discard_cosmetic_attributes=False*)
Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False.] Whether to discard non-spec parameter and header attributes in this ParameterHandler.

Returns

smirnoff_data [OrderedDict] SMIRNOFF-spec compliant representation of this ParameterHandler and its internal ParameterList.

openforcefield.typing.engines.smirnoff.parameters.ElectrostaticsHandler

class openforcefield.typing.engines.smirnoff.parameters.**ElectrostaticsHandler**(*allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)

Handles SMIRNOFF <Electrostatics> tags.

Warning: This API is experimental and subject to change.

Attributes

cutoff A descriptor for ParameterType attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have None as a default value, required attributes have the default set to the special type UNDEFINED.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a Quantity.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
```

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```
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

`known_kwargs` List of kwargs that can be parsed by the function.

method A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
```

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```
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

parameters The ParameterList that holds this ParameterHandler's parameter objects

scale12 A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
```

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```
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

scale13 A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

scale14 A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
```

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```
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

scale15 A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

switch_width A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
```

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```
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

version A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.
check_handler_compatibility(self, other_handler)	Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the elements of the topology/molecule matched by a parameter type.
get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument
postprocess_system(self, topology, system, ...)	Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

create_force	

__init__(*self*, *allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)
Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.

Parameters

allow_cosmetic_attributes [bool, optional. Default = False] Whether to permit non-spec kwargs. If True, non-spec kwargs will be stored as attributes of this object and can be accessed and modified. Otherwise an exception will be raised if a non-spec kwarg is encountered.

skip_version_check: bool, optional. Default = False If False, the SMIRNOFF section version will not be checked, and the ParameterHandler will be initialized with version set to _MAX_SUPPORTED_SECTION_VERSION.

****kwargs** [dict] The dict representation of the SMIRNOFF data source

Methods

__init__(self[, allow_cosmetic_attributes, ...])	Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.
check_handler_compatibility(self, other_handler)	Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler.
create_force(self, system, topology, **kwargs)	
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the elements of the topology/molecule matched by a parameter type.
get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument
postprocess_system(self, topology, system, ...)	Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Attributes

cutoff	A descriptor for ParameterType attributes.
known_kwargs	List of kwargs that can be parsed by the function.
method	A descriptor for ParameterType attributes.
parameters	The ParameterList that holds this ParameterHandler's parameter objects
scale12	A descriptor for ParameterType attributes.
scale13	A descriptor for ParameterType attributes.
scale14	A descriptor for ParameterType attributes.
scale15	A descriptor for ParameterType attributes.

Continued on next page

Table 80 – continued from previous page

switch_width	A descriptor for ParameterType attributes.
version	A descriptor for ParameterType attributes.

check_handler_compatibility(*self*, *other_handler*)
Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler. This is called if a second handler is attempted to be initialized for the same tag.

Parameters

other_handler [a ParameterHandler object] The handler to compare to.

Raises

IncompatibleParameterError if handler_kwargs are incompatible with existing parameters.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)
Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

add_parameter(*self*, *parameter_kwargs*)
Add a parameter to the forcefield, ensuring all parameters are valid.

Parameters

parameter_kwargs [dict] The kwargs to pass to the ParameterHandler.INFOTYPE (a ParameterType) constructor

assign_parameters(*self*, *topology*, *system*)
Assign parameters for the given Topology to the specified System object.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

find_matches(*self*, *entity*)
Find the elements of the topology/molecule matched by a parameter type.

Parameters

entity [openforcefield.topology.Topology] Topology to search.

Returns

matches [ValenceDict[Tuple[int], ParameterHandler._Match]] `matches[particle_indices]` is the `ParameterType` object matching the tuple of particle indices in `entity`.

get_parameter(*self*, *parameter_attrs*)
Return the parameters in this ParameterHandler that match the parameter_attrs argument

Parameters

parameter_attrs [dict of {attr: value}] The attrs mapped to desired values (for example {"smirks": "[*:1]~[#16:2]=,:[#6:3]~[*:4]", "id": "t105"})

Returns

list of ParameterType objects A list of matching ParameterType objects

property known_kwargs
List of kwargs that can be parsed by the function.

property parameters
The ParameterList that holds this ParameterHandler's parameter objects

postprocess_system(*self*, *topology*, *system*, ***kwargs*)
Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

to_dict(*self*, *discard_cosmetic_attributes=False*)
Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False.] Whether to discard non-spec parameter and header attributes in this ParameterHandler.

Returns

smirnoff_data [OrderedDict] SMIRNOFF-spec compliant representation of this ParameterHandler and its internal ParameterList.

openforcefield.typing.engines.smirnoff.parameters.ToolkitAM1BCCHandler

class openforcefield.typing.engines.smirnoff.parameters.**ToolkitAM1BCCHandler**(*allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)

Handle SMIRNOFF <ToolkitAM1BCC> tags

Warning: This API is experimental and subject to change.

Attributes

known_kwargs List of kwargs that can be parsed by the function.

parameters The ParameterList that holds this ParameterHandler's parameter objects

version A descriptor for ParameterType attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have None as a default value, required attributes have the default set to the special type UNDEFINED.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a Quantity.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

IndexedParameterAttribute A parameter attribute with multiple terms.

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0␣
↪dimensionless should have units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Methods

add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_charge_from_molecules(self, molecule, ...)	Given an input molecule, checks against a list of molecules for an isomorphic match.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.
check_handler_compatibility(self, other_handler)	Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler.
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the elements of the topology/molecule matched by a parameter type.
get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument
postprocess_system(self, system, topology, ...)	Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

create_force

__init__(*self*, *allow_cosmetic_attributes=False*, *skip_version_check=False*, ***kwargs*)
Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.

Parameters

allow_cosmetic_attributes [bool, optional. Default = False] Whether to permit non-spec kwargs. If True, non-spec kwargs will be stored as attributes of this object and can be accessed and modified. Otherwise an exception will be raised if a non-spec kwarg is encountered.

skip_version_check: bool, optional. Default = False If False, the SMIRNOFF section version will not be checked, and the ParameterHandler will be initialized with version set to _MAX_SUPPORTED_SECTION_VERSION.

****kwargs** [dict] The dict representation of the SMIRNOFF data source

Methods

__init__(self[, allow_cosmetic_attributes, ...])	Initialize a ParameterHandler, optionally with a list of parameters and other kwargs.
add_cosmetic_attribute(self, attr_name, ...)	Add a cosmetic attribute to this object.
add_parameter(self, parameter_kwargs)	Add a parameter to the forcefield, ensuring all parameters are valid.
assign_charge_from_molecules(self, molecule, ...)	Given an input molecule, checks against a list of molecules for an isomorphic match.
assign_parameters(self, topology, system)	Assign parameters for the given Topology to the specified System object.

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Table 82 – continued from previous page

check_handler_compatibility(self, other_handler)	Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler.
create_force(self, system, topology, **kwargs)	
delete_cosmetic_attribute(self, attr_name)	Delete a cosmetic attribute from this object.
find_matches(self, entity)	Find the elements of the topology/molecule matched by a parameter type.
get_parameter(self, parameter_attrs)	Return the parameters in this ParameterHandler that match the parameter_attrs argument
postprocess_system(self, system, topology, ...)	Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.
to_dict(self[, discard_cosmetic_attributes])	Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Attributes

known_kwargs	List of kwargs that can be parsed by the function.
parameters	The ParameterList that holds this ParameterHandler's parameter objects
version	A descriptor for ParameterType attributes.

check_handler_compatibility(*self*, *other_handler*, *assume_missing_is_default=True*)

Checks whether this ParameterHandler encodes compatible physics as another ParameterHandler. This is called if a second handler is attempted to be initialized for the same tag.

Parameters

other_handler [a ParameterHandler object] The handler to compare to.

Raises

IncompatibleParameterError if handler_kwargs are incompatible with existing parameters.

assign_charge_from_molecules(*self*, *molecule*, *charge_mols*)

Given an input molecule, checks against a list of molecules for an isomorphic match. If found, assigns partial charges from the match to the input molecule.

Parameters

molecule [an openforcefield.topology.FrozenMolecule] The molecule to have partial charges assigned if a match is found.

charge_mols [list of [openforcefield.topology.FrozenMolecule]] A list of molecules with charges already assigned.

Returns

match_found [bool] Whether a match was found. If True, the input molecule will have been modified in-place.

postprocess_system(*self*, *system*, *topology*, ***kwargs*)

Allow the force to perform a a final post-processing pass on the System following parameter assignment, if needed.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

add_cosmetic_attribute(*self*, *attr_name*, *attr_value*)
Add a cosmetic attribute to this object.

This attribute will not have a functional effect on the object in the Open Force Field toolkit, but can be written out during output.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the attribute to define for this object.

attr_value [str] The value of the attribute to define for this object.

add_parameter(*self*, *parameter_kwargs*)
Add a parameter to the forcefield, ensuring all parameters are valid.

Parameters

parameter_kwargs [dict] The kwargs to pass to the ParameterHandler.INFOTYPE (a ParameterType) constructor

assign_parameters(*self*, *topology*, *system*)
Assign parameters for the given Topology to the specified System object.

Parameters

topology [openforcefield.topology.Topology] The Topology for which parameters are to be assigned. Either a new Force will be created or parameters will be appended to an existing Force.

system [simtk.openmm.System] The OpenMM System object to add the Force (or append new parameters) to.

delete_cosmetic_attribute(*self*, *attr_name*)
Delete a cosmetic attribute from this object.

> **Warning:** The API for modifying cosmetic attributes is experimental

and may change in the future (see issue #338).

Parameters

attr_name [str] Name of the cosmetic attribute to delete.

find_matches(*self*, *entity*)
Find the elements of the topology/molecule matched by a parameter type.

Parameters

entity [openforcefield.topology.Topology] Topology to search.

Returns

matches [ValenceDict[Tuple[int], ParameterHandler._Match]] `matches[particle_indices]` is the `ParameterType` object matching the tuple of particle indices in `entity`.

get_parameter(*self*, *parameter_attrs*)
Return the parameters in this ParameterHandler that match the parameter_attrs argument

Parameters

parameter_attrs [dict of {attr: value}] The attrs mapped to desired values (for example {"smirks": "[*:1]~[#16:2]=,:[#6:3]~[*:4]", "id": "t105"})

Returns

list of ParameterType objects A list of matching ParameterType objects

property known_kwargs
List of kwargs that can be parsed by the function.

property parameters
The ParameterList that holds this ParameterHandler's parameter objects

to_dict(*self*, *discard_cosmetic_attributes=False*)
Convert this ParameterHandler to an OrderedDict, compliant with the SMIRNOFF data spec.

Parameters

discard_cosmetic_attributes [bool, optional. Default = False.] Whether to discard non-spec parameter and header attributes in this ParameterHandler.

Returns

smirnoff_data [OrderedDict] SMIRNOFF-spec compliant representation of this ParameterHandler and its internal ParameterList.

Parameter I/O Handlers

`ParameterIOHandler` objects handle reading and writing of serialzied SMIRNOFF data sources.

`ParameterIOHandler`	Base class for handling serialization/deserialization of SMIRNOFF ForceField objects
`XMLParameterIOHandler`	Handles serialization/deserialization of SMIRNOFF ForceField objects from OFFXML format.

openforcefield.typing.engines.smirnoff.io.ParameterIOHandler

class openforcefield.typing.engines.smirnoff.io.**ParameterIOHandler**
Base class for handling serialization/deserialization of SMIRNOFF ForceField objects

Methods

parse_file(self, file_path)	**Parameters**
parse_string(self, data)	Parse a SMIRNOFF force field definition in a seriaized format
to_file(self, file_path, smirnoff_data)	Write the current forcefield parameter set to a file.
to_string(self, smirnoff_data)	Render the forcefield parameter set to a string

__init__(*self*)
Create a new ParameterIOHandler.

Methods

__init__(self)	Create a new ParameterIOHandler.
parse_file(self, file_path)	**Parameters**
parse_string(self, data)	Parse a SMIRNOFF force field definition in a seriaized format
to_file(self, file_path, smirnoff_data)	Write the current forcefield parameter set to a file.
to_string(self, smirnoff_data)	Render the forcefield parameter set to a string

parse_file(*self*, *file_path*)

Parameters

file_path

parse_string(*self*, *data*)
Parse a SMIRNOFF force field definition in a seriaized format

Parameters

data

to_file(*self*, *file_path*, *smirnoff_data*)
Write the current forcefield parameter set to a file.

Parameters

file_path [str] The path to the file to write to.

smirnoff_data [dict] A dictionary structured in compliance with the SMIRNOFF spec

to_string(*self*, *smirnoff_data*)
Render the forcefield parameter set to a string

Parameters

smirnoff_data [dict] A dictionary structured in compliance with the SMIRNOFF spec

Returns

str

openforcefield.typing.engines.smirnoff.io.XMLParameterIOHandler

class openforcefield.typing.engines.smirnoff.io.**XMLParameterIOHandler**

Handles serialization/deserialization of SMIRNOFF ForceField objects from OFFXML format.

Methods

parse_file(self, source)	Parse a SMIRNOFF force field definition in XML format, read from a file.
parse_string(self, data)	Parse a SMIRNOFF force field definition in XML format.
to_file(self, file_path, smirnoff_data)	Write the current forcefield parameter set to a file.
to_string(self, smirnoff_data)	Write the current forcefield parameter set to an XML string.

__init__(*self*)

Create a new ParameterIOHandler.

Methods

__init__(self)	Create a new ParameterIOHandler.
parse_file(self, source)	Parse a SMIRNOFF force field definition in XML format, read from a file.
parse_string(self, data)	Parse a SMIRNOFF force field definition in XML format.
to_file(self, file_path, smirnoff_data)	Write the current forcefield parameter set to a file.
to_string(self, smirnoff_data)	Write the current forcefield parameter set to an XML string.

parse_file(*self*, *source*)

Parse a SMIRNOFF force field definition in XML format, read from a file.

Parameters

source [str or io.RawIOBase] File path of file-like object implementing a `read()` method specifying a SMIRNOFF force field definition in the SMIRNOFF XML format.

Raises

ParseError If the XML cannot be processed.

FileNotFoundError If the file could not found.

parse_string(*self*, *data*)

Parse a SMIRNOFF force field definition in XML format.

A `ParseError` is raised if the XML cannot be processed.

Parameters

data [str] A SMIRNOFF force field definition in the SMIRNOFF XML format.

to_file(*self*, *file_path*, *smirnoff_data*)
Write the current forcefield parameter set to a file.

Parameters

file_path [str] The path to the file to be written. The *.offxml* or *.xml* file extension must be present.

smirnoff_data [dict] A dict structured in compliance with the SMIRNOFF data spec.

to_string(*self*, *smirnoff_data*)
Write the current forcefield parameter set to an XML string.

Parameters

smirnoff_data [dict] A dictionary structured in compliance with the SMIRNOFF spec

Returns

serialized_forcefield [str] XML String representation of this forcefield.

Parameter Attributes

`ParameterAttribute` and `IndexedParameterAttribute` provide a standard backend for ParameterHandler and Parameter attributes, while also enforcing validation of types and units.

`ParameterAttribute`	A descriptor for `ParameterType` attributes.
`IndexedParameterAttribute`	The attribute of a parameter with an unspecified number of terms.

openforcefield.typing.engines.smirnoff.parameters.ParameterAttribute

class openforcefield.typing.engines.smirnoff.parameters.**ParameterAttribute**(*default=<class 'openforcefield.typing.engines.smirnoff.parameters unit=None*, *converter=None*)

A descriptor for `ParameterType` attributes.

The descriptors allows associating to the parameter a default value, which makes the attribute optional, a unit, and a custom converter.

Because we may want to have `None` as a default value, required attributes have the `default` set to the special type `UNDEFINED`.

Converters can be both static or instance functions/methods with respective signatures

converter(value): -> converted_value converter(instance, parameter_attribute, value): -> converted_value

A decorator syntax is available (see example below).

Parameters

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only quantities with compatible units are allowed to be set, and string expressions are automatically parsed into a `Quantity`.

converter [callable, optional] An optional function that can be used to convert values before setting the attribute.

See also:

`IndexedParameterAttribute` A parameter attribute with multiple terms.

Examples

Create a parameter type with an optional and a required attribute.

```
>>> class MyParameter:
...     attr_required = ParameterAttribute()
...     attr_optional = ParameterAttribute(default=2)
...
>>> my_par = MyParameter()
```

Even without explicit assignment, the default value is returned.

```
>>> my_par.attr_optional
2
```

If you try to access an attribute without setting it first, an exception is raised.

```
>>> my_par.attr_required
Traceback (most recent call last):
...
AttributeError: 'MyParameter' object has no attribute '_attr_required'
```

The attribute allow automatic conversion and validation of units.

```
>>> from simtk import unit
>>> class MyParameter:
...     attr_quantity = ParameterAttribute(unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.attr_quantity = '1.0 * nanometer'
>>> my_par.attr_quantity
Quantity(value=1.0, unit=nanometer)
>>> my_par.attr_quantity = 3.0
Traceback (most recent call last):
...
openforcefield.utils.utils.IncompatibleUnitError: attr_quantity=3.0 dimensionless should have␣
↪units of angstrom
```

You can attach a custom converter to an attribute.

```
>>> class MyParameter:
...     # Both strings and integers convert nicely to floats with float().
...     attr_all_to_float = ParameterAttribute(converter=float)
...     attr_int_to_float = ParameterAttribute()
...     @attr_int_to_float.converter
...     def attr_int_to_float(self, attr, value):
```

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```
...         # This converter converts only integers to float
...         # and raise an exception for the other types.
...         if isinstance(value, int):
...             return float(value)
...         elif not isinstance(value, float):
...             raise TypeError(f"Cannot convert '{value}' to float")
...         return value
...
>>> my_par = MyParameter()
```

attr_all_to_float accepts and convert to float both strings and integers

```
>>> my_par.attr_all_to_float = 1
>>> my_par.attr_all_to_float
1.0
>>> my_par.attr_all_to_float = '2.0'
>>> my_par.attr_all_to_float
2.0
```

The custom converter associated to attr_int_to_float converts only integers instead. >>> my_par.attr_int_to_float = 3 >>> my_par.attr_int_to_float 3.0 >>> my_par.attr_int_to_float = '4.0' Traceback (most recent call last): ... TypeError: Cannot convert '4.0' to float

Attributes

name

Methods

UNDEFINED	Custom type used by ParameterAttribute to differentiate between None and undeclared default.
converter(self, converter)	Create a new ParameterAttribute with an associated converter.

__init__(*self*, *default=<class 'openforcefield.typing.engines.smirnoff.parameters.ParameterAttribute.UNDEFINED'>*, *unit=None*, *converter=None*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(self[, default, unit, converter])	Initialize self.
converter(self, converter)	Create a new ParameterAttribute with an associated converter.

Attributes

name

class UNDEFINED
Custom type used by ParameterAttribute to differentiate between None and undeclared default.

converter(*self*, *converter*)
Create a new ParameterAttribute with an associated converter.

This is meant to be used as a decorator (see main examples).

openforcefield.typing.engines.smirnoff.parameters.IndexedParameterAttribute

class openforcefield.typing.engines.smirnoff.parameters.**IndexedParameterAttribute**(*default=<class 'openforcefield.typing.engines.smirnoff.pa unit=None, converter=None*)

The attribute of a parameter with an unspecified number of terms.

Some parameters can be associated to multiple terms, For example, torsions have parameters such as k1, k2, ..., and `IndexedParameterAttribute` can be used to encapsulate the sequence of terms.

The only substantial difference with `ParameterAttribute` is that only sequences are supported as values and converters and units are checked on each element of the sequence.

Currently, the descriptor makes the sequence immutable. This is to avoid that an element of the sequence could be set without being properly validated. In the future, the data could be wrapped in a safe list that would safely allow mutability.

Parameters

default [object, optional] When specified, the descriptor makes this attribute optional by attaching a default value to it.

unit [simtk.unit.Quantity, optional] When specified, only sequences of quantities with compatible units are allowed to be set.

converter [callable, optional] An optional function that can be used to validate and cast each element of the sequence before setting the attribute.

See also:

`ParameterAttribute` A simple parameter attribute.

Examples

Create an optional indexed attribute with unit of angstrom.

```
>>> from simtk import unit
>>> class MyParameter:
...     length = IndexedParameterAttribute(default=None, unit=unit.angstrom)
...
>>> my_par = MyParameter()
>>> my_par.length is None
True
```

Strings are parsed into Quantity objects.

```
>>> my_par.length = ['1 * angstrom', 0.5 * unit.nanometer]
>>> my_par.length[0]
Quantity(value=1, unit=angstrom)
```

Similarly, custom converters work as with `ParameterAttribute`, but they are used to validate each value in the sequence.

```
>>> class MyParameter:
...     attr_indexed = IndexedParameterAttribute(converter=float)
...
>>> my_par = MyParameter()
>>> my_par.attr_indexed = [1, '1.0', '1e-2', 4.0]
>>> my_par.attr_indexed
[1.0, 1.0, 0.01, 4.0]
```

Attributes

name

Methods

`UNDEFINED`	Custom type used by `ParameterAttribute` to differentiate between `None` and undeclared default.
`converter`(self, converter)	Create a new ParameterAttribute with an associated converter.

__init__(*self*, *default=<class 'openforcefield.typing.engines.smirnoff.parameters.ParameterAttribute.UNDEFINED'>*, *unit=None*, *converter=None*)
Initialize self. See help(type(self)) for accurate signature.

Methods

`__init__`(self[, default, unit, converter])	Initialize self.
`converter`(self, converter)	Create a new ParameterAttribute with an associated converter.

Attributes

`name`

class UNDEFINED
Custom type used by `ParameterAttribute` to differentiate between `None` and undeclared default.

converter(*self*, *converter*)
Create a new ParameterAttribute with an associated converter.

This is meant to be used as a decorator (see main examples).

2.3 Utilities

2.3.1 Toolkit wrappers

The toolkit wrappers provide a simple uniform API for accessing minimal functionality of cheminformatics toolkits.

These toolkit wrappers are generally used through a `ToolkitRegistry`, which can be constructed with a desired precedence of toolkits:

```
from openforcefield.utils.toolkits import ToolkitRegistry
toolkit_registry = ToolkitRegistry()
toolkit_precedence = [OpenEyeToolkitWrapper, RDKitToolkitWrapper, AmberToolsToolkitWrapper]
[ toolkit_registry.register(toolkit) for toolkit in toolkit_precedence if toolkit.is_available() ]
```

Alternatively, the global toolkit registry (which will attempt to register any available toolkits) can be used:

```
from openforcefield.utils.toolkits import DEFAULT_TOOLKIT_REGISTRY as toolkit_registry
```

The toolkit wrappers can then be accessed through the registry:

```
molecule = Molecule.from_smiles('Cc1ccccc1')
smiles = toolkit_registry.call('to_smiles', molecule)
```

ToolkitRegistry	Registry for ToolkitWrapper objects
ToolkitWrapper	Toolkit wrapper base class.
OpenEyeToolkitWrapper	OpenEye toolkit wrapper
RDKitToolkitWrapper	RDKit toolkit wrapper
AmberToolsToolkitWrapper	AmberTools toolkit wrapper

openforcefield.utils.toolkits.ToolkitRegistry

class openforcefield.utils.toolkits.**ToolkitRegistry**(*register_imported_toolkit_wrappers=False*, *toolkit_precedence=None*, *exception_if_unavailable=True*)

Registry for ToolkitWrapper objects

Examples

Register toolkits in a specified order, skipping if unavailable

```
>>> from openforcefield.utils.toolkits import ToolkitRegistry
>>> toolkit_registry = ToolkitRegistry()
>>> toolkit_precedence = [OpenEyeToolkitWrapper, RDKitToolkitWrapper, AmberToolsToolkitWrapper]
>>> for toolkit in toolkit_precedence:
...     if toolkit.is_available():
...         toolkit_registry.register_toolkit(toolkit)
```

Register specified toolkits, raising an exception if one is unavailable

```
>>> toolkit_registry = ToolkitRegistry()
>>> toolkits = [OpenEyeToolkitWrapper, AmberToolsToolkitWrapper]
```

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```
>>> for toolkit in toolkits:
...     toolkit_registry.register_toolkit(toolkit)
```

Register all available toolkits in arbitrary order

```
>>> from openforcefield.utils import all_subclasses
>>> toolkits = all_subclasses(ToolkitWrapper)
>>> for toolkit in toolkit_precedence:
...     if toolkit.is_available():
...         toolkit_registry.register_toolkit(toolkit)
```

Retrieve the global singleton toolkit registry, which is created when this module is imported from all available toolkits:

```
>>> from openforcefield.utils.toolkits import GLOBAL_TOOLKIT_REGISTRY as toolkit_registry
>>> available_toolkits = toolkit_registry.registered_toolkits
```

Warning: This API is experimental and subject to change.

Attributes

registered_toolkits List registered toolkits.

Methods

add_toolkit(self, toolkit_wrapper)	Append a ToolkitWrapper onto the list of toolkits in this ToolkitRegistry
call(self, method_name, *args, **kwargs)	Execute the requested method by attempting to use all registered toolkits in order of precedence.
register_toolkit(self, toolkit_wrapper[, ...])	Register the provided toolkit wrapper class, instantiating an object of it.
resolve(self, method_name)	Resolve the requested method name by checking all registered toolkits in order of precedence for one that provides the requested method.

__init__(*self*, *register_imported_toolkit_wrappers=False*, *toolkit_precedence=None*, *exception_if_unavailable=True*)
Create an empty toolkit registry.

Parameters

register_imported_toolkit_wrappers [bool, optional, default=False]

If True, will attempt to register all imported ToolkitWrapper subclasses that can be found, in no p
order.

toolkit_precedence [list, optional, default=None] List of toolkit wrapper classes, in order of desired precedence when performing molecule operations. If None, defaults to [OpenEyeToolkitWrapper, RDKitToolkitWrapper, AmberToolsToolkitWrapper].

exception_if_unavailable [bool, optional, default=True] If True, an exception will be raised if the toolkit is unavailable

Methods

`__init__`(self[, ...])	Create an empty toolkit registry.
`add_toolkit`(self, toolkit_wrapper)	Append a ToolkitWrapper onto the list of toolkits in this ToolkitRegistry
`call`(self, method_name, *args, **kwargs)	Execute the requested method by attempting to use all registered toolkits in order of precedence.
`register_toolkit`(self, toolkit_wrapper[, ...])	Register the provided toolkit wrapper class, instantiating an object of it.
`resolve`(self, method_name)	Resolve the requested method name by checking all registered toolkits in order of precedence for one that provides the requested method.

Attributes

`registered_toolkits`	List registered toolkits.

property registered_toolkits
List registered toolkits.

> **Warning:** This API is experimental and subject to change.

Returns

toolkits [iterable of toolkit objects]

register_toolkit(*self*, *toolkit_wrapper*, *exception_if_unavailable=True*)
Register the provided toolkit wrapper class, instantiating an object of it.

> **Warning:** This API is experimental and subject to change.

Parameters

toolkit_wrapper [instance or subclass of ToolkitWrapper] The toolkit wrapper to register or its class.

exception_if_unavailable [bool, optional, default=True] If True, an exception will be raised if the toolkit is unavailable

add_toolkit(*self*, *toolkit_wrapper*)
Append a ToolkitWrapper onto the list of toolkits in this ToolkitRegistry

> **Warning:** This API is experimental and subject to change.

Parameters

toolkit_wrapper [openforcefield.utils.ToolkitWrapper] The ToolkitWrapper object to add to the list of registered toolkits

resolve(*self*, *method_name*)

Resolve the requested method name by checking all registered toolkits in order of precedence for one that provides the requested method.

Parameters

method_name [str] The name of the method to resolve

Returns

method The method of the first registered toolkit that provides the requested method name

Raises

NotImplementedError if the requested method cannot be found among the registered toolkits

Examples

Create a molecule, and call the toolkit `to_smiles()` method directly

```
>>> from openforcefield.topology import Molecule
>>> molecule = Molecule.from_smiles('Cc1ccccc1')
>>> toolkit_registry = ToolkitRegistry(register_imported_toolkit_wrappers=True)
>>> method = toolkit_registry.resolve('to_smiles')
>>> smiles = method(molecule)
```

call(*self*, *method_name*, **args*, ***kwargs*)

Execute the requested method by attempting to use all registered toolkits in order of precedence.

`*args` and `**kwargs` are passed to the desired method, and return values of the method are returned

This is a convenient shorthand for `toolkit_registry.resolve_method(method_name)(*args, **kwargs)`

Parameters

method_name [str] The name of the method to execute

Raises

NotImplementedError if the requested method cannot be found among the registered toolkits

Examples

Create a molecule, and call the toolkit `to_smiles()` method directly

```
>>> from openforcefield.topology import Molecule
>>> molecule = Molecule.from_smiles('Cc1ccccc1')
>>> toolkit_registry = ToolkitRegistry(register_imported_toolkit_wrappers=True)
>>> smiles = toolkit_registry.call('to_smiles', molecule)
```

openforcefield.utils.toolkits.ToolkitWrapper

class openforcefield.utils.toolkits.**ToolkitWrapper**

Toolkit wrapper base class.

> **Warning:** This API is experimental and subject to change.

Attributes

toolkit_file_read_formats List of file formats that this toolkit can read.

toolkit_file_write_formats List of file formats that this toolkit can write.

toolkit_installation_instructions classmethod(function) -> method

toolkit_name The name of the toolkit wrapped by this class.

Methods

from_file(self, file_path, file_format[, ...])	Return an openforcefield.topology.Molecule from a file using this toolkit.
from_file_obj(self, file_obj, file_format[, ...])	Return an openforcefield.topology.Molecule from a file-like object (an object with a ".read()" method using this
is_available()	Check whether the corresponding toolkit can be imported
requires_toolkit()	

__init__(*self*, */*, **args*, ***kwargs*)

Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(self, /, *args, **kwargs)	Initialize self.
from_file(self, file_path, file_format[, ...])	Return an openforcefield.topology.Molecule from a file using this toolkit.
from_file_obj(self, file_obj, file_format[, ...])	Return an openforcefield.topology.Molecule from a file-like object (an object with a ".read()" method using this
is_available()	Check whether the corresponding toolkit can be imported
requires_toolkit()	

Attributes

toolkit_file_read_formats	List of file formats that this toolkit can read.
toolkit_file_write_formats	List of file formats that this toolkit can write.
toolkit_installation_instructions	classmethod(function) -> method
toolkit_name	The name of the toolkit wrapped by this class.

property toolkit_name
The name of the toolkit wrapped by this class.

property toolkit_installation_instructions
classmethod(function) -> method

Convert a function to be a class method.

A class method receives the class as implicit first argument, just like an instance method receives the instance. To declare a class method, use this idiom:

class C: @classmethod def f(cls, arg1, arg2, ...):

...

It can be called either on the class (e.g. C.f()) or on an instance (e.g. C().f()). The instance is ignored except for its class. If a class method is called for a derived class, the derived class object is passed as the implied first argument.

Class methods are different than C++ or Java static methods. If you want those, see the staticmethod builtin.

property toolkit_file_read_formats
List of file formats that this toolkit can read.

property toolkit_file_write_formats
List of file formats that this toolkit can write.

static is_available()
Check whether the corresponding toolkit can be imported

Returns

is_installed [bool] True if corresponding toolkit is installed, False otherwise.

from_file(*self*, *file_path*, *file_format*, *allow_undefined_stereo=False*)
Return an openforcefield.topology.Molecule from a file using this toolkit.

Parameters

file_path [str] The file to read the molecule from

file_format [str] Format specifier, usually file suffix (eg. 'MOL2', 'SMI') Note that not all toolkits support all formats. Check ToolkitWrapper.toolkit_file_read_formats for details.

allow_undefined_stereo [bool, default=False] If false, raises an exception if any molecules contain undefined stereochemistry.

Returns

——-

molecules [Molecule or list of Molecules] a list of Molecule objects is returned.

from_file_obj(*self*, *file_obj*, *file_format*, *allow_undefined_stereo=False*)

Return an openforcefield.topology.Molecule from a file-like object (an object with a ".read()" method using
toolkit.

Parameters

file_obj [file-like object] The file-like object to read the molecule from

file_format [str] Format specifier, usually file suffix (eg. 'MOL2', 'SMI') Note that not all toolkits support all formats. Check ToolkitWrapper.toolkit_file_read_formats for details.

allow_undefined_stereo [bool, default=False] If false, raises an exception if any molecules contain undefined stereochemistry. If false, the function skips loading the molecule.

Returns

molecules [Molecule or list of Molecules] a list of Molecule objects is returned.

openforcefield.utils.toolkits.OpenEyeToolkitWrapper

class openforcefield.utils.toolkits.**OpenEyeToolkitWrapper**

OpenEye toolkit wrapper

> **Warning:** This API is experimental and subject to change.

Attributes

toolkit_file_read_formats List of file formats that this toolkit can read.

toolkit_file_write_formats List of file formats that this toolkit can write.

toolkit_installation_instructions classmethod(function) -> method

toolkit_name The name of the toolkit wrapped by this class.

Methods

compute_partial_charges(self, molecule[, ...])	Compute partial charges with OpenEye quacpac
compute_partial_charges_am1bcc(self, molecule)	Compute AM1BCC partial charges with OpenEye quacpac
compute_wiberg_bond_orders(self, molecule[, ...])	Update and store list of bond orders this molecule.
find_smarts_matches(self, molecule, smarts)	Find all SMARTS matches for the specified molecule, using the specified aromaticity model.
from_file(self, file_path, file_format[, ...])	Return an openforcefield.topology.Molecule from a file using this toolkit.
from_file_obj(self, file_obj, file_format[, ...])	Return an openforcefield.topology.Molecule from a file-like object (an object with a ".read()" method using this toolkit.
from_object(self, object[, ...])	If given an OEMol (or OEMol-derived object), this function will load it into an openforcefield.topology.molecule Otherwise, it will return False.
from_openeye(oemol[, allow_undefined_stereo])	Create a Molecule from an OpenEye molecule.
from_smiles(self, smiles[, ...])	Create a Molecule from a SMILES string using the OpenEye toolkit.

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generate_conformers(self, molecule[, ...])	Generate molecule conformers using OpenEye Omega.
is_available([oetools])	Check if the given OpenEye toolkit components are available.
requires_toolkit()	
to_file(self, molecule, file_path, file_format)	Writes an OpenFF Molecule to a file-like object
to_file_obj(self, molecule, file_obj, ...)	Writes an OpenFF Molecule to a file-like object
to_openeye(molecule[, aromaticity_model])	Create an OpenEye molecule using the specified aromaticity model
to_smiles(molecule)	Uses the OpenEye toolkit to convert a Molecule into a SMILES string.

__init__(*self*, */*, **args*, ***kwargs*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(self, /, *args, **kwargs)	Initialize self.
compute_partial_charges(self, molecule[, ...])	Compute partial charges with OpenEye quacpac
compute_partial_charges_am1bcc(self, molecule)	Compute AM1BCC partial charges with OpenEye quacpac
compute_wiberg_bond_orders(self, molecule[, ...])	Update and store list of bond orders this molecule.
find_smarts_matches(self, molecule, smarts)	Find all SMARTS matches for the specified molecule, using the specified aromaticity model.
from_file(self, file_path, file_format[, ...])	Return an openforcefield.topology.Molecule from a file using this toolkit.
from_file_obj(self, file_obj, file_format[, ...])	Return an openforcefield.topology.Molecule from a file-like object (an object with a ".read()" method using this toolkit.
from_object(self, object[, ...])	If given an OEMol (or OEMol-derived object), this function will load it into an openforcefield.topology.molecule Otherwise, it will return False.
from_openeye(oemol[, allow_undefined_stereo])	Create a Molecule from an OpenEye molecule.
from_smiles(self, smiles[, ...])	Create a Molecule from a SMILES string using the OpenEye toolkit.
generate_conformers(self, molecule[, ...])	Generate molecule conformers using OpenEye Omega.
is_available([oetools])	Check if the given OpenEye toolkit components are available.
requires_toolkit()	
to_file(self, molecule, file_path, file_format)	Writes an OpenFF Molecule to a file-like object
to_file_obj(self, molecule, file_obj, ...)	Writes an OpenFF Molecule to a file-like object
to_openeye(molecule[, aromaticity_model])	Create an OpenEye molecule using the specified aromaticity model
to_smiles(molecule)	Uses the OpenEye toolkit to convert a Molecule into a SMILES string.

Attributes

toolkit_file_read_formats	List of file formats that this toolkit can read.
toolkit_file_write_formats	List of file formats that this toolkit can write.
toolkit_installation_instructions	classmethod(function) -> method
toolkit_name	The name of the toolkit wrapped by this class.

static is_available(*oetools=('oechem', 'oequacpac', 'oeiupac', 'oeomega')*)
Check if the given OpenEye toolkit components are available.

If the OpenEye toolkit is not installed or no license is found for at least one the given toolkits , `False` is returned.

Parameters

oetools [str or iterable of strings, optional, default=('oechem', 'oequacpac', 'oeiupac', 'oeomega')] Set of tools to check by their Python module name. Defaults to the complete set of tools supported by this function. Also accepts a single tool to check as a string instead of an iterable of length 1.

Returns

all_installed [bool] `True` if all tools in `oetools` are installed and licensed, `False` otherwise

from_object(*self*, *object*, *allow_undefined_stereo=False*)
If given an OEMol (or OEMol-derived object), this function will load it into an openforcefield.topology.molecule Otherwise, it will return False.

Parameters

object [A molecule-like object] An object to by type-checked.

allow_undefined_stereo [bool, default=False] Whether to accept molecules with undefined stereocenters. If False, an exception will be raised if a molecule with undefined stereochemistry is passed into this function.

Returns

Molecule An openforcefield.topology.molecule Molecule.

Raises

NotImplementedError If the object could not be converted into a Molecule.

from_file(*self*, *file_path*, *file_format*, *allow_undefined_stereo=False*)
Return an openforcefield.topology.Molecule from a file using this toolkit.

Parameters

file_path [str] The file to read the molecule from

file_format [str] Format specifier, usually file suffix (eg. 'MOL2', 'SMI') Note that not all toolkits support all formats. Check ToolkitWrapper.toolkit_file_read_formats for details.

allow_undefined_stereo [bool, default=False] If false, raises an exception if oemol contains undefined stereochemistry.

Returns

molecules [List[Molecule]] The list of `Molecule` objects in the file.

Raises

GAFFAtomTypeWarning If the loaded mol2 file possibly uses GAFF atom types, which are not supported.

Examples

Load a mol2 file into an OpenFF `Molecule` object.

```
>>> from openforcefield.utils import get_data_file_path
>>> mol2_file_path = get_data_file_path('molecules/cyclohexane.mol2')
>>> toolkit = OpenEyeToolkitWrapper()
>>> molecule = toolkit.from_file(mol2_file_path, file_format='mol2')
```

from_file_obj(*self*, *file_obj*, *file_format*, *allow_undefined_stereo=False*)
Return an openforcefield.topology.Molecule from a file-like object (an object with a ".read()" method using this toolkit.

Parameters

file_obj [file-like object] The file-like object to read the molecule from

file_format [str] Format specifier, usually file suffix (eg. 'MOL2', 'SMI') Note that not all toolkits support all formats. Check ToolkitWrapper.toolkit_file_read_formats for details.

allow_undefined_stereo [bool, default=False] If false, raises an exception if oemol contains undefined stereochemistry.

Returns

molecules [List[Molecule]] The list of Molecule objects in the file object.

Raises

GAFFAtomTypeWarning If the loaded mol2 file possibly uses GAFF atom types, which are not supported.

to_file_obj(*self*, *molecule*, *file_obj*, *file_format*)
Writes an OpenFF Molecule to a file-like object

Parameters

molecule [an OpenFF Molecule] The molecule to write

file_obj The file-like object to write to

file_format The format for writing the molecule data

to_file(*self*, *molecule*, *file_path*, *file_format*)
Writes an OpenFF Molecule to a file-like object

Parameters

molecule [an OpenFF Molecule] The molecule to write

file_path The file path to write to.

file_format The format for writing the molecule data

static from_openeye(*oemol*, *allow_undefined_stereo=False*)
Create a Molecule from an OpenEye molecule. If the OpenEye molecule has implicit hydrogens, this function will make them explicit.

Warning: This API is experimental and subject to change.

Parameters

oemol [openeye.oechem.OEMol] An OpenEye molecule

allow_undefined_stereo [bool, default=False] If false, raises an exception if oemol contains undefined stereochemistry.

Returns

molecule [openforcefield.topology.Molecule] An openforcefield molecule

Examples

Create a Molecule from an OpenEye OEMol

```
>>> from openeye import oechem
>>> from openforcefield.tests.utils import get_data_file_path
>>> ifs = oechem.oemolistream(get_data_file_path('systems/monomers/ethanol.mol2'))
>>> oemols = list(ifs.GetOEGraphMols())
```

```
>>> toolkit_wrapper = OpenEyeToolkitWrapper()
>>> molecule = toolkit_wrapper.from_openeye(oemols[0])
```

static to_openeye(*molecule*, *aromaticity_model='OEAroModel_MDL'*)

Create an OpenEye molecule using the specified aromaticity model

Warning: This API is experimental and subject to change.

Parameters

molecule [openforcefield.topology.molecule.Molecule object]

The molecule to convert to an OEMol

aromaticity_model [str, optional, default=DEFAULT_AROMATICITY_MODEL] The aromaticity model to use

Returns

oemol [openeye.oechem.OEMol] An OpenEye molecule

Examples

Create an OpenEye molecule from a Molecule

```
>>> from openforcefield.topology import Molecule
>>> toolkit_wrapper = OpenEyeToolkitWrapper()
>>> molecule = Molecule.from_smiles('CC')
>>> oemol = toolkit_wrapper.to_openeye(molecule)
```

static to_smiles(*molecule*)

Uses the OpenEye toolkit to convert a Molecule into a SMILES string.

Parameters

molecule [An openforcefield.topology.Molecule] The molecule to convert into a SMILES.

Returns

smiles [str] The SMILES of the input molecule.

from_smiles(*self*, *smiles*, *hydrogens_are_explicit=False*, *allow_undefined_stereo=False*)
Create a Molecule from a SMILES string using the OpenEye toolkit.

> **Warning:** This API is experimental and subject to change.

Parameters

smiles [str] The SMILES string to turn into a molecule

hydrogens_are_explicit [bool, default = False] If False, OE will perform hydrogen addition using OEAddExplicitHydrogens

allow_undefined_stereo [bool, default=False] Whether to accept SMILES with undefined stereochemistry. If False, an exception will be raised if a SMILES with undefined stereochemistry is passed into this function.

Returns

molecule [openforcefield.topology.Molecule] An openforcefield-style molecule.

generate_conformers(*self*, *molecule*, *n_conformers=1*, *clear_existing=True*)
Generate molecule conformers using OpenEye Omega.

> **Warning:** This API is experimental and subject to change.

molecule [a `Molecule`] The molecule to generate conformers for.

n_conformers [int, default=1] The maximum number of conformers to generate.

clear_existing [bool, default=True] Whether to overwrite existing conformers for the molecule

compute_partial_charges(*self*, *molecule*, *quantum_chemical_method='AM1-BCC'*, *partial_charge_method='None'*)
Compute partial charges with OpenEye quacpac

> **Warning:** This API is experimental and subject to change.

Parameters

molecule [Molecule] Molecule for which partial charges are to be computed

charge_model [str, optional, default=None] The charge model to use. One of ['noop', 'mmff', 'mmff94', 'am1bcc', 'am1bccnosymspt', 'amber', 'amberff94', 'am1bccelf10'] If None, 'am1bcc' will be used.

Returns

charges [numpy.array of shape (natoms) of type float] The partial charges

compute_partial_charges_am1bcc(*self*, *molecule*)
Compute AM1BCC partial charges with OpenEye quacpac

> **Warning:** This API is experimental and subject to change.

Parameters

molecule [Molecule] Molecule for which partial charges are to be computed

Returns

charges [numpy.array of shape (natoms) of type float] The partial charges

compute_wiberg_bond_orders(*self*, *molecule*, *charge_model=None*)
Update and store list of bond orders this molecule. Can be used for initialization of bondorders list, or for updating bond orders in the list.

> **Warning:** This API is experimental and subject to change.

Parameters

molecule [openforcefield.topology.molecule Molecule] The molecule to assign wiberg bond orders to

charge_model [str, optional, default=None] The charge model to use. One of ['am1', 'pm3']. If None, 'am1' will be used.

find_smarts_matches(*self*, *molecule*, *smarts*, *aromaticity_model='OEAroModel_MDL'*)
Find all SMARTS matches for the specified molecule, using the specified aromaticity model.

> **Warning:** This API is experimental and subject to change.

Parameters

molecule [openforcefield.topology.Molecule] The molecule for which all specified SMARTS matches are to be located

smarts [str] SMARTS string with optional SMIRKS-style atom tagging

aromaticity_model [str, optional, default='OEAroModel_MDL'] Aromaticity model to use during matching

.. note :: Currently, the only supported "aromaticity_model" is "OEAroModel_MDL"

property toolkit_file_read_formats
List of file formats that this toolkit can read.

property toolkit_file_write_formats
List of file formats that this toolkit can write.

property toolkit_installation_instructions
classmethod(function) -> method

Convert a function to be a class method.

A class method receives the class as implicit first argument, just like an instance method receives the instance. To declare a class method, use this idiom:

class C: @classmethod def f(cls, arg1, arg2, . . .):

. . .

It can be called either on the class (e.g. C.f()) or on an instance (e.g. C().f()). The instance is ignored except for its class. If a class method is called for a derived class, the derived class object is passed as the implied first argument.

Class methods are different than C++ or Java static methods. If you want those, see the staticmethod builtin.

property toolkit_name
The name of the toolkit wrapped by this class.

openforcefield.utils.toolkits.RDKitToolkitWrapper

class openforcefield.utils.toolkits.**RDKitToolkitWrapper**
RDKit toolkit wrapper

> **Warning:** This API is experimental and subject to change.

Attributes

toolkit_file_read_formats	List of file formats that this toolkit can read.
toolkit_file_write_formats	List of file formats that this toolkit can write.
toolkit_installation_instructions	classmethod(function) -> method
toolkit_name	The name of the toolkit wrapped by this class.

Methods

find_smarts_matches(self, molecule, smarts)	Find all SMARTS matches for the specified molecule, using the specified aromaticity model.
from_file(self, file_path, file_format[, . . .])	Create an openforcefield.topology.Molecule from a file using this toolkit.
from_file_obj(self, file_obj, file_format[, . . .])	Return an openforcefield.topology.Molecule from a file-like object (an object with a ".read()" method using this toolkit.
from_object(self, object[, . . .])	If given an rdchem.Mol (or rdchem.Mol-derived object), this function will load it into an openforcefield.topology.molecule.
from_rdkit(self, rdmol[, allow_undefined_stereo])	Create a Molecule from an RDKit molecule.
from_smiles(self, smiles[, . . .])	Create a Molecule from a SMILES string using the RDKit toolkit.
generate_conformers(self, molecule[, . . .])	Generate molecule conformers using RDKit.
is_available()	Check whether the RDKit toolkit can be imported

Continued on next page

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requires_toolkit()	
to_file(self, molecule, file_path, file_format)	Writes an OpenFF Molecule to a file-like object
to_file_obj(self, molecule, file_obj, ...)	Writes an OpenFF Molecule to a file-like object
to_rdkit(molecule[, aromaticity_model])	Create an RDKit molecule
to_smiles(molecule)	Uses the RDKit toolkit to convert a Molecule into a SMILES string.

__init__(*self*, */*, **args*, ***kwargs*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(self, /, *args, **kwargs)	Initialize self.
find_smarts_matches(self, molecule, smarts)	Find all SMARTS matches for the specified molecule, using the specified aromaticity model.
from_file(self, file_path, file_format[, ...])	Create an openforcefield.topology.Molecule from a file using this toolkit.
from_file_obj(self, file_obj, file_format[, ...])	Return an openforcefield.topology.Molecule from a file-like object (an object with a ".read()" method using this toolkit.
from_object(self, object[, ...])	If given an rdchem.Mol (or rdchem.Mol-derived object), this function will load it into an openforcefield.topology.molecule.
from_rdkit(self, rdmol[, allow_undefined_stereo])	Create a Molecule from an RDKit molecule.
from_smiles(self, smiles[, ...])	Create a Molecule from a SMILES string using the RDKit toolkit.
generate_conformers(self, molecule[, ...])	Generate molecule conformers using RDKit.
is_available()	Check whether the RDKit toolkit can be imported
requires_toolkit()	
to_file(self, molecule, file_path, file_format)	Writes an OpenFF Molecule to a file-like object
to_file_obj(self, molecule, file_obj, ...)	Writes an OpenFF Molecule to a file-like object
to_rdkit(molecule[, aromaticity_model])	Create an RDKit molecule
to_smiles(molecule)	Uses the RDKit toolkit to convert a Molecule into a SMILES string.

Attributes

toolkit_file_read_formats	List of file formats that this toolkit can read.
toolkit_file_write_formats	List of file formats that this toolkit can write.
toolkit_installation_instructions	classmethod(function) -> method
toolkit_name	The name of the toolkit wrapped by this class.

static is_available()
Check whether the RDKit toolkit can be imported

Returns

is_installed [bool] True if RDKit is installed, False otherwise.

from_object(*self*, *object*, *allow_undefined_stereo=False*)
If given an rdchem.Mol (or rdchem.Mol-derived object), this function will load it into an openforcefield.topology.molecule. Otherwise, it will return False.

Parameters

object [A rdchem.Mol-derived object] An object to be type-checked and converted into a Molecule, if possible.

allow_undefined_stereo [bool, default=False] Whether to accept molecules with undefined stereocenters. If False, an exception will be raised if a molecule with undefined stereochemistry is passed into this function.

Returns

Molecule or False An openforcefield.topology.molecule Molecule.

Raises

NotImplementedError If the object could not be converted into a Molecule.

from_file(*self*, *file_path*, *file_format*, *allow_undefined_stereo=False*)
Create an openforcefield.topology.Molecule from a file using this toolkit.

Parameters

file_path [str] The file to read the molecule from

file_format [str] Format specifier, usually file suffix (eg. 'MOL2', 'SMI') Note that not all toolkits support all formats. Check ToolkitWrapper.toolkit_file_read_formats for details.

allow_undefined_stereo [bool, default=False] If false, raises an exception if oemol contains undefined stereochemistry.

Returns

molecules [iterable of Molecules] a list of Molecule objects is returned.

from_file_obj(*self*, *file_obj*, *file_format*, *allow_undefined_stereo=False*)
Return an openforcefield.topology.Molecule from a file-like object (an object with a ".read()" method using this toolkit.

> **Warning:** This API is experimental and subject to change.

Parameters

file_obj [file-like object] The file-like object to read the molecule from

file_format [str] Format specifier, usually file suffix (eg. 'MOL2', 'SMI') Note that not all toolkits support all formats. Check ToolkitWrapper.toolkit_file_read_formats for details.

allow_undefined_stereo [bool, default=False] If false, raises an exception if oemol contains undefined stereochemistry.

Returns

molecules [Molecule or list of Molecules] a list of Molecule objects is returned.

to_file_obj(*self*, *molecule*, *file_obj*, *file_format*)
Writes an OpenFF Molecule to a file-like object

Parameters

molecule [an OpenFF Molecule] The molecule to write

file_obj The file-like object to write to

file_format The format for writing the molecule data

`to_file`(*self*, *molecule*, *file_path*, *file_format*)
Writes an OpenFF Molecule to a file-like object

Parameters

molecule [an OpenFF Molecule] The molecule to write

file_path The file path to write to

file_format The format for writing the molecule data

Returns

——

`classmethod to_smiles`(*molecule*)
Uses the RDKit toolkit to convert a Molecule into a SMILES string.

Parameters

molecule [An openforcefield.topology.Molecule] The molecule to convert into a SMILES.

Returns

smiles [str] The SMILES of the input molecule.

`from_smiles`(*self*, *smiles*, *hydrogens_are_explicit=False*, *allow_undefined_stereo=False*)
Create a Molecule from a SMILES string using the RDKit toolkit.

> **Warning:** This API is experimental and subject to change.

Parameters

smiles [str] The SMILES string to turn into a molecule

hydrogens_are_explicit [bool, default=False] If False, RDKit will perform hydrogen addition using Chem.AddHs

allow_undefined_stereo [bool, default=False] Whether to accept SMILES with undefined stereochemistry. If False, an exception will be raised if a SMILES with undefined stereochemistry is passed into this function.

Returns

molecule [openforcefield.topology.Molecule] An openforcefield-style molecule.

`generate_conformers`(*self*, *molecule*, *n_conformers=1*, *clear_existing=True*)
Generate molecule conformers using RDKit.

> **Warning:** This API is experimental and subject to change.

molecule [a `Molecule`] The molecule to generate conformers for.

n_conformers [int, default=1] Maximum number of conformers to generate.

clear_existing [bool, default=True] Whether to overwrite existing conformers for the molecule.

from_rdkit(*self*, *rdmol*, *allow_undefined_stereo=False*)
Create a Molecule from an RDKit molecule.

Requires the RDKit to be installed.

> **Warning:** This API is experimental and subject to change.

Parameters

rdmol [rkit.RDMol] An RDKit molecule

allow_undefined_stereo [bool, default=False] If false, raises an exception if rdmol contains undefined stereochemistry.

Returns

molecule [openforcefield.Molecule] An openforcefield molecule

Examples

Create a molecule from an RDKit molecule

```
>>> from rdkit import Chem
>>> from openforcefield.tests.utils import get_data_file_path
>>> rdmol = Chem.MolFromMolFile(get_data_file_path('systems/monomers/ethanol.sdf'))
```

```
>>> toolkit_wrapper = RDKitToolkitWrapper()
>>> molecule = toolkit_wrapper.from_rdkit(rdmol)
```

classmethod to_rdkit(*molecule*, *aromaticity_model='OEAroModel_MDL'*)
Create an RDKit molecule

Requires the RDKit to be installed.

> **Warning:** This API is experimental and subject to change.

Parameters

aromaticity_model [str, optional, default=DEFAULT_AROMATICITY_MODEL] The aromaticity model to use

Returns

rdmol [rkit.RDMol] An RDKit molecule

Examples

Convert a molecule to RDKit

```
>>> from openforcefield.topology import Molecule
>>> ethanol = Molecule.from_smiles('CCO')
>>> rdmol = ethanol.to_rdkit()
```

find_smarts_matches(*self*, *molecule*, *smarts*, *aromaticity_model='OEAroModel_MDL'*)
Find all SMARTS matches for the specified molecule, using the specified aromaticity model.

> **Warning:** This API is experimental and subject to change.

Parameters

molecule [openforcefield.topology.Molecule] The molecule for which all specified SMARTS matches are to be located

smarts [str] SMARTS string with optional SMIRKS-style atom tagging

aromaticity_model [str, optional, default='OEAroModel_MDL'] Aromaticity model to use during matching

.. note :: Currently, the only supported "aromaticity_model" is "OEAroModel_MDL"

property toolkit_file_read_formats
List of file formats that this toolkit can read.

property toolkit_file_write_formats
List of file formats that this toolkit can write.

property toolkit_installation_instructions
classmethod(function) -> method

Convert a function to be a class method.

A class method receives the class as implicit first argument, just like an instance method receives the instance. To declare a class method, use this idiom:

class C: @classmethod def f(cls, arg1, arg2, ...):

...

It can be called either on the class (e.g. C.f()) or on an instance (e.g. C().f()). The instance is ignored except for its class. If a class method is called for a derived class, the derived class object is passed as the implied first argument.

Class methods are different than C++ or Java static methods. If you want those, see the staticmethod builtin.

property toolkit_name
The name of the toolkit wrapped by this class.

openforcefield.utils.toolkits.AmberToolsToolkitWrapper

class openforcefield.utils.toolkits.**AmberToolsToolkitWrapper**
AmberTools toolkit wrapper

> **Warning:** This API is experimental and subject to change.

Attributes

toolkit_file_read_formats List of file formats that this toolkit can read.

toolkit_file_write_formats List of file formats that this toolkit can write.

toolkit_installation_instructions classmethod(function) -> method

toolkit_name The name of the toolkit wrapped by this class.

Methods

compute_partial_charges(self, molecule[, ...])	Compute partial charges with AmberTools using antechamber/sqm
compute_partial_charges_am1bcc(self, molecule)	Compute partial charges with AmberTools using antechamber/sqm.
from_file(self, file_path, file_format[, ...])	Return an openforcefield.topology.Molecule from a file using this toolkit.
from_file_obj(self, file_obj, file_format[, ...])	Return an openforcefield.topology.Molecule from a file-like object (an object with a ".read()" method using this
is_available()	Check whether the AmberTools toolkit is installed
requires_toolkit()	

__init__(*self*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(self)	Initialize self.
compute_partial_charges(self, molecule[, ...])	Compute partial charges with AmberTools using antechamber/sqm
compute_partial_charges_am1bcc(self, molecule)	Compute partial charges with AmberTools using antechamber/sqm.
from_file(self, file_path, file_format[, ...])	Return an openforcefield.topology.Molecule from a file using this toolkit.
from_file_obj(self, file_obj, file_format[, ...])	Return an openforcefield.topology.Molecule from a file-like object (an object with a ".read()" method using this
is_available()	Check whether the AmberTools toolkit is installed
requires_toolkit()	

Attributes

toolkit_file_read_formats	List of file formats that this toolkit can read.
toolkit_file_write_formats	List of file formats that this toolkit can write.
toolkit_installation_instructions	classmethod(function) -> method
toolkit_name	The name of the toolkit wrapped by this class.

static is_available()
Check whether the AmberTools toolkit is installed

Returns

is_installed [bool] True if AmberTools is installed, False otherwise.

compute_partial_charges(*self*, *molecule*, *charge_model=None*)
Compute partial charges with AmberTools using antechamber/sqm

> **Warning:** This API experimental and subject to change.

Parameters

molecule [Molecule] Molecule for which partial charges are to be computed

charge_model [str, optional, default=None] The charge model to use. One of ['gas', 'mul', 'bcc']. If None, 'bcc' will be used.

Raises

ValueError if the requested charge method could not be handled

Notes

Currently only sdf file supported as input and mol2 as output https://github.com/choderalab/openmoltools/blob/master/openmoltools/packmol.py

compute_partial_charges_am1bcc(*self*, *molecule*)
Compute partial charges with AmberTools using antechamber/sqm. This will calculate AM1-BCC charges on the first conformer only.

> **Warning:** This API experimental and subject to change.

Parameters

molecule [Molecule] Molecule for which partial charges are to be computed

Raises

ValueError if the requested charge method could not be handled

from_file(*self*, *file_path*, *file_format*, *allow_undefined_stereo=False*)
Return an openforcefield.topology.Molecule from a file using this toolkit.

Parameters

file_path [str] The file to read the molecule from

file_format [str] Format specifier, usually file suffix (eg. 'MOL2', 'SMI') Note that not all toolkits support all formats. Check ToolkitWrapper.toolkit_file_read_formats for details.

allow_undefined_stereo [bool, default=False] If false, raises an exception if any molecules contain undefined stereochemistry.

Returns

———-

molecules [Molecule or list of Molecules] a list of Molecule objects is returned.

from_file_obj(*self*, *file_obj*, *file_format*, *allow_undefined_stereo=False*)

Return an openforcefield.topology.Molecule from a file-like object (an object with a ".read()" method using toolkit.

Parameters

file_obj [file-like object] The file-like object to read the molecule from

file_format [str] Format specifier, usually file suffix (eg. 'MOL2', 'SMI') Note that not all toolkits support all formats. Check ToolkitWrapper.toolkit_file_read_formats for details.

allow_undefined_stereo [bool, default=False] If false, raises an exception if any molecules contain undefined stereochemistry. If false, the function skips loading the molecule.

Returns

molecules [Molecule or list of Molecules] a list of Molecule objects is returned.

property toolkit_file_read_formats
List of file formats that this toolkit can read.

property toolkit_file_write_formats
List of file formats that this toolkit can write.

property toolkit_installation_instructions
classmethod(function) -> method

Convert a function to be a class method.

A class method receives the class as implicit first argument, just like an instance method receives the instance. To declare a class method, use this idiom:

class C: @classmethod def f(cls, arg1, arg2, ...):

...

It can be called either on the class (e.g. C.f()) or on an instance (e.g. C().f()). The instance is ignored except for its class. If a class method is called for a derived class, the derived class object is passed as the implied first argument.

Class methods are different than C++ or Java static methods. If you want those, see the staticmethod builtin.

property toolkit_name
The name of the toolkit wrapped by this class.

2.3.2 Serialization support

Serializable	Mix-in to add serialization and deserialization support via JSON, YAML, BSON, TOML, MessagePack, and XML.

openforcefield.utils.serialization.Serializable

class openforcefield.utils.serialization.**Serializable**

Mix-in to add serialization and deserialization support via JSON, YAML, BSON, TOML, MessagePack, and XML.

For more information on these formats, see: JSON, BSON, YAML, TOML, MessagePack, and XML.

To use this mix-in, the class inheriting from this class must have implemented `to_dict()` and `from_dict()` methods that utilize dictionaries containing only serialiable Python objects.

Warning: The serialization/deserialiation schemes used here place some strict constraints on what kinds of `dict` objects can be serialized. No effort is made to add further protection to ensure serialization is possible. Use with caution.

Examples

Example class using `Serializable` mix-in:

```
>>> from openforcefield.utils.serialization import Serializable
>>> class Thing(Serializable):
...     def __init__(self, description):
...         self.description = description
...
...     def to_dict(self):
...         return { 'description' : self.description }
...
...     @classmethod
...     def from_dict(cls, d):
...         return cls(d['description'])
...
>>> # Create an example object
>>> thing = Thing('blorb')
```

Get JSON representation:

```
>>> json_thing = thing.to_json()
```

Reconstruct an object from its JSON representation:

```
>>> thing_from_json = Thing.from_json(json_thing)
```

Get BSON representation:

```
>>> bson_thing = thing.to_bson()
```

Reconstruct an object from its BSON representation:

```
>>> thing_from_bson = Thing.from_bson(bson_thing)
```

Get YAML representation:

```
>>> yaml_thing = thing.to_yaml()
```

Reconstruct an object from its YAML representation:

```
>>> thing_from_yaml = Thing.from_yaml(yaml_thing)
```

Get MessagePack representation:

```
>>> messagepack_thing = thing.to_messagepack()
```

Reconstruct an object from its MessagePack representation:

```
>>> thing_from_messagepack = Thing.from_messagepack(messagepack_thing)
```

Get XML representation:

```
>>> xml_thing = thing.to_xml()
```

Methods

from_bson(serialized)	Instantiate an object from a BSON serialized representation.
from_json(serialized)	Instantiate an object from a JSON serialized representation.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.
from_pickle(serialized)	Instantiate an object from a pickle serialized representation.
from_toml(serialized)	Instantiate an object from a TOML serialized representation.
from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
to_bson(self)	Return a BSON serialized representation.
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_pickle(self)	Return a pickle serialized representation.
to_toml(self)	Return a TOML serialized representation.
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.

from_dict	
to_dict	

__init__(*self*, */*, **args*, ***kwargs*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(self, /, *args, **kwargs)	Initialize self.

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from_bson(serialized)	Instantiate an object from a BSON serialized representation.
from_dict(d)	
from_json(serialized)	Instantiate an object from a JSON serialized representation.
from_messagepack(serialized)	Instantiate an object from a MessagePack serialized representation.
from_pickle(serialized)	Instantiate an object from a pickle serialized representation.
from_toml(serialized)	Instantiate an object from a TOML serialized representation.
from_xml(serialized)	Instantiate an object from an XML serialized representation.
from_yaml(serialized)	Instantiate from a YAML serialized representation.
to_bson(self)	Return a BSON serialized representation.
to_dict(self)	
to_json(self[, indent])	Return a JSON serialized representation.
to_messagepack(self)	Return a MessagePack representation.
to_pickle(self)	Return a pickle serialized representation.
to_toml(self)	Return a TOML serialized representation.
to_xml(self[, indent])	Return an XML representation.
to_yaml(self)	Return a YAML serialized representation.

to_json(*self*, *indent=None*)
Return a JSON serialized representation.

Specification: https://www.json.org/

Parameters

indent [int, optional, default=None] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [str] A JSON serialized representation of the object

classmethod from_json(*serialized*)
Instantiate an object from a JSON serialized representation.

Specification: https://www.json.org/

Parameters

serialized [str] A JSON serialized representation of the object

Returns

instance [cls] An instantiated object

to_bson(*self*)
Return a BSON serialized representation.

Specification: http://bsonspec.org/

Returns

serialized [bytes] A BSON serialized representation of the objecft

classmethod from_bson(*serialized*)
Instantiate an object from a BSON serialized representation.

Specification: http://bsonspec.org/

Parameters

serialized [bytes] A BSON serialized representation of the object

Returns

instance [cls] An instantiated object

to_toml(*self*)
Return a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Returns

serialized [str] A TOML serialized representation of the object

classmethod from_toml(*serialized*)
Instantiate an object from a TOML serialized representation.

Specification: https://github.com/toml-lang/toml

Parameters

serlialized [str] A TOML serialized representation of the object

Returns

instance [cls] An instantiated object

to_yaml(*self*)
Return a YAML serialized representation.

Specification: http://yaml.org/

Returns

serialized [str] A YAML serialized representation of the object

classmethod from_yaml(*serialized*)
Instantiate from a YAML serialized representation.

Specification: http://yaml.org/

Parameters

serialized [str] A YAML serialized representation of the object

Returns

instance [cls] Instantiated object

to_messagepack(*self*)
Return a MessagePack representation.

Specification: https://msgpack.org/index.html

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation of the object

classmethod from_messagepack(*serialized*)
Instantiate an object from a MessagePack serialized representation.

Specification: https://msgpack.org/index.html

Parameters

serialized [bytes] A MessagePack-encoded bytes serialized representation

Returns

instance [cls] Instantiated object.

to_xml(*self*, *indent=2*)
Return an XML representation.

Specification: https://www.w3.org/XML/

Parameters

indent [int, optional, default=2] If not None, will pretty-print with specified number of spaces for indentation

Returns

serialized [bytes] A MessagePack-encoded bytes serialized representation.

classmethod from_xml(*serialized*)
Instantiate an object from an XML serialized representation.

Specification: https://www.w3.org/XML/

Parameters

serialized [bytes] An XML serialized representation

Returns

instance [cls] Instantiated object.

to_pickle(*self*)
Return a pickle serialized representation.

> **Warning:** This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Returns

serialized [str] A pickled representation of the object

classmethod from_pickle(*serialized*)
Instantiate an object from a pickle serialized representation.

> **Warning:** This is not recommended for safe, stable storage since the pickle specification may change between Python versions.

Parameters

serialized [str] A pickled representation of the object

Returns

instance [cls] An instantiated object

2.3.3 Miscellaneous utilities

Miscellaneous utility functions.

inherit_docstrings	Inherit docstrings from parent class
all_subclasses	Recursively retrieve all subclasses of the specified class
temporary_cd	Context to temporary change the working directory.
temporary_directory	Context for safe creation of temporary directories.
get_data_file_path	Get the full path to one of the reference files in test-systems.
convert_0_1_smirnoff_to_0_2	Convert an 0.1-compliant SMIRNOFF dict to an 0.2-compliant one.
convert_0_2_smirnoff_to_0_3	Convert an 0.2-compliant SMIRNOFF dict to an 0.3-compliant one.

openforcefield.utils.utils.inherit_docstrings

openforcefield.utils.utils.**inherit_docstrings**(*cls*)
Inherit docstrings from parent class

openforcefield.utils.utils.all_subclasses

openforcefield.utils.utils.**all_subclasses**(*cls*)
Recursively retrieve all subclasses of the specified class

openforcefield.utils.utils.temporary_cd

openforcefield.utils.utils.**temporary_cd**(*dir_path*)
Context to temporary change the working directory.

Parameters

dir_path [str] The directory path to enter within the context

Examples

```
>>> dir_path = '/tmp'
>>> with temporary_cd(dir_path):
...     pass  # do something in dir_path
```

openforcefield.utils.utils.temporary_directory

openforcefield.utils.utils.**temporary_directory**()
Context for safe creation of temporary directories.

openforcefield.utils.utils.get_data_file_path

openforcefield.utils.utils.**get_data_file_path**(*relative_path*)

Get the full path to one of the reference files in testsystems. In the source distribution, these files are in `openforcefield/data/`, but on installation, they're moved to somewhere in the user's python site-packages directory. Parameters ———- name : str

Name of the file to load (with respect to the repex folder).

openforcefield.utils.utils.convert_0_1_smirnoff_to_0_2

openforcefield.utils.utils.**convert_0_1_smirnoff_to_0_2**(*smirnoff_data_0_1*)

Convert an 0.1-compliant SMIRNOFF dict to an 0.2-compliant one. This involves renaming several tags, adding Electrostatics and ToolkitAM1BCC tags, and separating improper torsions into their own section.

Parameters

smirnoff_data_0_1 [dict] Hierarchical dict representing a SMIRNOFF data structure according the the 0.1 spec

Returns

smirnoff_data_0_2 Hierarchical dict representing a SMIRNOFF data structure according the the 0.2 spec

openforcefield.utils.utils.convert_0_2_smirnoff_to_0_3

openforcefield.utils.utils.**convert_0_2_smirnoff_to_0_3**(*smirnoff_data_0_2*)

Convert an 0.2-compliant SMIRNOFF dict to an 0.3-compliant one. This involves removing units from header tags and adding them to attributes of child elements. It also requires converting ProperTorsions and ImproperTorsions potentials from "charmm" to "fourier".

Parameters

smirnoff_data_0_2 [dict] Hierarchical dict representing a SMIRNOFF data structure according the the 0.2 spec

Returns

smirnoff_data_0_3 Hierarchical dict representing a SMIRNOFF data structure according the the 0.3 spec

2.3.4 Structure tools

Tools for manipulating molecules and structures

> **Warning:** These methods are deprecated and will be removed and replaced with integrated API methods. We recommend that no new code makes use of these functions.

get_molecule_parameterIDs	Process a list of molecules with a specified SMIRNOFF ffxml file and determine which parameters are used by which molecules, returning collated results.

openforcefield.utils.structure.get_molecule_parameterIDs

openforcefield.utils.structure.**get_molecule_parameterIDs**(*molecules*, *forcefield*)

Process a list of molecules with a specified SMIRNOFF ffxml file and determine which parameters are used by which molecules, returning collated results.

Parameters

molecules [list of openforcefield.topology.Molecule] List of molecules (with explicit hydrogens) to parse

forcefield [openforcefield.typing.engines.smirnoff.ForceField] The ForceField to apply

Returns

parameters_by_molecule [dict] Parameter IDs used in each molecule, keyed by isomeric SMILES generated from provided OEMols. Each entry in the dict is a list which does not necessarily have unique entries; i.e. parameter IDs which are used more than once will occur multiple times.

parameters_by_ID [dict] Molecules in which each parameter ID occur, keyed by parameter ID. Each entry in the dict is a set of isomeric SMILES for molecules in which that parameter occurs. No frequency information is stored.

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