OpenFF Units

The Open Force Field Initiative

Jun 14, 2023

CONTENTS

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*.

CHAPTER

ONE

INSTALLATION

We recommend installing OpenFF Units with the Conda or Mamba package managers. If you don't yet have a Conda distribution installed, we recommend MambaForge for most users; see the OpenFF install docs. The `openff-units` package can be installed from Conda Forge:

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

CHAPTER

TWO

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 an 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
```

(continues on next page)

(continued from previous page)

```
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*.

CHAPTER

THREE

CURRENT DEVELOPMENT

3.1 Behavior changes

- #62 Drops support for Python 3.8, following NEP 29.

openff.units	

3.1.1 openff.units

Module Attributes

unit	Registry of units provided by OpenFF Units.

unit

openff.units.**unit: openff.units.units.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.

Functions

Measurement	
ensure_quantity	Given a quantity that could be of a variety of types, attempt to coerce into a given type.

Measurement

openff.units.**Measurement**(**args*, ***kwargs*)

ensure_quantity

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

Given a quantity that could be of a variety of types, attempt to coerce into a given type.

Examples

```
>>> import numpy
>>> from openmm import unit as openmm_unit
>>> from openff.units import unit
>>> from openff.units.openmm import ensure_quantity
>>> # Create a 9 Angstrom quantity with each registry
>>> length1 = unit.Quantity(9.0, unit.angstrom)
>>> length2 = openmm_unit.Quantity(9.0, openmm_unit.angstrom)
>>> # Similar quantities are be coerced into requested type
>>> assert type(ensure_quantity(length1, "openmm")) == openmm_unit.Quantity
>>> assert type(ensure_quantity(length2, "openff")) == unit.Quantity
>>> # Seemingly-redundant "conversions" short-circuit
>>> assert ensure_quantity(length1, "openff") == ensure_quantity(length2, "openff")
>>> assert ensure_quantity(length1, "openmm") == ensure_quantity(length2, "openmm")
>>> # NumPy arrays and some primitives are automatically up-converted to `Quantity`␣
↪objects
>>> # Note that their units are set to "dimensionless"
>>> ensure_quantity(numpy.array([1, 2]), "openff")
<Quantity([1 2], 'dimensionless')>
>>> ensure_quantity(4.0, "openmm")
Quantity(value=4.0, unit=dimensionless)
```

Classes

Quantity

Unit

Quantity

class openff.units.**Quantity**(*value: MagnitudeT*, *units: Optional[UnitLike] = None*)
class openff.units.**Quantity**(*value: str*, *units: Optional[UnitLike] = None*)
class openff.units.**Quantity**(*value: Sequence[ScalarT]*, *units: Optional[UnitLike] = None*)
class openff.units.**Quantity**(*value: PlainQuantity[Any]*, *units: Optional[UnitLike] = None*)

Bases: Quantity

Methods

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

continues on next page

Table 1 – continued from previous page

to_base_units	Return PlainQuantity rescaled to plain units.
to_compact	"Return PlainQuantity rescaled to compact, human-readable units.
to_openmm	Convert the quantity to an `openmm.unit.Quantity`.
to_preferred	Return Quantity converted to a unit composed of the preferred units.
to_reduced_units	Return PlainQuantity scaled in place to reduced units, i.e. one unit per dimension.
to_root_units	Return PlainQuantity rescaled to root units.
to_timedelta	
to_tuple	
tolist	
visualize	Produce a visual representation of the Dask graph.

Attributes

T	
UnitsContainer	
default_format	Default formatting string.
dimensionality	returns: `dict` -- Dimensionality of the PlainQuantity, e.g.
dimensionless	
flat	
force_ndarray	
force_ndarray_like	
imag	
m	PlainQuantity's magnitude.
magnitude	PlainQuantity's magnitude.
ndim	
real	
shape	
u	PlainQuantity's units.
unitless	
units	PlainQuantity'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.PlainQuantity.

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

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

default_format: str = ''

Default formatting string.

property dimensionality: UnitsContainerT

returns: dict – Dimensionality of the PlainQuantity, 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[PlainQuantity[MagnitudeT]]*, *units=None*) → PlainQuantity[MagnitudeT]

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

Returns `pint.PlainQuantity`

classmethod from_sequence(*seq: Sequence[PlainQuantity[MagnitudeT]]*, *units=None*) → PlainQuantity[MagnitudeT]

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

Returns `pint.PlainQuantity`

classmethod from_tuple(*tup*)

property imag: pint.facets.numpy.quantity.NumpyQuantity

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 PlainQuantity, 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: Optional[QuantityOrUnitLike] = None*, **contexts*, ***ctx_kwargs*) → None

Inplace rescale to different units.

Parameters

- **other** (`pint.PlainQuantity`, `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 PlainQuantity rescaled to plain units.

ito_reduced_units() → None

Return PlainQuantity 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 PlainQuantity rescaled to root units.

property m: pint.facets.plain.quantity.MagnitudeT

PlainQuantity's magnitude. Short form for *magnitude*

m_as(*units*) → MagnitudeT

PlainQuantity's magnitude expressed in particular units.

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

property magnitude: pint.facets.plain.quantity.MagnitudeT

PlainQuantity's magnitude. Long form for *m*

property ndim: int

persist(***kwargs*)

Persist the Dask Array wrapped by pint.PlainQuantity.

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

Returns `pint.PlainQuantity` – A pint.PlainQuantity 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: pint.facets.numpy.quantity.NumpyQuantity

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

property shape: tuple[int, ...]

to(*other: Optional[QuantityOrUnitLike] = None*, **contexts*, ***ctx_kwargs*) → PlainQuantity

Return PlainQuantity rescaled to different units.

Parameters

- **other** (`pint.PlainQuantity`, `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.PlainQuantity`

to_base_units() → PlainQuantity[MagnitudeT]

Return PlainQuantity rescaled to plain units.

to_compact(*unit: Optional[UnitsContainer] = None*) → PlainQuantity

"Return PlainQuantity 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_preferred(*preferred_units: list[UnitLike]*) → PlainQuantity

Return Quantity converted to a unit composed of the preferred units.

Examples

```
>>> import pint
>>> ureg = pint.UnitRegistry()
>>> (1*ureg.acre).to_preferred([ureg.meters])
<Quantity(4046.87261, 'meter ** 2')>
>>> (1*(ureg.force_pound*ureg.m)).to_preferred([ureg.W])
<Quantity(4.44822162, 'second * watt')>
```

to_reduced_units() → PlainQuantity

Return PlainQuantity 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() → PlainQuantity[MagnitudeT]

Return PlainQuantity rescaled to root units.

to_timedelta() → timedelta

to_tuple() → tuple[MagnitudeT, tuple[tuple[str, ...]]]

tolist()

property u: *Unit*

PlainQuantity's units. Short form for *units*

property unitless: bool

property units: *Unit*

PlainQuantity'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`.

Unit

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

Bases: `Unit`

Methods

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

Attributes

default_format	Default formatting string.
dimensionality	returns: `dict` -- Dimensionality of the PlainUnit, e.g.
dimensionless	Return True if the PlainUnit is dimensionless; False otherwise.
systems	

compare(*other*, *op*) → bool

compatible_units(**contexts*)

default_format: str = ''

Default formatting string.

property dimensionality: UnitsContainer

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

property dimensionless: bool

Return True if the PlainUnit 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, PlainUnit 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

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

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

MASSES	Mapping from atomic number to atomic mass

MASSES

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

Mapping from atomic number to atomic mass

exceptions

Exceptions

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

openmm

Functions for converting between OpenFF and OpenMM units

Functions

from_openmm	Convert an OpenMM Quantity to an OpenFF Quantity
to_openmm	Convert an OpenFF Quantity to an OpenMM Quantity
openmm_unit_to_string	Convert a openmm.unit.Unit to a string representation.
string_to_openmm_unit	Deserializes a openmm.unit.Quantity from a string representation, for example: "kilocalories_per_mole / angstrom ** 2"
ensure_quantity	Given a quantity that could be of a variety of types, attempt to coerce into a given type.

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.

Examples

```
>>> from openff.units import Quantity as OpenFFQuantity
>>> from openff.units.openmm import from_openmm
>>> from openmm import unit
>>> length = unit.Quantity(9.0, unit.angstrom)
>>> from_openmm(length)
<Quantity(9.0, 'angstrom')>
>>> assert isinstance(from_openmm(length), OpenFFQuantity)
```

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.

Examples

```
>>> from openff.units import unit
>>> from openff.units.openmm import to_openmm
>>> from openmm import unit as openmm_unit
>>> length = unit.Quantity(9.0, unit.angstrom)
>>> to_openmm(length)
Quantity(value=9.0, unit=angstrom)
>>> assert isinstance(to_openmm(length), openmm_unit.Quantity)
```

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]

Given a quantity that could be of a variety of types, attempt to coerce into a given type.

Examples

```
>>> import numpy
>>> from openmm import unit as openmm_unit
>>> from openff.units import unit
>>> from openff.units.openmm import ensure_quantity
>>> # Create a 9 Angstrom quantity with each registry
>>> length1 = unit.Quantity(9.0, unit.angstrom)
>>> length2 = openmm_unit.Quantity(9.0, openmm_unit.angstrom)
>>> # Similar quantities are be coerced into requested type
>>> assert type(ensure_quantity(length1, "openmm")) == openmm_unit.Quantity
>>> assert type(ensure_quantity(length2, "openff")) == unit.Quantity
```

(continues on next page)

(continued from previous page)

```
>>> # Seemingly-redundant "conversions" short-circuit
>>> assert ensure_quantity(length1, "openff") == ensure_quantity(length2, "openff")
>>> assert ensure_quantity(length1, "openmm") == ensure_quantity(length2, "openmm")
>>> # NumPy arrays and some primitives are automatically up-converted to `Quantity`␣
↪objects
>>> # Note that their units are set to "dimensionless"
>>> ensure_quantity(numpy.array([1, 2]), "openff")
<Quantity([1 2], 'dimensionless')>
>>> ensure_quantity(4.0, "openmm")
Quantity(value=4.0, unit=dimensionless)
```

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

PYTHON MODULE INDEX

O

INDEX

P

Q

R

S

T

U

V