
OpenFF Units

The Open Force Field Initiative

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Units of measure for biomolecular software.

OpenFF Units is based on [Pint](#). Its *Quantity*, *Unit*, and *Measurement* types inherit from Pint's, and add improved support for serialization and deserialization. OpenFF Units improves support for biomolecular software by providing a *system of units* that are compatible with [OpenMM](#) and *providing functions* to convert to OpenMM units and back. It also provides *atomic masses* with units, as well as some *other useful maps*.

INSTALLATION

We recommend installing OpenFF Units with the [Conda](#) package manager. If you don't yet have a Conda distribution installed, we recommend [MambaForge](#) for most users. The `openff-units` package can be installed from Conda Forge:

```
conda install -c conda-forge openff-units
```


USING OPENFF UNITS

OpenFF Units provides the *Quantity* class, which represents a numerical value with units. A *Quantity* can be created by providing a value and units:

```
>>> from openff.units import unit, Quantity
>>>
>>> Quantity(1.007, unit.amu)
<Quantity(1.007, 'unified_atomic_mass_unit')>
```

The *unit* singleton value is a registry of units, but also exposes the *Quantity*, *Unit*, and *Measurement* classes so you don't have to import them individually. Even easier, multiplying a number by the appropriate unit also provides a *Quantity*:

```
>>> mass_proton = 1.007 * unit.amu
>>> mass_proton == unit.Quantity(1.007, unit.amu)
True
```

Quantity can also wrap NumPy arrays. It's best to wrap an array of floats in a quantity, rather than have an array of quantities:

```
>>> import numpy as np
>>>
>>> box_vectors = np.array([
...     [5.0, 0.0, 0.0],
...     [0.0, 5.0, 0.0],
...     [0.0, 0.0, 5.0],
... ]) * unit.nanometer
```

When constructed like this, *Quantity* is transparent; it will pass any attributes it doesn't have through to the inner value. This means that a quantity-wrapped array can be used exactly as though it were an array — the units are just checked silently in the background:

```
>>> from numpy.random import rand
>>>
>>> trajectory = 10 * rand(10, 10000, 3) * unit.nanometer
>>> centroids = trajectory.mean(axis=1)[..., None]
>>> last_water = trajectory[:, 97:99, :]
>>> last_water_recentered = last_water - centroids
```

This transparency works with most container types, so it's usually best to have *Quantity* be the outermost wrapper type.

Complex units can be constructed by combining units with the usual arithmetic operations:

```
>>> boltzmann_constant = 8.314462618e-3 * unit.kilojoule / unit.kelvin / unit.avogadro_
↳number
```

Some common constants are provided as units as well:

```
>>> boltzmann_constant = 1.0 * unit.boltzmann_constant
```

Adding or subtracting different units with the same dimensions just works:

```
>>> 1.0 * unit.angstrom + 1.0 * unit.nanometer
<Quantity(11.0, 'angstrom')>
```

But quantities with different dimensions raise an exception:

```
>>> 1.0 * unit.angstrom + 1.0 * unit.nanojoule
Traceback (most recent call last):
...
pint.errors.DimensionalityError: Cannot convert from 'angstrom' ([length]) to 'nanojoule'
↳ ' ([length] ** 2 * [mass] / [time] ** 2)
```

Quantities can be converted between units with the `.to()` method:

```
>>> (1.0 * unit.nanometer).to(unit.angstrom)
<Quantity(10.0, 'angstrom')>
```

Or with the `.ito()` method for in-place transformations:

```
>>> quantity = 10.0 * unit.angstrom
>>> quantity.ito(unit.nanometer)
>>> quantity
<Quantity(1.0, 'nanometer')>
```

The underlying value without units can be retrieved with the `.m` or `.magnitude` properties. Just make sure it's in the units you expect first:

```
>>> quantity = (1.0 * unit.k_B).to_base_units()
>>> assert quantity.units == unit.kilogram * unit.meter**2 / unit.kelvin / unit.second**2
>>> quantity.magnitude
1.380649e-23
```

Alternatively, specify the target units of the output magnitude with `.m_as`:

```
>>> quantity = 1.0 * unit.k_B
>>> quantity.m_as(unit.kilogram * unit.meter**2 / unit.kelvin / unit.second**2)
1.380649e-23
```

OpenFF Units also provides the `from_openmm` and `to_openmm` functions to convert between OpenFF quantities and OpenMM quantities:

```
>>> from openff.units.openmm import from_openmm, to_openmm
>>>
>>> quantity = 10.0 * unit.angstrom
>>> omm_quant = to_openmm(quantity)
>>> omm_quant
```

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```

Quantity(value=10.0, unit=angstrom)
>>> type(omm_quant)
<class 'openmm.unit.quantity.Quantity'>
>>> quant_roundtrip = from_openmm(omm_quant)
>>> quant_roundtrip
<Quantity(10.0, 'angstrom')>
>>> type(quant_roundtrip)
<class 'openff.units.units.Quantity'>

```

For more details, see the [API reference](#).

[openff.units](#)

2.1 openff.units

Module Attributes

unit	Registry of units provided by OpenFF Units.
----------------------	---

2.1.1 unit

`openff.units.unit: UnitRegistry`

Registry of units provided by OpenFF Units.

`unit` may be used similarly to a module. It makes constants and units of measure available as attributes. Available units can be found in the `constants` and `defaults` data files.

Classes

Quantity	A value with associated units.
Measurement	A value with associated units and uncertainty.
Unit	A unit of measure.

2.1.2 Quantity

`class openff.units.Quantity(value: str, units: Optional[UnitLike] = None)`

`class openff.units.Quantity(value: Sequence, units: Optional[UnitLike] = None)`

`class openff.units.Quantity(value: Quantity[Magnitude], units: Optional[UnitLike] = None)`

`class openff.units.Quantity(value: Magnitude, units: Optional[UnitLike] = None)`

Bases: `Quantity[_MagnitudeType]`

A value with associated units.

Methods

<i>check</i>	Return true if the quantity's dimension matches passed dimension.
<i>clip</i>	
<i>compare</i>	
<i>compatible_units</i>	
<i>compute</i>	Compute the Dask array wrapped by pint.Quantity.
<i>dot</i>	Dot product of two arrays.
<i>fill</i>	
<i>format_babel</i>	
<i>from_list</i>	Transforms a list of Quantities into an numpy.array quantity.
<i>from_sequence</i>	Transforms a sequence of Quantities into an numpy.array quantity.
<i>from_tuple</i>	
<i>is_compatible_with</i>	check if the other object is compatible
<i>ito</i>	Inplace rescale to different units.
<i>ito_base_units</i>	Return Quantity rescaled to base units.
<i>ito_reduced_units</i>	Return Quantity scaled in place to reduced units, i.e. one unit per dimension.
<i>ito_root_units</i>	Return Quantity rescaled to root units.
<i>m_as</i>	Quantity's magnitude expressed in particular units.
<i>persist</i>	Persist the Dask Array wrapped by pint.Quantity.
<i>plus_minus</i>	
<i>prod</i>	Return the product of quantity elements over a given axis
<i>put</i>	
<i>searchsorted</i>	
<i>to</i>	Return Quantity rescaled to different units.
<i>to_base_units</i>	Return Quantity rescaled to base units.
<i>to_compact</i>	"Return Quantity rescaled to compact, human-readable units.
<i>to_openmm</i>	Convert the quantity to an openmm.unit.Quantity.
<i>to_reduced_units</i>	Return Quantity scaled in place to reduced units, i.e. one unit per dimension.
<i>to_root_units</i>	Return Quantity rescaled to root units.
<i>to_timedelta</i>	
<i>to_tuple</i>	

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Table 1 – continued from previous page

<i>tolist</i>	
<i>visualize</i>	Produce a visual representation of the Dask graph.
Attributes	
<i>T</i>	
<i>UnitsContainer</i>	
<i>debug_used</i>	
<i>default_format</i>	Default formatting string.
<i>dimensionality</i>	returns: <code>dict</code> -- Dimensionality of the Quantity, e.g.
<i>dimensionless</i>	
<i>flat</i>	
<i>force_ndarray</i>	
<i>force_ndarray_like</i>	
<i>imag</i>	
<i>m</i>	Quantity's magnitude.
<i>magnitude</i>	Quantity's magnitude.
<i>real</i>	
<i>shape</i>	
<i>u</i>	Quantity's units.
<i>unitless</i>	
<i>units</i>	Quantity's units.

property T**property UnitsContainer:** Callable[..., UnitsContainerT]**check**(*dimension: UnitLike*) → bool

Return true if the quantity's dimension matches passed dimension.

clip(*min=None, max=None, out=None, **kwargs*)**compare**(**args, **kwargs*)**compatible_units**(**contexts*)**compute**(***kwargs*)

Compute the Dask array wrapped by pint.Quantity.

Parameters ***kwargs* (`dict`) – Any keyword arguments to pass to `dask.compute`.

Returns `pint.Quantity` – A `pint.Quantity` wrapped numpy array.

property `debug_used`

default_format: `str` = ''

Default formatting string.

property `dimensionality`: `UnitsContainerT`

returns: `dict` – Dimensionality of the Quantity, e.g. `{length: 1, time: -1}`

property `dimensionless`: `bool`

`dot(b)`

Dot product of two arrays.

Wraps `np.dot()`.

`fill(value)` → `None`

property `flat`

property `force_ndarray`: `bool`

property `force_ndarray_like`: `bool`

`format_babel(spec: str = "", **kwspec: Any) → str`

classmethod `from_list(quant_list: List[Quantity], units=None) → Quantity[ndarray]`

Transforms a list of Quantities into an `numpy.array` quantity. If no units are specified, the unit of the first element will be used. Same as `from_sequence`.

If units is not specified and list is empty, the unit cannot be determined and a `ValueError` is raised.

Parameters

- `quant_list` (list of `pint.Quantity`) – list of `pint.Quantity`
- `units` (`UnitsContainer`, `str` or `pint.Quantity`) – units of the physical quantity to be created (Default value = `None`)

Returns `pint.Quantity`

classmethod `from_sequence(seq: Sequence[Quantity], units=None) → Quantity[ndarray]`

Transforms a sequence of Quantities into an `numpy.array` quantity. If no units are specified, the unit of the first element will be used.

If units is not specified and sequence is empty, the unit cannot be determined and a `ValueError` is raised.

Parameters

- `seq` (sequence of `pint.Quantity`) – sequence of `pint.Quantity`
- `units` (`UnitsContainer`, `str` or `pint.Quantity`) – units of the physical quantity to be created (Default value = `None`)

Returns `pint.Quantity`

classmethod `from_tuple(tup)`

property `imag`: `Quantity[pint._typing._MagnitudeType]`

is_compatible_with(*other*: Any, **contexts*: Union[str, Context], ***ctx_kwargs*: Any) → bool

check if the other object is compatible

Parameters

- **other** – The object to check. Treated as dimensionless if not a Quantity, Unit or str.
- ***contexts** (str or pint.Context) – Contexts to use in the transformation.
- ****ctx_kwargs** – Values for the Context/s

Returns bool

ito(*other=None*, **contexts*, ***ctx_kwargs*) → None

Inplace rescale to different units.

Parameters

- **other** (pint.Quantity, str or dict) – Destination units. (Default value = None)
- ***contexts** (str or pint.Context) – Contexts to use in the transformation.
- ****ctx_kwargs** – Values for the Context/s

ito_base_units() → None

Return Quantity rescaled to base units.

ito_reduced_units() → None

Return Quantity scaled in place to reduced units, i.e. one unit per dimension. This will not reduce compound units (e.g., 'J/kg' will not be reduced to m**2/s**2), nor can it make use of contexts at this time.

ito_root_units() → None

Return Quantity rescaled to root units.

property m: pint._typing._MagnitudeType

Quantity's magnitude. Short form for *magnitude*

m_as(*units*) → _MagnitudeType

Quantity's magnitude expressed in particular units.

Parameters *units* (pint.Quantity, str or dict) – destination units

property magnitude: pint._typing._MagnitudeType

Quantity's magnitude. Long form for *m*

persist(***kwargs*)

Persist the Dask Array wrapped by pint.Quantity.

Parameters ***kwargs* (dict) – Any keyword arguments to pass to `dask.persist`.

Returns pint.Quantity – A pint.Quantity wrapped Dask array.

plus_minus(*error*, *relative=False*)

prod(*axis=None*, *dtype=None*, *out=None*, *keepdims=np._NoValue*, *initial=np._NoValue*, *where=np._NoValue*)

Return the product of quantity elements over a given axis

Wraps `np.prod()`.

put(*indices*, *values*, *mode='raise'*) → None

property real: Quantity[pint._typing._MagnitudeType]

`searchsorted(v, side='left', sorter=None)`

property shape: `Tuple[int, ...]`

`to(other=None, *contexts, **ctx_kwargs) → Quantity[_MagnitudeType]`

Return Quantity rescaled to different units.

Parameters

- **other** (`pint.Quantity`, `str` or `dict`) – destination units. (Default value = None)
- ***contexts** (`str` or `pint.Context`) – Contexts to use in the transformation.
- ****ctx_kwargs** – Values for the Context/s

Returns `pint.Quantity`

`to_base_units() → Quantity[_MagnitudeType]`

Return Quantity rescaled to base units.

`to_compact(unit=None) → Quantity[_MagnitudeType]`

“Return Quantity rescaled to compact, human-readable units.

To get output in terms of a different unit, use the unit parameter.

Examples

```
>>> import pint
>>> ureg = pint.UnitRegistry()
>>> (200e-9*ureg.s).to_compact()
<Quantity(200.0, 'nanosecond')>
>>> (1e-2*ureg('kg m/s^2')).to_compact('N')
<Quantity(10.0, 'millinewton')>
```

`to_openmm() → OpenMMQuantity`

Convert the quantity to an `openmm.unit.Quantity`.

Returns `openmm_quantity` (`openmm.unit.quantity.Quantity`) – The OpenMM compatible quantity.

`to_reduced_units() → Quantity[_MagnitudeType]`

Return Quantity scaled in place to reduced units, i.e. one unit per dimension. This will not reduce compound units (intentionally), nor can it make use of contexts at this time.

`to_root_units() → Quantity[_MagnitudeType]`

Return Quantity rescaled to root units.

`to_timedelta() → timedelta`

`to_tuple() → Tuple[_MagnitudeType, Tuple[Tuple[str]]]`

`tolist()`

property u: `Unit`

Quantity’s units. Short form for *units*

property unitless: `bool`

property units: *Unit*

Quantity's units. Long form for *u*

visualize(kwargs)**

Produce a visual representation of the Dask graph.

The graphviz library is required.

Parameters ****kwargs** (*dict*) – Any keyword arguments to pass to `dask.visualize`.

2.1.3 Measurement

class `openff.units.Measurement` (*value, error, units=MISSING*)

Bases: *Measurement*

A value with associated units and uncertainty.

Methods

<i>check</i>	Return true if the quantity's dimension matches passed dimension.
<i>clip</i>	
<i>compare</i>	
<i>compatible_units</i>	
<i>compute</i>	Compute the Dask array wrapped by <code>pint.Quantity</code> .
<i>dot</i>	Dot product of two arrays.
<i>fill</i>	
<i>format_babel</i>	
<i>from_list</i>	Transforms a list of Quantities into an <code>numpy.array</code> quantity.
<i>from_sequence</i>	Transforms a sequence of Quantities into an <code>numpy.array</code> quantity.
<i>from_tuple</i>	
<i>is_compatible_with</i>	check if the other object is compatible
<i>ito</i>	Inplace rescale to different units.
<i>ito_base_units</i>	Return Quantity rescaled to base units.
<i>ito_reduced_units</i>	Return Quantity scaled in place to reduced units, i.e. one unit per dimension.
<i>ito_root_units</i>	Return Quantity rescaled to root units.
<i>m_as</i>	Quantity's magnitude expressed in particular units.
<i>persist</i>	Persist the Dask Array wrapped by <code>pint.Quantity</code> .
<i>plus_minus</i>	
<i>prod</i>	Return the product of quantity elements over a given axis

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Table 2 – continued from previous page

<i>put</i>	
<i>searchsorted</i>	
<i>to</i>	Return Quantity rescaled to different units.
<i>to_base_units</i>	Return Quantity rescaled to base units.
<i>to_compact</i>	"Return Quantity rescaled to compact, human-readable units.
<i>to_reduced_units</i>	Return Quantity scaled in place to reduced units, i.e. one unit per dimension.
<i>to_root_units</i>	Return Quantity rescaled to root units.
<i>to_timedelta</i>	
<i>to_tuple</i>	
<i>tolist</i>	
<i>visualize</i>	Produce a visual representation of the Dask graph.

Attributes

<i>T</i>	
<i>UnitsContainer</i>	
<i>debug_used</i>	
<i>default_format</i>	Default formatting string.
<i>dimensionality</i>	returns: <code>dict</code> -- Dimensionality of the Quantity, e.g.
<i>dimensionless</i>	
<i>error</i>	
<i>flat</i>	
<i>force_ndarray</i>	
<i>force_ndarray_like</i>	
<i>imag</i>	
<i>m</i>	Quantity's magnitude.
<i>magnitude</i>	Quantity's magnitude.
<i>real</i>	
<i>rel</i>	
<i>shape</i>	
<i>u</i>	Quantity's units.
<i>unitless</i>	
<i>units</i>	Quantity's units.
<i>value</i>	

property T

property UnitsContainer: `Callable[..., UnitsContainerT]`

check(*dimension: UnitLike*) \rightarrow `bool`

Return true if the quantity's dimension matches passed dimension.

clip(*min=None, max=None, out=None, **kwargs*)

compare(**args, **kwargs*)

compatible_units(**contexts*)

compute(***kwargs*)

Compute the Dask array wrapped by `pint.Quantity`.

Parameters ***kwargs* (`dict`) – Any keyword arguments to pass to `dask.compute`.

Returns `pint.Quantity` – A `pint.Quantity` wrapped numpy array.

property `debug_used`

default_format: `str` = ''

Default formatting string.

property `dimensionality`: `UnitsContainerT`

returns: `dict` – Dimensionality of the Quantity, e.g. `{length: 1, time: -1}`

property `dimensionless`: `bool`

`dot(b)`

Dot product of two arrays.

Wraps `np.dot()`.

property `error`

`fill(value)` → `None`

property `flat`

property `force_ndarray`: `bool`

property `force_ndarray_like`: `bool`

`format_babel(spec: str = "", **kwspec: Any) → str`

classmethod `from_list(quant_list: List[Quantity], units=None) → Quantity[ndarray]`

Transforms a list of Quantities into an `numpy.array` quantity. If no units are specified, the unit of the first element will be used. Same as `from_sequence`.

If units is not specified and list is empty, the unit cannot be determined and a `ValueError` is raised.

Parameters

- **quant_list** (list of `pint.Quantity`) – list of `pint.Quantity`
- **units** (`UnitsContainer`, `str` or `pint.Quantity`) – units of the physical quantity to be created (Default value = `None`)

Returns `pint.Quantity`

classmethod `from_sequence(seq: Sequence[Quantity], units=None) → Quantity[ndarray]`

Transforms a sequence of Quantities into an `numpy.array` quantity. If no units are specified, the unit of the first element will be used.

If units is not specified and sequence is empty, the unit cannot be determined and a `ValueError` is raised.

Parameters

- **seq** (sequence of `pint.Quantity`) – sequence of `pint.Quantity`
- **units** (`UnitsContainer`, `str` or `pint.Quantity`) – units of the physical quantity to be created (Default value = `None`)

Returns `pint.Quantity`

classmethod `from_tuple(tup)`

property `imag`: `Quantity[pint._typing.MagnitudeType]`

is_compatible_with(*other: Any, *contexts: Union[str, Context], **ctx_kwargs: Any*) → bool

check if the other object is compatible

Parameters

- **other** – The object to check. Treated as dimensionless if not a Quantity, Unit or str.
- ***contexts** (str or pint.Context) – Contexts to use in the transformation.
- ****ctx_kwargs** – Values for the Context/s

Returns bool

ito(*other=None, *contexts, **ctx_kwargs*) → None

Inplace rescale to different units.

Parameters

- **other** (pint.Quantity, str or dict) – Destination units. (Default value = None)
- ***contexts** (str or pint.Context) – Contexts to use in the transformation.
- ****ctx_kwargs** – Values for the Context/s

ito_base_units() → None

Return Quantity rescaled to base units.

ito_reduced_units() → None

Return Quantity scaled in place to reduced units, i.e. one unit per dimension. This will not reduce compound units (e.g., 'J/kg' will not be reduced to m**2/s**2), nor can it make use of contexts at this time.

ito_root_units() → None

Return Quantity rescaled to root units.

property m: pint._typing._MagnitudeType

Quantity's magnitude. Short form for *magnitude*

m_as(*units*) → _MagnitudeType

Quantity's magnitude expressed in particular units.

Parameters *units* (pint.Quantity, str or dict) – destination units

property magnitude: pint._typing._MagnitudeType

Quantity's magnitude. Long form for *m*

persist(***kwargs*)

Persist the Dask Array wrapped by pint.Quantity.

Parameters ****kwargs** (dict) – Any keyword arguments to pass to dask.persist.

Returns pint.Quantity – A pint.Quantity wrapped Dask array.

plus_minus(*error, relative=False*)

prod(*axis=None, dtype=None, out=None, keepdims=np._NoValue, initial=np._NoValue, where=np._NoValue*)

Return the product of quantity elements over a given axis

Wraps np.prod().

put(*indices, values, mode='raise'*) → None

property real: Quantity[pint._typing._MagnitudeType]

property `rel`

searchsorted(`v`, `side='left'`, `sorter=None`)

property `shape`: `Tuple[int, ...]`

to(`other=None`, `*contexts`, `**ctx_kwargs`) → `Quantity[_MagnitudeType]`

Return Quantity rescaled to different units.

Parameters

- **other** (`pint.Quantity`, `str` or `dict`) – destination units. (Default value = None)
- ***contexts** (`str` or `pint.Context`) – Contexts to use in the transformation.
- ****ctx_kwargs** – Values for the Context/s

Returns `pint.Quantity`

to_base_units() → `Quantity[_MagnitudeType]`

Return Quantity rescaled to base units.

to_compact(`unit=None`) → `Quantity[_MagnitudeType]`

“Return Quantity rescaled to compact, human-readable units.

To get output in terms of a different unit, use the unit parameter.

Examples

```
>>> import pint
>>> ureg = pint.UnitRegistry()
>>> (200e-9*ureg.s).to_compact()
<Quantity(200.0, 'nanosecond')>
>>> (1e-2*ureg('kg m/s^2')).to_compact('N')
<Quantity(10.0, 'millinewton')>
```

to_reduced_units() → `Quantity[_MagnitudeType]`

Return Quantity scaled in place to reduced units, i.e. one unit per dimension. This will not reduce compound units (intentionally), nor can it make use of contexts at this time.

to_root_units() → `Quantity[_MagnitudeType]`

Return Quantity rescaled to root units.

to_timedelta() → `timedelta`

to_tuple() → `Tuple[_MagnitudeType, Tuple[Tuple[str]]]`

tolist()

property `u`: `Unit`

Quantity’s units. Short form for *units*

property `unitless`: `bool`

property `units`: `Unit`

Quantity’s units. Long form for *u*

property `value`

visualize(**kwargs)

Produce a visual representation of the Dask graph.

The graphviz library is required.

Parameters **kwargs (dict) – Any keyword arguments to pass to dask.visualize.

2.1.4 Unit

class openff.units.Unit(*args, **kwargs)

Bases: Unit

A unit of measure.

Methods

<i>compare</i>	
<i>compatible_units</i>	
<i>format_babel</i>	
<i>from_</i>	Converts a numerical value or quantity to this unit
<i>is_compatible_with</i>	check if the other object is compatible
<i>m_from</i>	Converts a numerical value or quantity to this unit, then returns the magnitude of the converted value

Attributes

<i>debug_used</i>	
<i>default_format</i>	Default formatting string.
<i>dimensionality</i>	returns: dict -- Dimensionality of the Unit, e.g.
<i>dimensionless</i>	Return True if the Unit is dimensionless; False otherwise.
<i>systems</i>	

compare(other, op) → bool

compatible_units(*contexts)

property debug_used: Any

default_format: str = ''

Default formatting string.

property dimensionality: UnitsContainer

returns: dict – Dimensionality of the Unit, e.g. {length: 1, time: -1}

property dimensionless: `bool`

Return True if the Unit is dimensionless; False otherwise.

format_babel(*spec=""*, *locale=None*, ***kwspec: Any*) → `str`

from_(*value*, *strict=True*, *name='value'*)

Converts a numerical value or quantity to this unit

Parameters

- **value** – a Quantity (or numerical value if `strict=False`) to convert
- **strict** – boolean to indicate that only quantities are accepted (Default value = `True`)
- **name** – descriptive name to use if an exception occurs (Default value = “value”)

Returns `type` – The converted value as this unit

is_compatible_with(*other: Any*, **contexts: Union[str, Context]*, ***ctx_kwargs: Any*) → `bool`

check if the other object is compatible

Parameters

- **other** – The object to check. Treated as dimensionless if not a Quantity, Unit or str.
- ***contexts** (`str` or `pint.Context`) – Contexts to use in the transformation.
- ****ctx_kwargs** – Values for the Context/s

Returns `bool`

m_from(*value*, *strict=True*, *name='value'*)

Converts a numerical value or quantity to this unit, then returns the magnitude of the converted value

Parameters

- **value** – a Quantity (or numerical value if `strict=False`) to convert
- **strict** – boolean to indicate that only quantities are accepted (Default value = `True`)
- **name** – descriptive name to use if an exception occurs (Default value = “value”)

Returns `type` – The magnitude of the converted value

property systems

Modules

<code>elements</code>	Symbols and masses for the chemical elements.
<code>exceptions</code>	
<code>openmm</code>	Functions for converting between OpenFF and OpenMM units
<code>utilities</code>	Utility methods for OpenFF Units

2.1.5 elements

Symbols and masses for the chemical elements.

This module provides mappings from atomic number to atomic mass and symbol. These dicts were seeded from running the below script using OpenMM 7.7.

It's not completely clear where OpenMM sourced these values from [1] but they are generally consistent with recent IUPAC values [2].

1. <https://github.com/openmm/openmm/issues/3434#issuecomment-1023406296>
2. <https://www.ciaaw.org/publications.htm>

```
import openmm.app

masses = {
    atomic_number: openmm.app.element.Element.getByAtomicNumber(
        atomic_number
    ).mass._value
    for atomic_number in range(1, 117)
}

symbols = {
    atomic_number: openmm.app.element.Element.getByAtomicNumber(atomic_number).symbol
    for atomic_number in range(1, 117)
}
```

Module Attributes

<i>MASSES</i>	Mapping from atomic number to atomic mass
<i>SYMBOLS</i>	Mapping from atomic number to element symbol

MASSES

`openff.units.elements.MASSES: Dict[int, Quantity]`

Mapping from atomic number to atomic mass

SYMBOLS

`openff.units.elements.SYMBOLS: Dict[int, str]`

Mapping from atomic number to element symbol

2.1.6 exceptions

Exceptions

<i>MissingOpenMMUnitError</i>	Raised when a unit cannot be converted to an equivalent OpenMM unit
<i>NoneQuantityError</i>	Raised when attempting to convert <i>None</i> between unit packages as a quantity object
<i>NoneUnitError</i>	Raised when attempting to convert <i>None</i> between unit packages as a unit object

MissingOpenMMUnitError

exception `openff.units.exceptions.MissingOpenMMUnitError`

Bases: `Exception`

Raised when a unit cannot be converted to an equivalent OpenMM unit

NoneQuantityError

exception `openff.units.exceptions.NoneQuantityError`

Bases: `Exception`

Raised when attempting to convert *None* between unit packages as a quantity object

NoneUnitError

exception `openff.units.exceptions.NoneUnitError`

Bases: `Exception`

Raised when attempting to convert *None* between unit packages as a unit object

2.1.7 openmm

Functions for converting between OpenFF and OpenMM units

Functions

<i>from_openmm</i>	Convert an OpenMM Quantity to an OpenFF Quantity
<i>to_openmm</i>	Convert an OpenFF Quantity to an OpenMM Quantity
<i>openmm_unit_to_string</i>	Convert a <code>openmm.unit.Unit</code> to a string representation.
<i>string_to_openmm_unit</i>	Deserializes a <code>openmm.unit.Quantity</code> from a string representation, for example: "kilocalories_per_mole / angstrom ** 2"
<i>ensure_quantity</i>	

from_openmm

`openff.units.openmm.from_openmm(openmm_quantity: openmm_unit.Quantity) → Quantity`

Convert an OpenMM Quantity to an OpenFF Quantity

`openmm.unit.quantity.Quantity` from OpenMM and `openff.units.Quantity` from this package both represent a numerical value with units.

to_openmm

`openff.units.openmm.to_openmm(quantity: Quantity) → openmm_unit.Quantity`

Convert an OpenFF Quantity to an OpenMM Quantity

`openmm.unit.quantity.Quantity` from OpenMM and `openff.units.Quantity` from this package both represent a numerical value with units. The units available in the two packages differ; when a unit is missing from the target package, the resulting quantity will be in base units (kg/m/s/A/K/mole), which are shared between both packages. This may cause the resulting value to be slightly different to the input due to the limited precision of floating point numbers.

openmm_unit_to_string

`openff.units.openmm.openmm_unit_to_string(input_unit: openmm_unit.Unit) → str`

Convert a `openmm.unit.Unit` to a string representation.

Parameters `input_unit` (`A openmm.unit`) – The unit to serialize

Returns `unit_string` (`str`) – The serialized unit.

string_to_openmm_unit

`openff.units.openmm.string_to_openmm_unit(unit_string: str) → openmm_unit.Unit`

Deserializes a `openmm.unit.Quantity` from a string representation, for example: “kilocalories_per_mole / angstrom ** 2”

Parameters `unit_string` (`dict`) – Serialized representation of a `openmm.unit.Quantity`.

Returns `output_unit` (`openmm.unit.Quantity`) – The deserialized unit from the string

Raises `MissingOpenMMUnitError` – if the unit is unavailable in OpenMM.

ensure_quantity

`openff.units.openmm.ensure_quantity(unknown_quantity: Union[Quantity, openmm_unit.Quantity], type_to_ensure: Literal['openmm', 'openff']) → Union[Quantity, openmm_unit.Quantity]`

2.1.8 utilities

Utility methods for OpenFF Units

Functions

`get_defaults_path`

Get the full path to the `defaults.txt` file

`get_defaults_path`

`openff.units.utilities.get_defaults_path()` → `str`

Get the full path to the `defaults.txt` file

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