OpenSCM-Units Documentation

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DOCUMENTATION

1	Installation	3				
2	Usage					
3	Development3.1Contributing3.2Getting setup3.3Formatting3.4Buiding the docs3.5Releasing3.6Why is there a Makefile in a pure Python repository?	7 8 9 10 11				
4	Unit Registry API	13				
5	Data API 5.1 Mixtures API	23 23				
6	Changelog 6.1 master 6.2 v0.3.0 6.3 v0.2.0 6.4 v0.1.4 6.5 v0.1.3 6.6 v0.1.2 6.7 v0.1.1 6.8 v0.1.0	25 25 25 25 26 26 26 26				
7	Index	27				
Ру	Python Module Index					
In	Index					

OpenSCM-Units is a repository for handling of units related to simple climate modelling. OpenSCM-Units is free software under a BSD 3-Clause License, see LICENSE.

ONE

INSTALLATION

OpenSCM-Runner can be installed with pip

pip install openscm-units

If you also want to run the example notebooks install additional dependencies using

pip install openscm-units[notebooks]

OpenSCM-Units can also be installed with conda

conda install -c conda-forge openscm-units

TWO

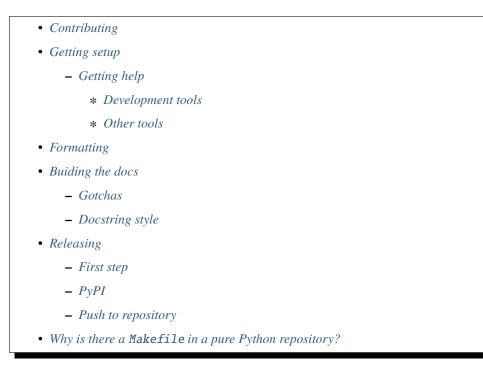
USAGE

All of our usage examples are included in openscm-units/notebooks.

THREE

DEVELOPMENT

If you're interested in contributing to OpenSCM-Units, we'd love to have you on board! This section of the docs will (once we've written it) detail how to get setup to contribute and how best to communicate.



3.1 Contributing

All contributions are welcome, some possible suggestions include:

- tutorials (or support questions which, once solved, result in a new tutorial :D)
- blog posts
- improving the documentation
- bug reports
- feature requests
- pull requests

Please report issues or discuss feature requests in the OpenSCM-Units issue tracker. If your issue is a feature request or a bug, please use the templates available, otherwise, simply open a normal issue :)

As a contributor, please follow a couple of conventions:

- Create issues in the OpenSCM-Units issue tracker for changes and enhancements, this ensures that everyone in the community has a chance to comment
- Be welcoming to newcomers and encourage diverse new contributors from all backgrounds: see the Python Community Code of Conduct
- Only push to your own branches, this allows people to force push to their own branches as they need without fear or causing others headaches
- Start all pull requests as draft pull requests and only mark them as ready for review once they've been rebased onto master, this makes it much simpler for reviewers
- Try and make lots of small pull requests, this makes it easier for reviewers and faster for everyone as review time grows exponentially with the number of lines in a pull request

3.2 Getting setup

To get setup as a developer, we recommend the following steps (if any of these tools are unfamiliar, please see the resources we recommend in *Development tools*):

- 1. Install conda and make
- 2. Run make virtual-environment, if that fails you can try doing it manually
 - 1. Change your current directory to OpenSCM-Units's root directory (i.e. the one which contains README. rst), cd openscm-units
 - 2. Create a virtual environment to use with OpenSCM-Units python3 -m venv venv
 - 3. Activate your virtual environment source ./venv/bin/activate
 - 4. Upgrade pip pip intall --upgrade pip
 - 5. Install the development dependencies (very important, make sure your virtual environment is active before doing this) pip install -e .[dev]
- 3. Make sure the tests pass by running make test-all, if that fails the commands are
 - 1. Activate your virtual environment source ./venv/bin/activate
 - 2. Run the unit and integration tests pytest --cov -r a --cov-report term-missing
 - 3. Test the notebooks pytest -r a --nbval ./notebooks --sanitize ./notebooks/ tests_sanitize.cfg

3.2.1 Getting help

Whilst developing, unexpected things can go wrong (that's why it's called 'developing', if we knew what we were doing, it would already be 'developed'). Normally, the fastest way to solve an issue is to contact us via the issue tracker. The other option is to debug yourself. For this purpose, we provide a list of the tools we use during our development as starting points for your search to find what has gone wrong.

Development tools

This list of development tools is what we rely on to develop OpenSCM-Units reliably and reproducibly. It gives you a few starting points in case things do go inexplicably wrong and you want to work out why. We include links with each of these tools to starting points that we think are useful, in case you want to learn more.

- Git
- Make
- Conda virtual environments
- Pip and pip virtual environments
- Tests
 - we use a blend of pytest and the inbuilt Python testing capabilities for our tests so checkout what we've already done in tests to get a feel for how it works
- Continuous integration (CI) (also brief intro blog post and a longer read)
 - we use GitHub CI for our CI but there are a number of good providers
- Jupyter Notebooks
 - Jupyter is automatically included in your virtual environment if you follow our Getting setup instructions
- Sphinx

Other tools

We also use some other tools which aren't necessarily the most familiar. Here we provide a list of these along with useful resources.

- · Regular expressions
 - we use regex101.com to help us write and check our regular expressions, make sure the language is set to Python to make your life easy!

3.3 Formatting

To help us focus on what the code does, not how it looks, we use a couple of automatic formatting tools. These automatically format the code for us and tell use where the errors are. To use them, after setting yourself up (see *Getting setup*), simply run make format (and make format-notebooks to format notebook code). Note that make format can only be run if you have committed all your work i.e. your working directory is 'clean'. This restriction is made to ensure that you don't format code without being able to undo it, just in case something goes wrong.

3.4 Buiding the docs

After setting yourself up (see *Getting setup*), building the docs is as simple as running make docs (note, run make -B docs to force the docs to rebuild and ignore make when it says '... index.html is up to date'). This will build the docs for you. You can preview them by opening docs/build/html/index.html in a browser.

For documentation we use Sphinx. To get ourselves started with Sphinx, we started with this example then used Sphinx's getting started guide.

3.4.1 Gotchas

To get Sphinx to generate pdfs (rarely worth the hassle), you require Latexmk. On a Mac this can be installed with sudo tlmgr install latexmk. You will most likely also need to install some other packages (if you don't have the full distribution). You can check which package contains any missing files with tlmgr search --global --file [filename]. You can then install the packages with sudo tlmgr install [package].

3.4.2 Docstring style

For our docstrings we use numpy style docstrings. For more information on these, here is the full guide and the quick reference we also use.

3.5 Releasing

3.5.1 First step

- 1. Test installation with dependencies make test-install
- 2. Update CHANGELOG.rst
 - add a header for the new version between master and the latest bullet point
 - this should leave the section underneath the master header empty
- 3. git add .
- 4. git commit -m "Prepare for release of vX.Y.Z"
- 5. git tag vX.Y.Z
- 6. Test version updated as intended with make test-install

3.5.2 PyPI

If uploading to PyPI, do the following (otherwise skip these steps)

- 1. make publish-on-testpypi
- 2. Go to test PyPI and check that the new release is as intended. If it isn't, stop and debug.
- 3. Test the install with make test-testpypi-install (this doesn't test all the imports as most required packages are not on test PyPI).

Assuming test PyPI worked, now upload to the main repository

- 1. make publish-on-pypi
- 2. Go to OpenSCM-Units's PyPI and check that the new release is as intended.
- 3. Test the install with make test-pypi-install

3.5.3 Push to repository

Finally, push the tags and the repository state

- 1. git push
- 2. git push --tags

3.6 Why is there a Makefile in a pure Python repository?

Whilst it may not be standard practice, a Makefile is a simple way to automate general setup (environment setup in particular). Hence we have one here which basically acts as a notes file for how to do all those little jobs which we often forget e.g. setting up environments, running tests (and making sure we're in the right environment), building docs, setting up auxillary bits and pieces.

UNIT REGISTRY API

Unit handling makes use of the Pint library. This allows us to easily define units as well as contexts. Contexts allow us to perform conversions which would not normally be allowed e.g. in the 'AR4GWP100' context we can convert from CO2 to CH4 using the AR4GWP100 equivalence metric.

An illustration of how the unit_registry can be used is shown below:

More details on emissions units

Emissions are a flux composed of three parts: mass, the species being emitted and the time period e.g. "t CO2 / yr". As mass and time are part of SI units, all we need to define here are emissions units i.e. the stuff. Here we include as many of the canonical emissions units, and their conversions, as possible.

For emissions units, there are a few cases to be considered:

- fairly obvious ones e.g. carbon dioxide emissions can be provided in 'C' or 'CO2' and converting between the two is possible
- less obvious ones e.g. NOx emissions can be provided in 'N' or 'NOx' (a short-hand which is assumed to be NO2), we provide conversions between these two
- case-sensitivity. In order to provide a simplified interface, using all uppercase versions of any unit is also valid e.g. unit_registry("HFC4310mee") is the same as unit_registry("HFC4310MEE")
- hyphens and underscores in units. In order to be Pint compatible and to simplify things, we strip all hyphens and underscores from units.

As a convenience, we allow users to combine the mass and the type of emissions to make a 'joint unit' e.g. "tCO2". It should be recognised that this joint unit is a derived unit and not a base unit.

By defining these three separate components, it is much easier to track what conversions are valid and which are not. For example, as the emissions units are all defined as emissions units, and not as atomic masses, we are able to prevent

invalid conversions. If emissions units were simply atomic masses, it would be possible to convert between e.g. C and N2O which would be a problem. Conventions such as allowing carbon dioxide emissions to be reported in C or CO2, despite the fact that they are fundamentally different chemical species, is a convention which is particular to emissions (as far as we can tell).

Pint's contexts are particularly useful for emissions as they facilitate metric conversions. With a context, a conversion which wouldn't normally be allowed (e.g. $tCO2 \rightarrow tN2O$) is allowed and will use whatever metric conversion is appropriate for that context (e.g. AR4GWP100).

Finally, we discuss namespace collisions.

CH4

Methane emissions are defined as 'CH4'. In order to prevent inadvertent conversions of 'CH4' to e.g. 'CO2' via 'C', the conversion 'CH4' <-> 'C' is by default forbidden. However, it can be performed within the context 'CH4_conversions' as shown below:

```
>>> from openscm_units import unit_registry
>>> unit_registry("CH4").to("C")
pint.errors.DimensionalityError: Cannot convert from 'CH4' ([methane]) to 'C' ([carbon])
# with a context, the conversion becomes legal again
>>> with unit_registry.context("CH4_conversions"):
... unit_registry("CH4").to("C")
<Quantity(0.75, 'C')>
# as an unavoidable side effect, this also becomes possible
>>> with unit_registry.context("CH4_conversions"):
... unit_registry("CH4").to("C02")
<Quantity(2.75, 'C02')>
```

N20

Nitrous oxide emissions are typically reported with units of 'N2O'. However, they are also reported with units of 'N2ON' (a short-hand which indicates that only the mass of the nitrogen is being counted). Reporting nitrous oxide emissions with units of simply 'N' is ambiguous (do you mean the mass of nitrogen, so 1 N = 28 / 44 N2O or just the mass of a single N atom, so 1 N = 14 / 44 N2O). By default, converting 'N2O' <-> 'N' is forbidden to prevent this ambiguity. However, the conversion can be performed within the context 'N2O_conversions', in which case it is assumed that 'N' just means a single N atom i.e. 1 N = 14 / 44 N2O, as shown below:

NOx

Like for methane, NOx emissions also suffer from a namespace collision. In order to prevent inadvertent conversions from 'NOx' to e.g. 'N2O', the conversion 'NOx' \rightarrow 'N' is by default forbidden. It can be performed within the 'NOx_conversions' context:

```
>>> from openscm_units import unit_registry
>>> unit_registry("NOx").to("N")
pint.errors.DimensionalityError: Cannot convert from 'NOx' ([NOx]) to 'N' ([nitrogen])
# with a context, the conversion becomes legal again
>>> with unit_registry.context("NOx_conversions"):
... unit_registry("NOx").to("N")
<Quantity(0.30434782608695654, 'N')>
```

NH3

In order to prevent inadvertent conversions from 'NH3' to 'CO2', the conversion 'NH3' $\langle - \rangle$ 'N' is by default forbidden. It can be performed within the 'NH3_conversions' context analogous to the 'NOx_conversions' context:

```
>>> from openscm_units import unit_registry
>>> unit_registry("NH3").to("N")
pint.errors.DimensionalityError: Cannot convert from 'NH3' ([NH3]) to 'N' ([nitrogen])
# with a context, the conversion becomes legal again
>>> with unit_registry.context("NH3_conversions"):
... unit_registry("NH3").to("N")
<Quantity(0.823529412, 'N')>
```

```
class openscm_units._unit_registry.ScmUnitRegistry(*args, **kwargs)
Bases: pint.registry.UnitRegistry
```

Unit registry class.

Provides some convenience methods to add standard units and contexts with lazy loading from disk.

UnitsContainer(*args, **kwargs)

add_context(context: pint.context.Context) \rightarrow None

Add a context object to the registry.

The context will be accessible by its name and aliases.

Notice that this method will NOT enable the context; see enable_contexts().

add_standards()

Add standard units.

Has to be done separately because of pint's weird initializing.

auto_reduce_dimensions

Determines if dimensionality should be reduced on appropriate operations.

case_sensitive

Default unit case sensitivity

check(*args)

Decorator to for quantity type checking for function inputs.

Use it to ensure that the decorated function input parameters match the expected dimension of pint quantity.

The wrapper function raises:

• pint.DimensionalityError if an argument doesn't match the required dimensions.

ureg [UnitRegistry] a UnitRegistry instance.

args [str or UnitContainer or None] Dimensions of each of the input arguments. Use *None* to skip argument conversion.

Returns the wrapped function.

Return type callable

Raises

- **TypeError** If the number of given dimensions does not match the number of function parameters.
- ValueError If the any of the provided dimensions cannot be parsed as a dimension.

context(*names, **kwargs)

Used as a context manager, this function enables to activate a context which is removed after usage.

Parameters

- ***names** name(s) of the context(s).
- ****kwargs** keyword arguments for the contexts.

Examples

Context can be called by their name:

```
>>> import pint
>>> ureg = pint.UnitRegistry()
>>> ureg.add_context(pint.Context('one'))
>>> ureg.add_context(pint.Context('two'))
>>> with ureg.context('one'):
... pass
```

If a context has an argument, you can specify its value as a keyword argument:

```
>>> with ureg.context('one', n=1):
... pass
```

Multiple contexts can be entered in single call:

```
>>> with ureg.context('one', 'two', n=1):
... pass
```

Or nested allowing you to give different values to the same keyword argument:

```
>>> with ureg.context('one', n=1):
... with ureg.context('two', n=2):
... pass
```

A nested context inherits the defaults from the containing context:

```
>>> with ureg.context('one', n=1):
... # Here n takes the value of the outer context
... with ureg.context('two'):
... pass
```

convert(value, src, dst, inplace=False)

Convert value from some source to destination units.

Parameters

- value value
- **src** (*pint.Quantity or str*) source units.
- dst (pint.Quantity or str) destination units.
- **inplace** (Default value = False)

Returns converted value

Return type type

default_as_delta

When performing a multiplication of units, interpret non-multiplicative units as their *delta* counterparts.

property default_format

Default formatting string for quantities.

property default_system

define(definition)

Add unit to the registry.

Parameters definition (str or Definition) – a dimension, unit or prefix definition.

 $disable_contexts(n: Optional[int] = None) \rightarrow None$

Disable the last n enabled contexts.

Parameters n (int) – Number of contexts to disable. Default: disable all contexts.

enable_contexts(*names_or_contexts, **kwargs)

Overload pint's *enable_contexts()* to load contexts once (the first time they are used) to avoid (unnecessary) file operations on import.

fmt_locale = None

Babel.Locale instance or None

get_base_units(input_units, check_nonmult=True, system=None) Convert unit or dict of units to the base units.

If any unit is non multiplicative and check_converter is True, then None is returned as the multiplicative factor.

Unlike BaseRegistry, in this registry root_units might be different from base_units

Parameters

- input_units (UnitsContainer or str) units
- **check_nonmult** (*bool*) if True, None will be returned as the multiplicative factor if a non-multiplicative units is found in the final Units. (Default value = True)
- **system** (Default value = None)

Returns multiplicative factor, base units

Return type type

get_compatible_units(input_units, group_or_system=None)

get_dimensionality(input_units)

Convert unit or dict of units or dimensions to a dict of base dimensions dimensions

get_group(name, create_if_needed=True)
 Return a Group.

Parameters

- **name** (*str*) Name of the group to be
- **create_if_needed** (*boo1*) If True, create a group if not found. If False, raise an Exception. (Default value = True)

Returns Group

Return type type

get_name(name_or_alias, case_sensitive=None)
 Return the canonical name of a unit.

get_root_units(input_units, check_nonmult=True)

Convert unit or dict of units to the root units.

If any unit is non multiplicative and check_converter is True, then None is returned as the multiplicative factor.

Parameters

- input_units (UnitsContainer or str) units
- **check_nonmult** (*bool*) if True, None will be returned as the multiplicative factor if a non-multiplicative units is found in the final Units. (Default value = True)

Returns multiplicative factor, base units

Return type Number, pint.Unit

- get_symbol(name_or_alias, case_sensitive=None)
 Return the preferred alias for a unit.
- get_system(name, create_if_needed=True)
 Return a Group.

Parameters

- **name** (*str*) Name of the group to be
- **create_if_needed** (*bool*) If True, create a group if not found. If False, raise an Exception. (Default value = True)

Returns System

Return type type

Parameters

- **obj1** The objects to check against each other. Treated as dimensionless if not a Quantity, Unit or str.
- **obj2** The objects to check against each other. 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

Return type bool

load_definitions(file, is_resource=False)

Add units and prefixes defined in a definition text file.

Parameters

- **file** can be a filename or a line iterable.
- **is_resource** used to indicate that the file is a resource file and therefore should be loaded from the package. (Default value = False)

non_int_type

Numerical type used for non integer values.

parse_expression(input_string, case_sensitive=None, use_decimal=False, **values)

Parse a mathematical expression including units and return a quantity object.

Numerical constants can be specified as keyword arguments and will take precedence over the names defined in the registry.

Parameters

- input_string -
- **case_sensitive** (Default value = None, which uses registry setting)
- **use_decimal** (Default value = False)
- **values -
- parse_pattern(input_string, pattern, case_sensitive=None, use_decimal=False, many=False)
 Parse a string with a given regex pattern and returns result.

Parameters

- input_string -
- pattern_string The regex parse string
- **case_sensitive** (Default value = None, which uses registry setting)
- **use_decimal** (Default value = False)
- **many** Match many results (Default value = False)

parse_unit_name(unit_name, case_sensitive=None)

Parse a unit to identify prefix, unit name and suffix by walking the list of prefix and suffix. In case of equivalent combinations (e.g. ('kilo', 'gram', '') and ('', 'kilogram', ''), prefer those with prefix.

Parameters

- unit_name -
- **case_sensitive** (*bool or None*) Control if unit lookup is case sensitive. Defaults to None, which uses the registry's case_sensitive setting

Returns all non-equivalent combinations of (prefix, unit name, suffix)

Return type tuple of tuples (str, str, str)

parse_units(input_string, as_delta=None, case_sensitive=None)

Parse a units expression and returns a UnitContainer with the canonical names.

The expression can only contain products, ratios and powers of units.

Parameters

- input_string (str) -
- **as_delta** (*bool or None*) if the expression has multiple units, the parser will interpret non multiplicative units as their *delta_* counterparts. (Default value = None)
- **case_sensitive** (*bool or None*) Control if unit parsing is case sensitive. Defaults to None, which uses the registry's setting.

pi_theorem(quantities)

Builds dimensionless quantities using the Buckingham theorem

Parameters quantities (dict) - mapping between variable name and units

Returns a list of dimensionless quantities expressed as dicts

```
Return type list
```

```
remove_context(name_or_alias: str) \rightarrow pint.context.Context
Remove a context from the registry and return it.
```

Notice that this methods will not disable the context; see *disable_contexts()*.

set_fmt_locale(loc)

Change the locale used by default by *format_babel*.

Parameters loc (*str or None*) – None` (do not translate), 'sys' (detect the system locale) or a locale id string.

setup_matplotlib(enable=True)

Set up handlers for matplotlib's unit support.

Parameters enable (*bool*) – whether support should be enabled or disabled (Default value = True)

```
split_gas_mixture(quantity: pint.quantity.Quantity) \rightarrow list
```

Split a gas mixture into constituent gases.

Given a pint quantity with the units containing a gas mixture, returns a list of the constituents as pint quantities.

property sys

```
with_context(name, **kwargs)
```

Decorator to wrap a function call in a Pint context.

Use it to ensure that a certain context is active when calling a function:

```
:param name: name of the context.
:param \*\*kwargs: keyword arguments for the context
```

Returns the wrapped function.

Return type callable

Example

wraps(ret, args, strict=True)

Wraps a function to become pint-aware.

Use it when a function requires a numerical value but in some specific units. The wrapper function will take a pint quantity, convert to the units specified in *args* and then call the wrapped function with the resulting magnitude.

The value returned by the wrapped function will be converted to the units specified in ret.

Parameters

- **ureg** (*pint.UnitRegistry*) a UnitRegistry instance.
- **ret** (*str*, *pint*.*Unit*, *iterable* of *str*, *or iterable* of *pint*.*Unit*) Units of each of the return values. Use *None* to skip argument conversion.
- **args** (*str*, *pint*.*Unit*, *iterable* of *str*, *or iterable* of *pint*.*Unit*) Units of each of the input arguments. Use *None* to skip argument conversion.
- **strict** (*bool*) Indicates that only quantities are accepted. (Default value = True)

Returns the wrapper function.

Return type callable

Raises TypeError – if the number of given arguments does not match the number of function parameters. if the any of the provided arguments is not a unit a string or Quantity

```
openscm_units._unit_registry.unit_registry =
<openscm_units._unit_registry.ScmUnitRegistry object>
Standard unit registry
```

The unit registry contains all of the recognised units. Be careful, if you edit this registry in one place then it will also be edited in any other places that use openscm_units. If you want multiple, separate registries, create multiple instances of ScmUnitRegistry.

FIVE

DATA API

Data used within OpenSCM Units

For example, metric conversions and breakdownss of mixture substances into their constituents.

5.1 Mixtures API

openscm_units.data.mixtures.MIXTURES

Gas mixtures supported by OpenSCM Units

Last update: 2020-12-16

Each key is the mixture's name. Each value is itself a dictionary where each key is the name of a component of the mixture and the value is a list in which the first element is the standard composition, the second element is the positive composition tolerance and the third element is the negative composition tolerance. All values are given in mass percentage.

Sources:

- ANSI/ASHRAE Standard 34-2019, p. 9ff, ISSN 1041-2336, https://www.techstreet.com/ashrae/standards/ ashrae-15-2019-packaged-w-34-2019?product_id=2046531
- https://en.wikipedia.org/wiki/List_of_refrigerants (for common names)

Type dict

SIX

CHANGELOG

6.1 master

6.2 v0.3.0

- (#25) Add "N2O_conversions" context to remove ambiguity in N2O conversions
- (#23) Add AR5 GWPs with climate-carbon cycle feedbacks (closes #22)
- (#20) Make openscm_units.data a module by adding an __init__.py file to it and add docs for openscm_units.data (closes #19)
- (#18) Made NH3 a separate dimension to avoid accidental conversion to CO2 in GWP contexts. Also added an nh3_conversions context to convert to nitrogen (closes #12)
- (#16) Added refrigerant mixtures as units, including automatic GWP calculation from the GWP of their constituents. Also added the unit_registry.split_gas_mixtures function which can be used to split quantities containing a gas mixture into their constituents (closes #10)

6.3 v0.2.0

- (#15) Update CI so that it runs on pull requests from forks too
- (#14) Renamed openscm_units.unit_registry module to openscm_units._unit_registry to avoid name collision and lift ScmUnitRegistry to openscm_units.ScmUnitRegistry (closes #13)

6.4 v0.1.4

• (#7) Added C7F16, C8F18 and SO2F2 AR5GWP100 (closes #8)

6.5 v0.1.3

- (#7) Include metric conversions data in package
- (#6) Add conda install instructions

6.6 v0.1.2

- (#5) Update MANIFEST.in to ensure LICENSE, README.rst and CHANGELOG.rst are included in source distributions
- (#4) Update README and url to point to openscm organisation

6.7 v0.1.1

• (#2) Hotfix so that 'Tt' is terra tonne rather than 'tex'

6.8 v0.1.0

• (#1) Setup repository

SEVEN

INDEX

- genindex
- modindex
- search

PYTHON MODULE INDEX

0

openscm_units._unit_registry, 13
openscm_units.data, 23

INDEX

A

add_context()	(open-
scm_unitsunit_registry.ScmU	nitRegistry
method), 15	
add_standards()	(open-
scm_unitsunit_registry.ScmU	nitRegistry
method), 15	
auto_reduce_dimensions	(open-
scm_unitsunit_registry.ScmU	nitRegistry
attribute), 15	
0	

С

```
case_sensitive (open-
scm_units._unit_registry.ScmUnitRegistry
attribute), 15
check() (openscm_units._unit_registry.ScmUnitRegistry
method), 15
context() (openscm_units._unit_registry.ScmUnitRegistry
method), 16
convert() (openscm_units._unit_registry.ScmUnitRegistry
method), 16
```

D

```
default_as_delta
                                              (open-
         scm_units._unit_registry.ScmUnitRegistry
        attribute), 17
default format
                                              (open-
        scm_units._unit_registry.ScmUnitRegistry
        property), 17
default_system
                                              (open-
        scm_units._unit_registry.ScmUnitRegistry
        property), 17
define() (openscm_units._unit_registry.ScmUnitRegistry
        method), 17
disable_contexts()
                                              (open-
        scm_units._unit_registry.ScmUnitRegistry
        method), 17
Ε
enable_contexts()
                                              (open-
```

scm_units._unit_registry.ScmUnitRegistry

method), 17

F

```
fmt_locale(openscm_units._unit_registry.ScmUnitRegistry
         attribute), 17
G
get_base_units()
                                               (open-
         scm_units._unit_registry.ScmUnitRegistry
         method), 17
get_compatible_units()
                                               (open-
         scm units. unit registry.ScmUnitRegistry
         method), 17
get_dimensionality()
                                               (open-
         scm_units._unit_registry.ScmUnitRegistry
         method), 17
get_group() (openscm_units._unit_registry.ScmUnitRegistry
         method), 17
get_name() (openscm_units._unit_registry.ScmUnitRegistry
         method), 18
get_root_units()
                                               (open-
         scm_units._unit_registry.ScmUnitRegistry
         method), 18
get_symbol() (openscm_units._unit_registry.ScmUnitRegistry
         method), 18
get_system() (openscm_units._unit_registry.ScmUnitRegistry
         method), 18
I
```

is_compatible_with() (openscm_units._unit_registry.ScmUnitRegistry method), 18

-

load_definitions() (openscm_units._unit_registry.ScmUnitRegistry method), 19

Μ

MIXTURES (in module openscm_units.data.mixtures), 23
module
 openscm_units._unit_registry, 13
 openscm_units.data, 23

Ν		W	
<pre>non_int_type (openscm_unitsunit_registry.</pre>	ScmUnitReg	g <i>iatirt</i> yh_co	ntext() (open-
attribute), 19			scm_unitsunit_registry.ScmUnitRegistry
0		wraps()	<pre>method), 20 (openscm_unitsunit_registry.ScmUnitRegistry</pre>
<pre>openscm_unitsunit_registry module, 13</pre>			method), 21
openscm_units.data module,23			
Р			
<pre>parse_expression()</pre>	(open-		
scm_unitsunit_registry.ScmUnitReg method), 19	gistry		
parse_pattern()	(open-		
scm_unitsunit_registry.ScmUnitReg method), 19	gistry		
<pre>parse_unit_name()</pre>	(open-		
scm_unitsunit_registry.ScmUnitReg method), 19	gistry		
<pre>parse_units()</pre>	(open-		
scm_unitsunit_registry.ScmUnitReg method), 19	gistry		
<pre>pi_theorem() (openscm_unitsunit_registry.</pre>	.ScmUnitReg	gistry	
R			
remove_context()	(open-		
scm_unitsunit_registry.ScmUnitReg method), 20	gistry		
S			
ScmUnitRegistry (class in scm_unitsunit_registry), 15	open-		
<pre>set_fmt_locale()</pre>	(open-		
scm_unitsunit_registry.ScmUnitReg method), 20	· •		
<pre>setup_matplotlib()</pre>	(open-		
scm_unitsunit_registry.ScmUnitReg method), 20	gistry		
<pre>split_gas_mixture()</pre>	(open-		
scm_unitsunit_registry.ScmUnitReg method), 20	gistry		
sys (openscm_unitsunit_registry.ScmUn property), 20	nitRegistry		
U			
unit_registry (in module	open-		
<pre>scm_unitsunit_registry), 21</pre>	(-		
UnitsContainer() scm_unitsunit_registry.ScmUnitReg	(open- gistry		
method), 15			