
InterMol Documentation

Release 0.2a1

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Installation

1.1 Installation

1.1.1 Install with pip (coming soon!)

InterMol will be added to PyPI as soon as we get our first stable release up and running.

1.1.2 Install from source

```
$ git clone https://github.com/shirtsgroup/InterMol.git
$ cd InterMol
$ python setup.py install
```

Or if you plan on contributing something:

```
$ python setup.py develop
```

1.1.3 Dependencies

To use InterMol, the following libraries and software will need to be installed.

Linux, Mac OS X or Windows operating system We develop mainly on 64-bit Mac and CentOS machines. TravisCI is currently only set up to perform testing on Debian.

Python == 2.7 Once our unit tests flesh out a bit more, we intend to add support for ≥ 2.6 .

NumPy $\geq 1.6.0$ Numpy is the base package for numerical computing in python.

simtk.unit ≥ 0.1 Python unit classes for dimensional analysis and unit conversion.

2.1 Contributing

Contributions are welcome and they are greatly appreciated! Every little bit helps and credit will always be given.

2.1.1 Bug Reports

If you find a bug, please file a detailed issue [here](#) and **provide input files** so that we can try to reproduce the problem.

2.1.2 Code Style

PEP8 describes the style guide for python code. Please try to follow it when reasonable, in particular the naming conventions (e.g. public methods should use `lower_case_with_underscores` instead of `camelCase`).

Two helpful tools for checking your code are `flake8` and `pylint`. The latter is a lot pickier but generally, your code should pass most `flake8` tests:

```
$ pip install flake8 pylint
```

Also some IDE's like [PyCharm](#) will notify you of PEP8 violations as you code.

Note: Some older chunks of the code do not yet adhere to PEP8. If you find something easily fixable, please do so!

2.1.3 Running our tests

InterMol uses `py.test` for unit testing. To run them simply type run the following while in the base directory:

```
$ py.test
```

We need a LOT more tests so any help here is especially welcome!

To debug failing tests, you typically get a clearer output by running a subset of the tests, e.g.:

```
$ python test_gromacs.py --type unit
```

which prints out log files to `intermol/tests/unit_test_outputs/from_gromacs/[system name]/debug.log`. Re-running a single test is best done directly via the `convert.py` script, e.g.:

```
$ python convert.py --gro_in tests/gromacs/unit_tests/[system name]/[system name].{top,gro} --gromacs
```

Note: If you have any ideas or suggestions for streamlining the testing process please let us know by filing an issue or opening a pull request!

2.1.4 Git Flow

Because we are supporting multiple molecular dynamics engines that should all work independently, we try to keep development of each engine in a separate branch until the basics are working.

To this end, we've started working with the [git flow branching model](#). The basic things to know are:

1. The `master` branch is strictly used for releases.
2. The `develop` branch is where (!!!) development happens.
3. When we start working on a new engine, we create a feature branch. E.g., at the time of this writing, there are branches called `feature/lammps` and `feature/desmond`. Once the overall structure in this branch is fairly stable and has a good amounts of tests, we merge it into `develop`.

So what do you, the interested developer, need to know?

1. Don't make pull requests against `master`.
2. Choose either `develop` or the appropriate `feature/*` branch to pull against.

For more reading and a neat tool to help with branching see:

<http://jeffkreeftmeijer.com/2010/why-arent-you-using-git-flow/>

<https://github.com/nvie/gitflow>

<http://danielkummer.github.io/git-flow-cheatsheet/>

3.1 intermol package

3.1.1 Subpackages

intermol.forces package

Submodules

intermol.forces.abstract_2_virtual_type module

class `intermol.forces.abstract_2_virtual_type.Abstract2VirtualType` (*bondingtype1, bondingtype2, bondingtype3*)

Bases: `intermol.forces.abstract_type.AbstractType`

bondingtype1

bondingtype2

placeholder

intermol.forces.abstract_3_virtual_type module

class `intermol.forces.abstract_3_virtual_type.Abstract3VirtualType` (*bondingtype1, bondingtype2, bondingtype3, bondingtype4*)

Bases: `intermol.forces.abstract_type.AbstractType`

bondingtype1

bondingtype2

bondingtype3

bondingtype4

placeholder

intermol.forces.abstract_4_virtual_type module

class `intermol.forces.abstract_4_virtual_type.Abstract4VirtualType` (*bondingtype1, bondingtype2, bondingtype3, bondingtype4, bondingtype5*)

Bases: `intermol.forces.abstract_type.AbstractType`

bondingtype1

bondingtype2

bondingtype3

bondingtype4

intermol.forces.abstract_angle_type module

class `intermol.forces.abstract_angle_type.AbstractAngleType` (*bondingtype1, bondingtype2, bondingtype3, c=False*)

Bases: `intermol.forces.abstract_type.AbstractType`

bondingtype1

bondingtype2

bondingtype3

c

intermol.forces.abstract_atom_type module

class `intermol.forces.abstract_atom_type.AbstractAtomType` (*atomtype, bondtype=None, atomic_number=None, mass=None, charge=None, ptype=None*)

Bases: `intermol.forces.abstract_type.AbstractType`

atomic_number

atomtype

bondtype

charge

mass

ptype

intermol.forces.abstract_bond_type module

class `intermol.forces.abstract_bond_type.AbstractBondType` (*bondingtype1, bondingtype2, order=1, c=False*)

Bases: `intermol.forces.abstract_type.AbstractType`

bondingtype1

bondingtype2

c

order

intermol.forces.abstract_dihedral_type module

```
class intermol.forces.abstract_dihedral_type.AbstractDihedralType (bondingtype1,
                                                                    bondingtype2,
                                                                    bondingtype3,
                                                                    bonding-
                                                                    type4, im-
                                                                    proper=False)
```

Bases: `intermol.forces.abstract_type.AbstractType`

bondingtype1

bondingtype2

bondingtype3

bondingtype4

improper

intermol.forces.abstract_nonbonded_type module

```
class intermol.forces.abstract_nonbonded_type.AbstractNonbondedType (atom1,
                                                                    atom2,
                                                                    type)
```

Bases: `intermol.forces.abstract_type.AbstractType`

atom1

atom2

type

intermol.forces.abstract_pair_type module

```
class intermol.forces.abstract_pair_type.AbstractPairType (bondingtype1, bonding-
                                                                    type2, scaleLJ=None,
                                                                    scaleQQ=None,
                                                                    long=False)
```

Bases: `intermol.forces.abstract_type.AbstractType`

bondingtype1

bondingtype2

long

scaleLJ

scaleQQ

intermol.forces.abstract_type module

```
class intermol.forces.abstract_type.AbstractType
```

Bases: `object`

```
__repr__ ()
```

Print the object and all of its non-magic attributes.

intermol.forces.atom_c_type module

class `intermol.forces.atom_c_type.AtomCType` (**args, **kws*)
Bases: `intermol.forces.abstract_atom_type.AbstractAtomType`

intermol.forces.atom_sigeps_type module

class `intermol.forces.atom_sigeps_type.AtomSigepsType` (**args, **kws*)
Bases: `intermol.forces.abstract_atom_type.AbstractAtomType`

intermol.forces.buckingham_nonbonded_type module

class `intermol.forces.buckingham_nonbonded_type.BuckinghamNonbonded` (*atom1, atom2, bonding-type1=None, bonding-type2=None, a=Quantity(value=0.0, unit=kilojoule/mole), b=Quantity(value=0.0, unit=nanometer), C6=Quantity(value=0.0, unit=nanometer**6*kilojoule/mole), type=False*)
Bases: `intermol.forces.buckingham_nonbonded_type.BuckinghamNonbondedType`

stub documentation

class `intermol.forces.buckingham_nonbonded_type.BuckinghamNonbondedType` (**args, **kws*)
Bases: `intermol.forces.abstract_nonbonded_type.AbstractNonbondedType`

C6

a

b

type

intermol.forces.connection_bond_type module

class `intermol.forces.connection_bond_type.ConnectionBond` (*atom1, atom2, bonding-type1=None, bonding-type2=None, order=1, c=False*)
Bases: `intermol.forces.connection_bond_type.ConnectionBondType`

stub documentation

class `intermol.forces.connection_bond_type.ConnectionBondType` (**args, **kws*)
Bases: `intermol.forces.abstract_bond_type.AbstractBondType`

c

order

intermol.forces.convert_dihedrals module

`intermol.forces.convert_dihedrals.convert_dihedral_from_OPLS_to_RB` (*f*)

`intermol.forces.convert_dihedrals.convert_dihedral_from_RB_to_OPLS` (*c*)

`intermol.forces.convert_dihedrals.convert_dihedral_from_RB_to_trig` (*c*)

```

intermol.forces.convert_dihedrals.convert_dihedral_from_fourier_to_trig (f)
intermol.forces.convert_dihedrals.convert_dihedral_from_proper_to_trig (p)
intermol.forces.convert_dihedrals.convert_dihedral_from_trig_to_RB (fcs)
intermol.forces.convert_dihedrals.convert_dihedral_from_trig_to_fourier (fcs)
intermol.forces.convert_dihedrals.convert_dihedral_from_trig_to_proper (fcs,
                                                                    con-
                                                                    ven-
                                                                    tion='0')

intermol.forces.convert_dihedrals.convert_nothing (x)
    useful utility for not converting anything

```

intermol.forces.cosine_angle_type module

```

class intermol.forces.cosine_angle_type.CosineAngle (atom1, atom2, atom3, bond-
                                                    ingtype1=None, bonding-
                                                    type2=None, bondingtype3=None,
                                                    k=Quantity(value=0.0,
                                                    unit=kilojoule/mole), c=False)

    Bases: intermol.forces.cosine_angle_type.CosineAngleType

```

http://lammps.sandia.gov/doc/angle_cosine.html

```

class intermol.forces.cosine_angle_type.CosineAngleType (*args, **kwds)
    Bases: intermol.forces.abstract_angle_type.AbstractAngleType

```

c

k

intermol.forces.cosine_squared_angle_type module

```

class intermol.forces.cosine_squared_angle_type.CosineSquaredAngle (atom1,
                                                                    atom2,
                                                                    atom3,
                                                                    bonding-
                                                                    type1=None,
                                                                    bonding-
                                                                    type2=None,
                                                                    bonding-
                                                                    type3=None,
                                                                    theta=Quantity(value=0.0,
                                                                    unit=degree),
                                                                    k=Quantity(value=0.0,
                                                                    unit=kilojoule/mole),
                                                                    c=False)

    Bases: intermol.forces.cosine_squared_angle_type.CosineSquaredAngleType

```

stub documentation

```

class intermol.forces.cosine_squared_angle_type.CosineSquaredAngleType (*args,
                                                                    **kwds)

    Bases: intermol.forces.abstract_angle_type.AbstractAngleType

```

c

k

theta

intermol.forces.cross_bond_angle_angle_type module

```
class intermol.forces.cross_bond_angle_angle_type.CrossBondAngleAngle (atom1,  
                                                                    atom2,  
                                                                    atom3,  
                                                                    bonding-  
                                                                    type1=None,  
                                                                    bonding-  
                                                                    type2=None,  
                                                                    bonding-  
                                                                    type3=None,  
                                                                    r1=Quantity(value=0.0,  
                                                                    unit=nanometer),  
                                                                    r2=Quantity(value=0.0,  
                                                                    unit=nanometer),  
                                                                    r3=Quantity(value=0.0,  
                                                                    unit=nanometer),  
                                                                    k=Quantity(value=0.0,  
                                                                    unit=kilojoule/(nanometer**2*mole),  
                                                                    c=False)
```

Bases: `intermol.forces.cross_bond_angle_angle_type.CrossBondAngleAngleType`

stub documentation

```
class intermol.forces.cross_bond_angle_angle_type.CrossBondAngleAngleType (*args,  
                                                                    **kwargs)
```

Bases: `intermol.forces.abstract_angle_type.AbstractAngleType`

c

k

r1

r2

r3

intermol.forces.cross_bond_bond_angle_type module

```
class intermol.forces.cross_bond_bond_angle_type.CrossBondBondAngle (atom1,  
                                                                    atom2,  
                                                                    atom3,  
                                                                    bonding-  
                                                                    type1=None,  
                                                                    bonding-  
                                                                    type2=None,  
                                                                    bonding-  
                                                                    type3=None,  
                                                                    r1=Quantity(value=0.0,  
                                                                    unit=nanometer),  
                                                                    r2=Quantity(value=0.0,  
                                                                    unit=nanometer),  
                                                                    k=Quantity(value=0.0,  
                                                                    unit=kilojoule/(nanometer**2*mole),  
                                                                    c=False)
```

Bases: `intermol.forces.cross_bond_bond_angle_type.CrossBondBondAngleType`

stub documentation

```

class intermol.forces.cross_bond_bond_angle_type.CrossBondBondAngleType (*args,
                                                                    **kwds)
    Bases: intermol.forces.abstract_angle_type.AbstractAngleType
    c
    k
    r1
    r2

```

intermol.forces.cubic_bond_type module

```

class intermol.forces.cubic_bond_type.CubicBond (atom1,          atom2,          bonding-
                                                    type1=None,          bondingtype2=None,
                                                    length=Quantity(value=0.0,
                                                            unit=nanometer),
                                                    C2=Quantity(value=0.0,
                                                       unit=kilojoule/(nanometer**2*mole)),
                                                    C3=Quantity(value=0.0,
                                                       unit=kilojoule/(nanometer**3*mole)),
                                                    order=1, c=False)
    Bases: intermol.forces.cubic_bond_type.CubicBondType

```

stub documentation

```

class intermol.forces.cubic_bond_type.CubicBondType (*args, **kwds)
    Bases: intermol.forces.abstract_bond_type.AbstractBondType
    C2
    C3
    c
    length
    order

```

intermol.forces.fene_bond_type module

```

class intermol.forces.fene_bond_type.FeneBond (atom1, atom2, bondingtype1=None, bond-
                                                    ingtype2=None, length=Quantity(value=0.0,
                                                            unit=nanometer), kb=Quantity(value=0.0,
                                                            unit=kilojoule/(nanometer**2*mole)),
                                                    order=1, c=False)
    Bases: intermol.forces.fene_bond_type.FeneBondType

```

stub documentation

```

class intermol.forces.fene_bond_type.FeneBondType (*args, **kwds)
    Bases: intermol.forces.abstract_bond_type.AbstractBondType
    c
    kb
    length
    order

```

intermol.forces.fene_expandable_bond_type module

```
class intermol.forces.fene_expandable_bond_type.FeneExpandableBond (atom1,  
atom2,  
bonding-  
type1=None,  
bonding-  
type2=None,  
k=Quantity(value=0.0,  
unit=kilojoule/(nanometer**2*mole)),  
length=Quantity(value=0.0,  
unit=nanometer),  
ep-  
silon=Quantity(value=0.0,  
unit=kilojoule/mole),  
sigma=Quantity(value=0.0,  
unit=nanometer),  
delta=Quantity(value=0.0,  
unit=nanometer),  
order=1,  
c=False)
```

Bases: `intermol.forces.fene_expandable_bond_type.FeneExpandableBondType`

stub documentation

```
class intermol.forces.fene_expandable_bond_type.FeneExpandableBondType (*args,  
**kwds)
```

Bases: `intermol.forces.abstract_bond_type.AbstractBondType`

c

delta

epsilon

k

length

order

sigma

intermol.forces.forcedata module**intermol.forces.forcefunctions module**

```
intermol.forces.forcefunctions.build_paramlist (program)
```

Create a paramlist specific for a given program.

```
intermol.forces.forcefunctions.build_unitvars (program, paramlist, dumself=None)
```

Takes a string program name (one of the supported programs), and a 'self' object it looks like the keyword is not being used, but it is used in the line eval(unit). The test name 'dumself' needs to match what is in the force data arrays. Currently only used for lammmps.

```
intermol.forces.forcefunctions.capifyname (forcename)
```

Return name of the class in camelCase.

```
intermol.forces.forcefunctions.create_kwd_dict (unitvars, paramlist, force_type_object,  
values, optvalues=None)
```



```
intermol.forces.forcefunctions.create_kwds_from_entries(unitvars, paramlist, entries, force_type, offset=0)
```

Create a keyword dictionary given an array of information from a file format

requires the master set of units, the master set of parameter lists, an object (either a force_class or force_type), the list of information to be converted into a keyword, and an offset.

Parameters *offset* (*int*) – how far over from the first entry we translate

```
intermol.forces.forcefunctions.get_parameter_kwds_from_force(force, forceparams, paramlist)
```

```
intermol.forces.forcefunctions.get_parameter_list_from_force(force, paramlist)
```

Create a function that returns the parameters of a function type.

First, we need make some additions to the parameter list dictionary, which we do once when the forcedata script is imported. Useful to put the forces here as well. We won't make this a function for now since it's needed in this module.

```
intermol.forces.forcefunctions.get_parameter_list_from_kwds(force, kwds, paramlist)
```

```
intermol.forces.forcefunctions.optforceparams(force_type, forcetype_object=None)
```

Return the dictionary of optional parameters of an abstract force type.

If no object is given, we fill with blanks.

```
intermol.forces.forcefunctions.optparamkeylookup(force_type)
```

Given a force_type object, determine the key associated with the optional parameters.

```
intermol.forces.forcefunctions.optparamlookup(force_type_object, object_default=False)
```

A wrapper for optforceparams that takes a force_type object and returns the optional parameter dictionary.

```
intermol.forces.forcefunctions.specify(program_units, unitset, dumself=None, shouldEval=True)
```

Takes the dict of units, and a set of dimensions and replaces the dimensions with the appropriate units.

intermol.forces.four_fdn_virtual_type module

```
class intermol.forces.four_fdn_virtual_type.FourFdnVirtual(atom1, atom2, atom3, atom4, atom5, bondingtype1=None, bondingtype2=None, bondingtype3=None, bondingtype4=None, bondingtype5=None, a=Quantity(value=0.0, unit=dimensionless), b=Quantity(value=0.0, unit=dimensionless), c=Quantity(value=0.0, unit=nanometer), placeholder=False)
```

Bases: `intermol.forces.four_fdn_virtual_type.FourFdnVirtualType`

stub documentation

```
class intermol.forces.four_fdn_virtual_type.FourFdnVirtualType(*args, **kwargs)
```

Bases: `intermol.forces.abstract_4_virtual_type.Abstract4VirtualType`

a

b

c

placeholder

intermol.forces.fourier_dihedral_type module

```
class intermol.forces.fourier_dihedral_type.FourierDihedral (atom1, atom2, atom3,
                                                            atom4,          bonding-
                                                            type1=None,    bond-
                                                            ingtype2=None,
                                                            bondingtype3=None,
                                                            bondingtype4=None,
                                                            c1=Quantity(value=0.0,
                                                            unit=kilojoule/mole),
                                                            c2=Quantity(value=0.0,
                                                            unit=kilojoule/mole),
                                                            c3=Quantity(value=0.0,
                                                            unit=kilojoule/mole),
                                                            c4=Quantity(value=0.0,
                                                            unit=kilojoule/mole),
                                                            c5=Quantity(value=0.0,
                                                            unit=kilojoule/mole),
                                                            improper=False)
```

Bases: `intermol.forces.fourier_dihedral_type.FourierDihedralType`

stub documentation

```
class intermol.forces.fourier_dihedral_type.FourierDihedralType (*args, **kwds)
```

Bases: `intermol.forces.abstract_dihedral_type.AbstractDihedralType`

c1

c2

c3

c4

c5

improper

intermol.forces.g96_bond_type module

```
class intermol.forces.g96_bond_type.G96Bond (atom1, atom2, bondingtype1=None, bond-
                                                            ingtype2=None,   length=Quantity(value=0.0,
                                                            unit=nanometer),    k=Quantity(value=0.0,
                                                            unit=kilojoule/(nanometer**4*mole)), order=1,
                                                            c=False)
```

Bases: `intermol.forces.g96_bond_type.G96BondType`

stub documentation

```
class intermol.forces.g96_bond_type.G96BondType (*args, **kwds)
```

Bases: `intermol.forces.abstract_bond_type.AbstractBondType`

c

k

length

order

intermol.forces.harmonic_angle_type module

```
class intermol.forces.harmonic_angle_type.HarmonicAngle (atom1, atom2, atom3,
                                                         bondingtype1=None,
                                                         bondingtype2=None,
                                                         bondingtype3=None,
                                                         theta=Quantity(value=0.0,
                                                         unit=degree),
                                                         k=Quantity(value=0.0,
                                                         unit=kilojoule/(mole*radian**2)),
                                                         c=False)
```

Bases: `intermol.forces.harmonic_angle_type.HarmonicAngleType`

stub documentation

```
class intermol.forces.harmonic_angle_type.HarmonicAngleType (*args, **kwds)
```

Bases: `intermol.forces.abstract_angle_type.AbstractAngleType`

c

k

theta

intermol.forces.harmonic_bond_type module

```
class intermol.forces.harmonic_bond_type.HarmonicBond (atom1, atom2, bond-
                                                         ingtype1=None, bond-
                                                         ingtype2=None,
                                                         length=Quantity(value=0.0,
                                                         unit=nanometer),
                                                         k=Quantity(value=0.0,
                                                         unit=kilojoule/(nanometer**2*mole)),
                                                         order=1, c=False)
```

Bases: `intermol.forces.harmonic_bond_type.HarmonicBondType`

stub documentation

```
class intermol.forces.harmonic_bond_type.HarmonicBondType (*args, **kwds)
```

Bases: `intermol.forces.abstract_bond_type.AbstractBondType`

c

k

length

order

intermol.forces.harmonic_potential_bond_type module

```
class intermol.forces.harmonic_potential_bond_type.HarmonicPotentialBond (atom1,  
                                                                    atom2,  
                                                                    bond-  
                                                                    ing-  
                                                                    type1=None,  
                                                                    bond-  
                                                                    ing-  
                                                                    type2=None,  
                                                                    length=Quantity(value=0.0,  
                                                                    unit=nanometer),  
                                                                    k=Quantity(value=0.0,  
                                                                    unit=kilojoule/(nanometer**2,  
                                                                    or-  
                                                                    der=1,  
                                                                    c=False))
```

```
    Bases: intermol.forces.harmonic_potential_bond_type.HarmonicPotentialBondType
```

```
    stub documentation
```

```
class intermol.forces.harmonic_potential_bond_type.HarmonicPotentialBondType (*args,  
                                                                    **kwds)
```

```
    Bases: intermol.forces.abstract_bond_type.AbstractBondType
```

```
    c
```

```
    k
```

```
    length
```

```
    order
```

intermol.forces.improper_harmonic_dihedral_type module

```
class intermol.forces.improper_harmonic_dihedral_type.ImproperHarmonicDihedral (atom1,  
                                                                    atom2,  
                                                                    atom3,  
                                                                    atom4,  
                                                                    bond-  
                                                                    ing-  
                                                                    type1=None,  
                                                                    bond-  
                                                                    ing-  
                                                                    type2=None,  
                                                                    bond-  
                                                                    ing-  
                                                                    type3=None,  
                                                                    bond-  
                                                                    ing-  
                                                                    type4=None,  
                                                                    xi=Quantity(value=0,  
                                                                    unit=degree),  
                                                                    k=Quantity(value=0,  
                                                                    unit=kilojoule/(mole*degree**2,  
                                                                    im-  
                                                                    proper=False))
```

```
    Bases: intermol.forces.improper_harmonic_dihedral_type.ImproperHarmonicDihedralType
```

```
    stub documentation
```

```

class intermol.forces.improper_harmonic_dihedral_type.ImproperHarmonicDihedralType (*args,
                                                                                   **kwds)
    Bases: intermol.forces.abstract_dihedral_type.AbstractDihedralType
    improper
    k
    xi

```

intermol.forces.lj_c_nonbonded_type module

```

class intermol.forces.lj_c_nonbonded_type.LjCNonbonded (atom1, atom2, bondingtype1=None, bondingtype2=None,
                                                         C6=Quantity(value=0.0, unit=nanometer**6*kilojoule/mole),
                                                         C12=Quantity(value=0.0, unit=nanometer**12*kilojoule/mole),
                                                         type=False)
    Bases: intermol.forces.lj_c_nonbonded_type.LjCNonbondedType

```

stub documentation

```

class intermol.forces.lj_c_nonbonded_type.LjCNonbondedType (*args, **kwds)
    Bases: intermol.forces.abstract_nonbonded_type.AbstractNonbondedType
    C12
    C6
    type

```

intermol.forces.lj_c_pair_type module

```

class intermol.forces.lj_c_pair_type.LjCPair (atom1, atom2, bondingtype1=None, bondingtype2=None,
                                               C6=Quantity(value=0.0, unit=nanometer**6*kilojoule/mole),
                                               C12=Quantity(value=0.0, unit=nanometer**12*kilojoule/mole),
                                               scaleLJ=None, scaleQQ=None, long=False)
    Bases: intermol.forces.lj_c_pair_type.LjCPairType

```

stub documentation

```

class intermol.forces.lj_c_pair_type.LjCPairType (*args, **kwds)
    Bases: intermol.forces.abstract_pair_type.AbstractPairType
    C12
    C6
    long
    scaleLJ
    scaleQQ

```

intermol.forces.lj_default_pair_type module

```
class intermol.forces.lj_default_pair_type.LjDefaultPair(atom1, atom2, bonding-  
type1=None, bonding-  
type2=None, scaleLJ=None,  
scaleQQ=None,  
long=False)
```

Bases: `intermol.forces.lj_default_pair_type.LjDefaultPairType`

stub documentation

```
class intermol.forces.lj_default_pair_type.LjDefaultPairType(*args,**kwds)
```

Bases: `intermol.forces.abstract_pair_type.AbstractPairType`

long

scaleLJ

scaleQQ

intermol.forces.lj_sigeps_nonbonded_type module

```
class intermol.forces.lj_sigeps_nonbonded_type.LjSigepsNonbonded(atom1, atom2,  
bonding-  
type1=None,  
bonding-  
type2=None,  
sigma=Quantity(value=0.0,  
unit=nanometer),  
ep-  
silon=Quantity(value=0.0,  
unit=kilojoule/mole),  
type=False)
```

Bases: `intermol.forces.lj_sigeps_nonbonded_type.LjSigepsNonbondedType`

stub documentation

```
class intermol.forces.lj_sigeps_nonbonded_type.LjSigepsNonbondedType(*args,  
**kwds)
```

Bases: `intermol.forces.abstract_nonbonded_type.AbstractNonbondedType`

epsilon

sigma

type

intermol.forces.lj_sigeps_pair_type module

```
class intermol.forces.lj_sigeps_pair_type.LjSigepsPair(atom1, atom2, bond-  
ingtype1=None, bond-  
ingtype2=None,  
sigma=Quantity(value=0.0,  
unit=nanometer), ep-  
silon=Quantity(value=0.0,  
unit=kilojoule/mole),  
scaleLJ=None,  
scaleQQ=None, long=False)
```

Bases: `intermol.forces.lj_sigeps_pair_type.LjSigepsPairType`

stub documentation

```
class intermol.forces.lj_sigeps_pair_type.LjSigepsPairType(*args,**kwds)
```

Bases: `intermol.forces.abstract_pair_type.AbstractPairType`

epsilon

long
scaleLJ
scaleQQ
sigma

intermol.forces.ljq_c_pair_type module

```

class intermol.forces.ljq_c_pair_type.LjqCPair (atom1, atom2, bondingtype1=None, bondingtype2=None, qi=Quantity(value=0.0, unit=elementary charge), qj=Quantity(value=0.0, unit=elementary charge), C6=Quantity(value=0.0, unit=nanometer**6*kilojoule/mole), C12=Quantity(value=0.0, unit=nanometer**12*kilojoule/mole), scaleLJ=None, scaleQQ=None, long=False)

```

Bases: `intermol.forces.ljq_c_pair_type.LjqCPairType`

stub documentation

```

class intermol.forces.ljq_c_pair_type.LjqCPairType (*args, **kwds)
Bases: intermol.forces.abstract_pair_type.AbstractPairType

```

C12
C6
long
qi
qj
scaleLJ
scaleQQ

intermol.forces.ljq_default_pair_type module

```

class intermol.forces.ljq_default_pair_type.LjqDefaultPair (atom1, atom2, bondingtype1=None, bondingtype2=None, scaleLJ=None, scaleQQ=None, long=False)

```

Bases: `intermol.forces.ljq_default_pair_type.LjqDefaultPairType`

stub documentation

```

class intermol.forces.ljq_default_pair_type.LjqDefaultPairType (*args, **kwds)
Bases: intermol.forces.abstract_pair_type.AbstractPairType

```

long
scaleLJ
scaleQQ

intermol.forces.ljq_sigeps_pair_type module

```
class intermol.forces.ljq_sigeps_pair_type.LjqSigepsPair (atom1, atom2, bondingtype1=None, bondingtype2=None, qi=Quantity(value=0.0, unit=elementary charge), qj=Quantity(value=0.0, unit=elementary charge), sigma=Quantity(value=0.0, unit=nanometer), epsilon=Quantity(value=0.0, unit=kilojoule/mole), scaleLJ=None, scaleQQ=None, long=False)
```

Bases: `intermol.forces.ljq_sigeps_pair_type.LjqSigepsPairType`

stub documentation

```
class intermol.forces.ljq_sigeps_pair_type.LjqSigepsPairType (*args, **kwds)
```

Bases: `intermol.forces.abstract_pair_type.AbstractPairType`

epsilon

long

qi

qj

scaleLJ

scaleQQ

sigma

intermol.forces.make_forces module**intermol.forces.morse_bond_type module**

```
class intermol.forces.morse_bond_type.MorseBond (atom1, atom2, bondingtype1=None, bondingtype2=None, length=Quantity(value=0.0, unit=nanometer), D=Quantity(value=0.0, unit=kilojoule/mole), beta=Quantity(value=0.0, unit=nanometer), order=1, c=False)
```

Bases: `intermol.forces.morse_bond_type.MorseBondType`

stub documentation

```
class intermol.forces.morse_bond_type.MorseBondType (*args, **kwds)
```

Bases: `intermol.forces.abstract_bond_type.AbstractBondType`

D

beta

c

length

order

intermol.forces.nonlinear_bond_type module

```
class intermol.forces.nonlinear_bond_type.NonlinearBond (atom1, atom2, bond-
ingtype1=None, bond-
ingtype2=None, ep-
silon=Quantity(value=0.0,
unit=kilojoule/mole),
r0=Quantity(value=0.0,
unit=nanometer),
lamda=Quantity(value=0.0,
unit=nanometer), order=1,
c=False)
```

Bases: `intermol.forces.nonlinear_bond_type.NonlinearBondType`

http://lammps.sandia.gov/doc/bond_nonlinear.html

```
class intermol.forces.nonlinear_bond_type.NonlinearBondType (*args, **kwds)
```

Bases: `intermol.forces.abstract_bond_type.AbstractBondType`

c

epsilon

lamda

order

r0

intermol.forces.proper_periodic_dihedral_type module

```
class intermol.forces.proper_periodic_dihedral_type.ProperPeriodicDihedral (atom1,
atom2,
atom3,
atom4,
bond-
ing-
type1=None,
bond-
ing-
type2=None,
bond-
ing-
type3=None,
bond-
ing-
type4=None,
phi=Quantity(value=0.0,
unit=degree),
k=Quantity(value=0.0,
unit=kilojoule/mole),
mul-
ti-
plic-
ity=Quantity(value=0.0,
unit=dimensionless),
weight=Quantity(value=0
unit=dimensionless),
im-
proper=False)
```

Bases: `intermol.forces.proper_periodic_dihedral_type.ProperPeriodicDihedralType`
stub documentation

class `intermol.forces.proper_periodic_dihedral_type.ProperPeriodicDihedralType` (**args*,
***kws*)

Bases: `intermol.forces.abstract_dihedral_type.AbstractDihedralType`

improper

k

multiplicity

phi

weight

`intermol.forces.quartic_angle_type` module

class `intermol.forces.quartic_angle_type.QuarticAngle` (*atom1*, *atom2*, *atom3*,
bondingtype1=None,
bondingtype2=None,
bondingtype3=None,
theta=Quantity(value=0.0,
unit=degree),
C0=Quantity(value=0.0,
unit=kilojoule/mole),
C1=Quantity(value=0.0,
*unit=kilojoule/(mole*radian))*,
C2=Quantity(value=0.0,
*unit=kilojoule/(mole*radian**2))*,
C3=Quantity(value=0.0,
*unit=kilojoule/(mole*radian**3))*,
C4=Quantity(value=0.0,
*unit=kilojoule/(mole*radian**4))*,
c=False)

Bases: `intermol.forces.quartic_angle_type.QuarticAngleType`

stub documentation

class `intermol.forces.quartic_angle_type.QuarticAngleType` (**args*, ***kws*)

Bases: `intermol.forces.abstract_angle_type.AbstractAngleType`

C0

C1

C2

C3

C4

c

theta

`intermol.forces.quartic_bond_type` module

```
class intermol.forces.quartic_bond_type.QuarticBond (atom1, atom2, bonding-
    type1=None, bondingtype2=None,
    length=Quantity(value=0.0,
    unit=nanometer),
    C2=Quantity(value=0.0,
    unit=kilojoule/(nanometer**2*mole)),
    C3=Quantity(value=0.0,
    unit=kilojoule/(nanometer**3*mole)),
    C4=Quantity(value=0.0,
    unit=kilojoule/(nanometer**4*mole)),
    order=1, c=False)
```

Bases: `intermol.forces.quartic_bond_type.QuarticBondType`

stub documentation

```
class intermol.forces.quartic_bond_type.QuarticBondType (*args, **kws)
```

Bases: `intermol.forces.abstract_bond_type.AbstractBondType`

C2

C3

C4

c

length

order

intermol.forces.quartic_breakable_bond_type module

```
class intermol.forces.quartic_breakable_bond_type.QuarticBreakableBond (atom1,
    atom2,
    bond-
    ing-
    type1=None,
    bond-
    ing-
    type2=None,
    k=Quantity(value=0.0,
    unit=kilojoule/(nanometer**4*mole)),
    B1=Quantity(value=0.0,
    unit=nanometer),
    B2=Quantity(value=0.0,
    unit=nanometer),
    Rc=Quantity(value=0.0,
    unit=nanometer),
    U0=Quantity(value=0.0,
    unit=kilojoule/mole),
    or-
    der=1,
    c=False)
```

Bases: `intermol.forces.quartic_breakable_bond_type.QuarticBreakableBondType`

http://lammmps.sandia.gov/doc/bond_quartic.html

```
class intermol.forces.quartic_breakable_bond_type.QuarticBreakableBondType (*args,
    **kws)
```

Bases: `intermol.forces.abstract_bond_type.AbstractBondType`

B1

B2
Rc
U0
c
k
order

intermol.forces.rb_dihedral_type module

```
class intermol.forces.rb_dihedral_type.RbDihedral (atom1, atom2, atom3, atom4, bonding-
    type1=None,    bondingtype2=None,
    bondingtype3=None,    bonding-
    type4=None, C0=Quantity(value=0.0,
    unit=kilojoule/mole),
    C1=Quantity(value=0.0,
    unit=kilojoule/mole),
    C2=Quantity(value=0.0,
    unit=kilojoule/mole),
    C3=Quantity(value=0.0,
    unit=kilojoule/mole),
    C4=Quantity(value=0.0,
    unit=kilojoule/mole),
    C5=Quantity(value=0.0,
    unit=kilojoule/mole),
    C6=Quantity(value=0.0,
    unit=kilojoule/mole),
    proper=False)
    im-
Bases: intermol.forces.rb_dihedral_type.RbDihedralType
```

stub documentation

```
class intermol.forces.rb_dihedral_type.RbDihedralType (*args, **kwds)
    Bases: intermol.forces.abstract_dihedral_type.AbstractDihedralType
    C0
    C1
    C2
    C3
    C4
    C5
    C6
    improper
```

intermol.forces.settles module

```
class intermol.forces.settles.Settles (*args, **kwds)
    Bases: intermol.forces.abstract_type.AbstractType
```

intermol.forces.three_fad_virtual_type module

```
class intermol.forces.three_fad_virtual_type.ThreeFadVirtual (atom1, atom2, atom3,
                                                    atom4, bonding-
                                                    type1=None, bond-
                                                    ingtype2=None,
                                                    bondingtype3=None,
                                                    bondingtype4=None,
                                                    theta=Quantity(value=0.0,
                                                    unit=degree),
                                                    d=Quantity(value=0.0,
                                                    unit=nanometer),
                                                    placeholder=False)
```

Bases: `intermol.forces.three_fad_virtual_type.ThreeFadVirtualType`

stub documentation

```
class intermol.forces.three_fad_virtual_type.ThreeFadVirtualType (*args, **kws)
```

Bases: `intermol.forces.abstract_3_virtual_type.Abstract3VirtualType`

d

placeholder

theta

intermol.forces.three_fd_virtual_type module

```
class intermol.forces.three_fd_virtual_type.ThreeFdVirtual (atom1, atom2, atom3,
                                                    atom4, bonding-
                                                    type1=None, bond-
                                                    ingtype2=None,
                                                    bondingtype3=None,
                                                    bondingtype4=None,
                                                    a=Quantity(value=0.0,
                                                    unit=dimensionless),
                                                    d=Quantity(value=0.0,
                                                    unit=nanometer), place-
                                                    holder=False)
```

Bases: `intermol.forces.three_fd_virtual_type.ThreeFdVirtualType`

stub documentation

```
class intermol.forces.three_fd_virtual_type.ThreeFdVirtualType (*args, **kws)
```

Bases: `intermol.forces.abstract_3_virtual_type.Abstract3VirtualType`

a

d

placeholder

intermol.forces.three_linear_virtual_type module

```
class intermol.forces.three_linear_virtual_type.ThreeLinearVirtual (atom1,  
                                                                    atom2,  
                                                                    atom3,  
                                                                    atom4,  
                                                                    bonding-  
                                                                    type1=None,  
                                                                    bonding-  
                                                                    type2=None,  
                                                                    bonding-  
                                                                    type3=None,  
                                                                    bonding-  
                                                                    type4=None,  
                                                                    a=Quantity(value=0.0,  
                                                                    unit=dimensionless),  
                                                                    b=Quantity(value=0.0,  
                                                                    unit=dimensionless),  
                                                                    place-  
                                                                    holder=False)
```

```
    Bases: intermol.forces.three_linear_virtual_type.ThreeLinearVirtualType
```

```
    stub documentation
```

```
class intermol.forces.three_linear_virtual_type.ThreeLinearVirtualType (*args,  
                                                                    **kwds)
```

```
    Bases: intermol.forces.abstract_3_virtual_type.Abstract3VirtualType
```

```
    a
```

```
    b
```

```
    placeholder
```

intermol.forces.three_out_virtual_type module

```
class intermol.forces.three_out_virtual_type.ThreeOutVirtual (atom1, atom2, atom3,  
                                                                    atom4,      bonding-  
                                                                    type1=None,  bond-  
                                                                    ingtype2=None,  
                                                                    bondingtype3=None,  
                                                                    bondingtype4=None,  
                                                                    a=Quantity(value=0.0,  
                                                                    unit=dimensionless),  
                                                                    b=Quantity(value=0.0,  
                                                                    unit=dimensionless),  
                                                                    c=Quantity(value=0.0,  
                                                                    unit=/nanometer),  
                                                                    placeholder=False)
```

```
    Bases: intermol.forces.three_out_virtual_type.ThreeOutVirtualType
```

```
    stub documentation
```

```
class intermol.forces.three_out_virtual_type.ThreeOutVirtualType (*args, **kwds)
```

```
    Bases: intermol.forces.abstract_3_virtual_type.Abstract3VirtualType
```

```
    a
```

```
    b
```

```
    c
```

```
    placeholder
```

intermol.forces.trig_dihedral_type module

```
class intermol.forces.trig_dihedral_type.TrigDihedral (atom1,      atom2,      atom3,
                                                    atom4,      bondingtype1=None,
                                                    bondingtype2=None,
                                                    bondingtype3=None,
                                                    bondingtype4=None,
                                                    phi=Quantity(value=0.0,
                                                         unit=degree),
                                                    fc0=Quantity(value=0.0,
                                                         unit=kilojoule/mole),
                                                    fc1=Quantity(value=0.0,
                                                         unit=kilojoule/mole),
                                                    fc2=Quantity(value=0.0,
                                                         unit=kilojoule/mole),
                                                    fc3=Quantity(value=0.0,
                                                         unit=kilojoule/mole),
                                                    fc4=Quantity(value=0.0,
                                                         unit=kilojoule/mole),
                                                    fc5=Quantity(value=0.0,
                                                         unit=kilojoule/mole),
                                                    fc6=Quantity(value=0.0,
                                                         unit=kilojoule/mole),      im-
                                                    improper=False)
```

Bases: `intermol.forces.trig_dihedral_type.TrigDihedralType`

stub documentation

```
class intermol.forces.trig_dihedral_type.TrigDihedralType (*args, **kwds)
```

Bases: `intermol.forces.abstract_dihedral_type.AbstractDihedralType`

fc0

fc1

fc2

fc3

fc4

fc5

fc6

improper

phi

intermol.forces.two_virtual_type module

```
class intermol.forces.two_virtual_type.TwoVirtual (atom1,      atom2,      atom3,
                                                    bondingtype1=None,      bond-
                                                    bondingtype2=None,      bonding-
                                                    type3=None,      a=Quantity(value=0.0,
                                                         unit=dimensionless),      place-
                                                    holder=False)
```

Bases: `intermol.forces.two_virtual_type.TwoVirtualType`

stub documentation

```
class intermol.forces.two_virtual_type.TwoVirtualType (*args, **kwds)
```

Bases: `intermol.forces.abstract_2_virtual_type.Abstract2VirtualType`

a

placeholder

intermol.forces.urey_bradley_angle_type module

```
class intermol.forces.urey_bradley_angle_type.UreyBradleyAngle (atom1, atom2,  
atom3, bonding-  
type1=None, bond-  
ingtype2=None,  
bonding-  
type3=None,  
theta=Quantity(value=0.0,  
unit=degree),  
k=Quantity(value=0.0,  
unit=kilojoule/(mole*radian**2)),  
r=Quantity(value=0.0,  
unit=nanometer),  
kUB=Quantity(value=0.0,  
unit=kilojoule/(nanometer**2*mole)),  
c=False)
```

Bases: `intermol.forces.urey_bradley_angle_type.UreyBradleyAngleType`

stub documentation

```
class intermol.forces.urey_bradley_angle_type.UreyBradleyAngleType (*args,  
**kwds)
```

Bases: `intermol.forces.abstract_angle_type.AbstractAngleType`

c

k

kUB

r

theta

Module contents

intermol.gromacs package

Submodules

intermol.gromacs.grofile_parser module

```
class intermol.gromacs.grofile_parser.GromacsGroParser (gro_file)
```

Bases: `object`

GromacsGroParser reads and writes Gromacs .gro files

A .gro file also contains some topological information, such as elements and residue names, but not enough to construct a full Topology object. This information is recorded and stored in the object's public fields.

read()

write (*system*)

Write the system out in a Gromacs 4.6 format

Parameters *filename* (*str*) – the file to write out to

intermol.gromacs.gromacs_driver module

`intermol.gromacs.gromacs_driver.gromacs_energies` (*top=None, gro=None, mdp=None, gropath=None, grosuff=None, grompp_check=False*)
 gropath = path to gromacs binaries *grosuff* = suffix of gromacs binaries, usually “” or ‘_d’
`intermol.gromacs.gromacs_driver.read_file` (*top_in, gro_in, gropath*)
`intermol.gromacs.gromacs_driver.write_file` (*system, top_out, gro_out*)

intermol.gromacs.gromacs_parser module

class `intermol.gromacs.gromacs_parser.GromacsParser` (*top_file, gro_file, system=None, include_dir=None, defines=None*)

Bases: `object`

A class containing methods required to read in a Gromacs(4.5.4) Topology File

class TopMoleculeType

Bases: `object`

Inner class to store information about a molecule type.

`GromacsParser.canonical_angle` (*params, angle, direction='into'*)

Parameters

- **params** –
- **angle** –
- **direction** –

Returns:

`GromacsParser.canonical_bond` (*params, bond, direction='into'*)

Parameters

- **params** –
- **bond** –
- **direction** –

Returns:

`GromacsParser.canonical_dihedral` (*params, dihedral, direction='into'*)

We can fit everything into two types of dihedrals - `dihedral_trig`, and improper harmonic. Dihedral trig is of the form

$$fc0 + \sum_{i=1}^6 fci (\cos(nx-\phi))$$

Proper dihedrals can be stored easily in this form, since they have only 1 n. Improper dihedrals can as well (flag as improper). RB can be stored as well, assuming $\phi = 0$ or 180. Fourier can also be stored. A full dihedral trig can be decomposed into multiple proper dihedrals.

Will need to handle multiple dihedrals little differently in that we will need to add multiple 9 dihedrals together into a single `dihedral_trig`, as long as they have the same ϕ angle (seems to be always the case).

Parameters

- **params** –
- **dihedral** –
- **direction** –

Returns:

`GromacsParser.choose_parameter_kwds_from_forces` (*entries, n_atoms, force_type, gromacs_force*)

Extract a force's parameters into a keyword dictionary.

Parameters

- **entries** (*str*) – The *split()* line being parsed.
- **n_atoms** (*int*) – The number of atoms in the force.
- **force_type** – The type of the force.
- **gromacs_force** – The

Returns

kwds – The force's parameters, e.g.

```
{'length': Quantity(value=0.13, unit=nanometers), 'k': ...
}
```

Return type dict

`GromacsParser.create_angle` (*angle*)

`GromacsParser.create_atom` (*temp_atom*)

`GromacsParser.create_bond` (*bond*)

`GromacsParser.create_dihedral` (*dihedral*)

Create a dihedral object based on a [*dihedrals*] entry.

`GromacsParser.create_exclusion` (*exclusion*)

`GromacsParser.create_kwds_from_entries` (*entries, force_class, offset=0*)

`GromacsParser.create_molecule` (*top_moltype, mol_name*)

`GromacsParser.create_moleculetype` (*top_moltype, mol_name, mol_count*)

`GromacsParser.create_pair` (*pair*)

Create a pair force object based on a [*pairs*] entry

`GromacsParser.create_settle` (*settle*)

`GromacsParser.directive_before_moleculetype` ()

`GromacsParser.find_dihedralttype` (*bondingtypes, improper*)

Determine the type of dihedral interaction between four atoms.

`GromacsParser.find_forcetype` (*bondingtypes, types_of_kind*)

`GromacsParser.get_parameter_kwds_from_force` (*force*)

`GromacsParser.get_parameter_list_from_force` (*force*)

`GromacsParser.gromacs_angle_types` = {'1': <class 'intermol.forces.harmonic_angle_type.HarmonicAngleType'>

`GromacsParser.gromacs_angles` = {'1': <class 'intermol.forces.harmonic_angle_type.HarmonicAngle'>, '3': <class 'intermol.forces.harmonic_angle_type.HarmonicAngle'>

`GromacsParser.gromacs_bond_types` = {'1': <class 'intermol.forces.harmonic_bond_type.HarmonicBondType'>, '3': <class 'intermol.forces.harmonic_bond_type.HarmonicBondType'>

`GromacsParser.gromacs_bonds` = {'1': <class 'intermol.forces.harmonic_bond_type.HarmonicBond'>, '3': <class 'intermol.forces.harmonic_bond_type.HarmonicBond'>

`GromacsParser.gromacs_combination_rules` = {'1': 'Multiply-C6C12', '3': 'Multiply-Sigeps', '2': 'Lorentz-Berendsen'}

`GromacsParser.gromacs_dihedral_types` = {'Trig': <class 'intermol.forces.trig_dihedral_type.TrigDihedralType'>

GromacsParser.**process_line** (*top_file*, *line*)

Process one line from a file.

GromacsParser.**process_molecule** (*line*)

Process a line in the [molecules] category.

GromacsParser.**process_moleculetype** (*line*)

Process a line in the [moleculetypes] category.

GromacsParser.**process_nonbond_params** (*line*)

Process a line in the [nonbond_param] category.

GromacsParser.**process_pair** (*line*)

Process a line in the [pairs] category.

GromacsParser.**process_pairtype** (*line*)

Process a line in the [pairtypes] category.

GromacsParser.**process_settle** (*line*)

Process a line in the [settles] category.

GromacsParser.**read** ()

Returns system

GromacsParser.**too_few_fields** (*line*)

static GromacsParser.**type_parameters_are_unique** (*a*, *b*)

Check if two force types are unique.

Currently only tests TrigDihedralType and ImproperHarmonicDihedralType because these are the only two forcetypes that we currently allow to have multiple values for the same set of 4 atom bondingtypes.

GromacsParser.**unitvars** = {"QuarticBreakableBond": [Unit({BaseUnit(base_dim=BaseDimension("length"), name=

GromacsParser.**write** ()

Write this topology in GROMACS file format.

Parameters filename – the name of the file to write out to

GromacsParser.**write_angles** (*top*)

GromacsParser.**write_atoms** (*top*)

GromacsParser.**write_atomtypes** (*top*)

GromacsParser.**write_bonds** (*top*)

GromacsParser.**write_defaults** (*top*)

GromacsParser.**write_dihedrals** (*top*)

GromacsParser.**write_exclusions** (*top*)

GromacsParser.**write_molecules** (*top*)

GromacsParser.**write_moleculetypes** (*top*)

GromacsParser.**write_nonbonded_types** (*top*)

GromacsParser.**write_pairs** (*top*)

GromacsParser.**write_settles** (*top*)

GromacsParser.**write_system** (*top*)

```
intermol.gromacs.gromacs_parser.default_gromacs_include_dir()
```

Find the location where gromacs #include files are referenced from, by searching for (1) gromacs environment variables, (2) just using the default gromacs install location, /usr/local/gromacs/share/gromacs/top.

```
intermol.gromacs.gromacs_parser.load_gromacs(top_file, gro_file, include_dir=None, defines=None)
```

Load a set of GROMACS input files into a *System*.

Parameters

- **top_file** –
- **gro_file** –
- **include_dir** –
- **defines** –

Returns

Return type system

```
intermol.gromacs.gromacs_parser.write_gromacs(top_file, gro_file, system)
```

Load a set of GROMACS input files into a *System*.

Parameters

- **top_file** –
- **gro_file** –
- **include_dir** –
- **defines** –

Returns

Return type system

Module contents

intermol.lammps package

Submodules

intermol.lammps.lammps_driver module

```
intermol.lammps.lammps_driver.lammps_energies(input_file, lmppath='lmp_openmpi')
```

Evaluate energies of LAMMPS files

Parameters

- **= path to input file (expects data file in same folder) (input_file)** –
- **= path to LAMMPS binaries (lmppath)** –

```
intermol.lammps.lammps_driver.read_file(in_file)
```

```
intermol.lammps.lammps_driver.write_file(in_file, system, unit_set='real')
```

intermol.lammps.lammps_parser module

```
class intermol.lammps.lammps_parser.LammpsParser(in_file, system=None, unit_set='real')
```

Bases: object

A class containing methods to read and write LAMMPS files.

parse_bonds (*data_lines*)

parse_boundary (*line*)

parse_box (*line, dim*)

Read box information from data file.

Parameters

- **line** (*str*) – Current line in input file.
- **dim** (*int*) – Dimension specified in line.

parse_dihedral_coeffs (*data_lines*)

parse_dihedral_style (*line*)

parse_dihedrals (*data_lines*)

parse_dimension (*line*)

parse_force (*data_lines, force_classes, forceSet, n=0*)

Read bonds, angles, dihedrals, impropers from data file.

parse_force_coeffs (*data_lines, force_name, force_classes, force_style, lammmps_forces, canonical_force*)

Read force coefficients from data file.

parse_improper_coeffs (*data_lines*)

parse_improper_style (*line*)

parse_impropers (*data_lines*)

parse_kspace_style (*line*)

Note: Currently ignored.

parse_masses (*data_lines*)

Read masses from data file.

parse_pair_coeffs (*data_lines*)

Read pair coefficients from data file.

parse_pair_modify (*line*)

parse_pair_style (*line*)

parse_read_data (*line*)

parse_special_bonds (*line*)

parse_units (*line*)

parse_velocities (*data_lines*)

read ()

Reads a LAMMPS input file and a data file specified within.

Parameters **input_file** (*str*) – Name of LAMMPS input file to read in.

read_data (*data_file*)

Reads a LAMMPS data file.

Parameters **data_file** (*str*) – name of LAMMPS data file to read in.

read_input ()

Reads a LAMMPS input file.

Parameters **input_file** (*str*) – Name of LAMMPS input file to read in.

set_units (*unit_set*)

Set what unit set to use.

write (*unit_set='real'*)

Writes a LAMMPS data and corresponding input file.

Parameters

- **data_file** (*str*) – Name of LAMMPS data file to write to.
- **unit_set** (*str*) – LAMMPS unit set for output file.

write_angles (*mol_type, offset*)

write_bonds (*mol_type, offset*)

write_dihedrals (*mol_type, offset*)

Separate dihedrals from impropers.

write_forces (*forces, offset, force_name, lookup_lammps_force, lammps_force_types, canonical_force*)

The general force writing function.

Currently supports bonds, angles, dihedrals, impropers.

write_impropers (*mol_type, offset*)

Separate dihedrals from impropers.

write_virtuals (*mol_type, offset*)

`intermol.lammps.lammps_parser.load_lammps` (*in_file*)

Load a LAMMPS input file into a *System*.

Parameters

- **in_file** –
- **include_dir** –
- **defines** –

Returns

Return type `system`

`intermol.lammps.lammps_parser.write_lammps` (*in_file, system, unit_set='real'*)

Load a LAMMPS input file into a *System*.

Parameters

- **in_file** –
- **include_dir** –
- **defines** –

Returns

Return type `system`

Module contents

3.1.2 Submodules

intermol.atom module

class `intermol.atom.Atom` (*index, name=None, residue_index=-1, residue_name=None*)

Bases: `object`

atomic_number

atomtype

bondingtype

cgnr

charge

epsilon

force

Return the force on the atom

index

mass

name

position

Return the cartesian coordinates of the atom

ptype

residue_index

residue_name

sigma

velocity

Return the velocity of the atom

intermol.convert module

`intermol.convert.find_match` (*key, dictionary, unit*)

Helper function for *summarize_energy_results*.

`intermol.convert.get_diff` (*e_in, e_out*)

Returns difference in potential energy.

Parameters

- - **dictionary of energy groups from input file** (*e_in*) –
- - **dictionary of energy groups from output file** (*e_out*) –

Returns potential energy difference in units of the input

`intermol.convert.main` (*args=None*)

`intermol.convert.parse_args` (*args*)

`intermol.convert.summarize_energy_results` (*energy_input*, *energy_outputs*, *input_type*, *output_types*)

Creates a table comparing input and output energy groups.

Args: *energy_input* (dict): energy groups from input file *energy_output*(list): containing dictionary of energy groups or -1 for each output file

input_type (str): input engine *output_types* (list): containing output formats

Returns: out (list of strings): which forms a summary table using “
”.join(out)

intermol.decorators module

exception `intermol.decorators.UnitsException` (*value*)

Bases: `exceptions.Exception`

Exception denoting that an argument has the incorrect units.

exception `intermol.decorators.ValueException` (*value*)

Bases: `exceptions.Exception`

Exception denoting that an argument has the incorrect value.

`intermol.decorators.accepts` (**types*)

Decorator for class methods that should accept only specified types.

EXAMPLE

```
@accepts(float, int) def function(a, b):  
    return b*a
```

`intermol.decorators.accepts_compatible_units` (**units*, ***unitdict*)

Decorator for class methods that should accept only arguments compatible with specified units.

Each argument of the function will be matched with an argument of `@acceptunits`. Those arguments of the function that correspond `@acceptunits` which are not `None` will be checked to ensure they are compatible with the specified units.

EXAMPLE

```
@acceptunits(units.meter, None, units.kilocalories_per_mole) def function(a, b, c):  
    pass function(1.0 *  
    units.angstrom, 3, 1.0 * units.kilojoules_per_mole)
```

`intermol.decorators.returns` (*rtype*)

Decorator for functions that should only return specific types. EXAMPLE

```
@returns(int) def function(): return 7
```

intermol.molecule module

class `intermol.molecule.Molecule` (*name=None*)

Bases: `object`

An abstract molecule object.

add_atom (*atom*)

Add an atom

Parameters `atom` (*Atom*) – the atom to add into the molecule

atoms

Return an orderedset of atoms.

intermol.moleculetype module

class `intermol.moleculetype.MoleculeType` (*name=None*)

Bases: `object`

An abstract container for molecules of one type.

add_molecule (*molecule*)

Add a molecule into the moleculetype container

Parameters `molecule` (*Molecule*) – the molecule to append

intermol.orderedset module

class `intermol.orderedset.OrderedSet` (*iterable=()*)

Bases: `_abcoll.Set`

add (*key*)

difference_update (**args, **kwargs*)

discard (*key*)

intersection_update (**args, **kwargs*)

intermol.system module

class `intermol.system.System` (*name=None*)

Bases: `object`

add_atomtype (*atomtype*)

add_molecule (*molecule*)

Append a molecule into the System. :param molecule: The molecule object to be appended

add_molecule_type (*molecule_type*)

Append a molecule_type into the System. :param molecule_type: The MoleculeType object to be appended

atoms

atomtypes

box_vector

Return the box vector.

molecule_types

n_atoms

nonbonded_types

3.1.3 Module contents

3.2 intermol.gromacs package

3.2.1 Submodules

intermol.gromacs.grofile_parser module

class `intermol.gromacs.grofile_parser.GromacsGroParser` (*gro_file*)

Bases: `object`

GromacsGroParser reads and writes Gromacs .gro files

A .gro file also contains some topological information, such as elements and residue names, but not enough to construct a full Topology object. This information is recorded and stored in the object's public fields.

read ()

write (*system*)

Write the system out in a Gromacs 4.6 format

Parameters `filename` (*str*) – the file to write out to

intermol.gromacs.gromacs_driver module

`intermol.gromacs.gromacs_driver.gromacs_energies` (*top=None, gro=None, mdp=None, gropath=None, grosuff=None, grompp_check=False*)

`gropath` = path to gromacs binaries `grosuff` = suffix of gromacs binaries, usually ‘’ or ‘_d’

`intermol.gromacs.gromacs_driver.read_file` (*top_in, gro_in, gropath*)

`intermol.gromacs.gromacs_driver.write_file` (*system, top_out, gro_out*)

intermol.gromacs.gromacs_parser module

class `intermol.gromacs.gromacs_parser.GromacsParser` (*top_file, gro_file, system=None, include_dir=None, defines=None*)

Bases: `object`

A class containing methods required to read in a Gromacs(4.5.4) Topology File

class `TopMoleculeType`

Bases: `object`

Inner class to store information about a molecule type.

`GromacsParser.canonical_angle` (*params, angle, direction='into'*)

Parameters

- `params` –
- `angle` –
- `direction` –

Returns:

`GromacsParser.canonical_bond` (*params, bond, direction='into'*)

Parameters

- **params** –
- **bond** –
- **direction** –

Returns:

GromacsParser.**canonical_dihedral** (*params, dihedral, direction='into'*)

We can fit everything into two types of dihedrals - dihedral_trig, and improper harmonic. Dihedral trig is of the form

$$fc0 + \sum_{i=1}^6 fci (\cos(nx-\phi))$$

Proper dihedrals can be stored easily in this form, since they have only 1 n. Improper dihedrals can as well (flag as improper). RB can be stored as well, assuming $\phi = 0$ or 180 . Fourier can also be stored. A full dihedral trig can be decomposed into multiple proper dihedrals.

Will need to handle multiple dihedrals little differently in that we will need to add multiple 9 dihedrals together into a single dihedral_trig, as long as they have the same phi angle (seems to be always the case).

Parameters

- **params** –
- **dihedral** –
- **direction** –

Returns:

GromacsParser.**choose_parameter_kwds_from_forces** (*entries, n_atoms, force_type, gromacs_force*)

Extract a force's parameters into a keyword dictionary.

Parameters

- **entries** (*str*) – The *split()* line being parsed.
- **n_atoms** (*int*) – The number of atoms in the force.
- **force_type** – The type of the force.
- **gromacs_force** – The

Returns

kwds – The force's parameters, e.g.

```
{'length': Quantity(value=0.13, unit=nanometers), 'k': ...
}
```

Return type dict

GromacsParser.**create_angle** (*angle*)

GromacsParser.**create_atom** (*temp_atom*)

GromacsParser.**create_bond** (*bond*)

GromacsParser.**create_dihedral** (*dihedral*)

Create a dihedral object based on a [dihedrals] entry.

GromacsParser.**create_exclusion** (*exclusion*)

GromacsParser.**create_kwds_from_entries** (*entries, force_class, offset=0*)

GromacsParser.**process_bond** (*line*)

Process a line in the [bonds] category.

GromacsParser.**process_bondtype** (*line*)

Process a line in the [bondtypes] category.

GromacsParser.**process_cmap** (*line*)

Process a line in the [cmaps] category.

GromacsParser.**process_cmaptypes** (*line*)

Process a line in the [cmaptypes] category.

GromacsParser.**process_defaults** (*line*)

Process the [defaults] line.

GromacsParser.**process_dihedral** (*line*)

Process a line in the [dihedrals] category.

GromacsParser.**process_dihedraltypes** (*line*)

Process a line in the [dihedraltypes] category.

GromacsParser.**process_exclusion** (*line*)

Process a line in the [exclusions] category.

GromacsParser.**process_file** (*top_file*)

GromacsParser.**process_forcetype** (*bondingtypes*, *forcename*, *line*, *n_atoms*, *gromacs_force_types*, *canonical_force*)

GromacsParser.**process_implicittype** (*line*)

Process a line in the [implicit_genborn_params] category.

GromacsParser.**process_line** (*top_file*, *line*)

Process one line from a file.

GromacsParser.**process_molecule** (*line*)

Process a line in the [molecules] category.

GromacsParser.**process_moleculetypes** (*line*)

Process a line in the [moleculetypes] category.

GromacsParser.**process_nonbond_params** (*line*)

Process a line in the [nonbond_param] category.

GromacsParser.**process_pair** (*line*)

Process a line in the [pairs] category.

GromacsParser.**process_pairtypes** (*line*)

Process a line in the [pairtypes] category.

GromacsParser.**process_settle** (*line*)

Process a line in the [settles] category.

GromacsParser.**read** ()

Returns system

GromacsParser.**too_few_fields** (*line*)

static GromacsParser.**type_parameters_are_unique** (*a*, *b*)

Check if two force types are unique.

Currently only tests TrigDihedralType and ImproperHarmonicDihedralType because these are the only two forcetypes that we currently allow to have multiple values for the same set of 4 atom bondingtypes.

GromacsParser.**unitvars** = {'QuarticBreakableBond': [Unit({BaseUnit(base_dim=BaseDimension("length"), name=

GromacsParser.**write**()

Write this topology in GROMACS file format.

Parameters `filename` – the name of the file to write out to

GromacsParser.**write_angles** (*top*)

GromacsParser.**write_atoms** (*top*)

GromacsParser.**write_atomtypes** (*top*)

GromacsParser.**write_bonds** (*top*)

GromacsParser.**write_defaults** (*top*)

GromacsParser.**write_dihedrals** (*top*)

GromacsParser.**write_exclusions** (*top*)

GromacsParser.**write_molecules** (*top*)

GromacsParser.**write_moleculetypes** (*top*)

GromacsParser.**write_nonbonded_types** (*top*)

GromacsParser.**write_pairs** (*top*)

GromacsParser.**write_settles** (*top*)

GromacsParser.**write_system** (*top*)

intermol.gromacs.gromacs_parser.**default_gromacs_include_dir**()

Find the location where gromacs #include files are referenced from, by searching for (1) gromacs environment variables, (2) just using the default gromacs install location, /usr/local/gromacs/share/gromacs/top.

intermol.gromacs.gromacs_parser.**load_gromacs** (*top_file*, *gro_file*, *include_dir=None*, *defines=None*)

Load a set of GROMACS input files into a *System*.

Parameters

- `top_file` –
- `gro_file` –
- `include_dir` –
- `defines` –

Returns

Return type `system`

intermol.gromacs.gromacs_parser.**write_gromacs** (*top_file*, *gro_file*, *system*)

Load a set of GROMACS input files into a *System*.

Parameters

- `top_file` –
- `gro_file` –
- `include_dir` –
- `defines` –

Returns

Return type `system`


```
lammmps_dihedrals = {'charmm': <class 'intermol.forces.proper_periodic_dihedral_type.ProperPeriodicDihedral'>, 'r  
lammmps_improper_types = {'cvff': <class 'intermol.forces.trig_dihedral_type.TrigDihedralType'>, 'harmonic': <clas  
lammmps_impropers = {'cvff': <class 'intermol.forces.trig_dihedral_type.TrigDihedral'>, 'harmonic': <class 'intermol.  
lookup_lammmps_angles = {<class 'intermol.forces.harmonic_angle_type.HarmonicAngle'>: 'harmonic', <class 'inter  
lookup_lammmps_bonds = {<class 'intermol.forces.fene_expandable_bond_type.FeneExpandableBond'>: 'fene/expand  
lookup_lammmps_dihedrals = {<class 'intermol.forces.rb_dihedral_type.RbDihedral'>: 'multi/harmonic', <class 'int  
lookup_lammmps_impropers = {<class 'intermol.forces.trig_dihedral_type.TrigDihedral'>: 'cvff', <class 'intermol.for  
parse_angle_coeffs (data_lines)  
parse_angle_style (line)  
parse_angles (data_lines)  
parse_atom_style (line)
```

Note: Assuming 'full' as default for everything else.

```
parse_atoms (data_lines)  
    Read atoms from data file.  
parse_bond_coeffs (data_lines)  
parse_bond_style (line)  
parse_bonded_style (line)  
parse_bonds (data_lines)  
parse_boundary (line)  
parse_box (line, dim)  
    Read box information from data file.
```

Parameters

- **line** (*str*) – Current line in input file.
- **dim** (*int*) – Dimension specified in line.

```
parse_dihedral_coeffs (data_lines)  
parse_dihedral_style (line)  
parse_dihedrals (data_lines)  
parse_dimension (line)  
parse_force (data_lines, force_classes, forceSet, n=0)  
    Read bonds, angles, dihedrals, impropers from data file.  
parse_force_coeffs (data_lines, force_name, force_classes, force_style, lammmps_forces, canoni-  
    cal_force)  
    Read force coefficients from data file.  
parse_improper_coeffs (data_lines)  
parse_improper_style (line)  
parse_impropers (data_lines)
```

parse_kspace_style (*line*)

Note: Currently ignored.

parse_masses (*data_lines*)

Read masses from data file.

parse_pair_coeffs (*data_lines*)

Read pair coefficients from data file.

parse_pair_modify (*line*)

parse_pair_style (*line*)

parse_read_data (*line*)

parse_special_bonds (*line*)

parse_units (*line*)

parse_velocities (*data_lines*)

read ()

Reads a LAMMPS input file and a data file specified within.

Parameters **input_file** (*str*) – Name of LAMMPS input file to read in.

read_data (*data_file*)

Reads a LAMMPS data file.

Parameters **data_file** (*str*) – name of LAMMPS data file to read in.

read_input ()

Reads a LAMMPS input file.

Parameters **input_file** (*str*) – Name of LAMMPS input file to read in.

set_units (*unit_set*)

Set what unit set to use.

write (*unit_set='real'*)

Writes a LAMMPS data and corresponding input file.

Parameters

- **data_file** (*str*) – Name of LAMMPS data file to write to.
- **unit_set** (*str*) – LAMMPS unit set for output file.

write_angles (*mol_type, offset*)

write_bonds (*mol_type, offset*)

write_dihedrals (*mol_type, offset*)

Separate dihedrals from impropers.

write_forces (*forces, offset, force_name, lookup_lammps_force, lammps_force_types, canonical_force*)

The general force writing function.

Currently supports bonds, angles, dihedrals, impropers.

write_impropers (*mol_type, offset*)

Separate dihedrals from impropers.

write_virtuals (*mol_type*, *offset*)

`intermol.lammps.lammps_parser.load_lammps` (*in_file*)

Load a LAMMPS input file into a *System*.

Parameters

- **in_file** –
- **include_dir** –
- **defines** –

Returns

Return type `system`

`intermol.lammps.lammps_parser.write_lammps` (*in_file*, *system*, *unit_set='real'*)

Load a LAMMPS input file into a *System*.

Parameters

- **in_file** –
- **include_dir** –
- **defines** –

Returns

Return type `system`

3.3.2 Module contents

3.4 intermol.forces package

3.4.1 Submodules

`intermol.forces.abstract_2_virtual_type` module

`class intermol.forces.abstract_2_virtual_type.Abstract2VirtualType` (*bondingtype1*,
bonding-
type2, *bond-*
ingtype3)

Bases: `intermol.forces.abstract_type.AbstractType`

`bondingtype1`

`bondingtype2`

`placeholder`

intermol.forces.abstract_3_virtual_type module

```
class intermol.forces.abstract_3_virtual_type.Abstract3VirtualType (bondingtype1,
                                                                    bonding-
                                                                    type2, bond-
                                                                    ingtype3,
                                                                    bonding-
                                                                    type4)
```

```
    Bases: intermol.forces.abstract_type.AbstractType
```

```
    bondingtype1
```

```
    bondingtype2
```

```
    bondingtype3
```

```
    bondingtype4
```

```
    placeholder
```

intermol.forces.abstract_4_virtual_type module

```
class intermol.forces.abstract_4_virtual_type.Abstract4VirtualType (bondingtype1,
                                                                    bonding-
                                                                    type2, bond-
                                                                    ingtype3,
                                                                    bonding-
                                                                    type4, bond-
                                                                    ingtype5)
```

```
    Bases: intermol.forces.abstract_type.AbstractType
```

```
    bondingtype1
```

```
    bondingtype2
```

```
    bondingtype3
```

```
    bondingtype4
```

intermol.forces.abstract_angle_type module

```
class intermol.forces.abstract_angle_type.AbstractAngleType (bondingtype1, bonding-
                                                                    type2, bondingtype3,
                                                                    c=False)
```

```
    Bases: intermol.forces.abstract_type.AbstractType
```

```
    bondingtype1
```

```
    bondingtype2
```

```
    bondingtype3
```

```
    c
```

intermol.forces.abstract_atom_type module

```
class intermol.forces.abstract_atom_type.AbstractAtomType (atomtype, bondtype=None,
atomic_number=None,
mass=None, charge=None,
ptype=None)
```

```
    Bases: intermol.forces.abstract_type.AbstractType
```

```
    atomic_number
```

```
    atomtype
```

```
    bondtype
```

```
    charge
```

```
    mass
```

```
    ptype
```

intermol.forces.abstract_bond_type module

```
class intermol.forces.abstract_bond_type.AbstractBondType (bondingtype1, bonding-
type2, order=1, c=False)
```

```
    Bases: intermol.forces.abstract_type.AbstractType
```

```
    bondingtype1
```

```
    bondingtype2
```

```
    c
```

```
    order
```

intermol.forces.abstract_dihedral_type module

```
class intermol.forces.abstract_dihedral_type.AbstractDihedralType (bondingtype1,
bondingtype2,
bondingtype3,
bonding-
type4, im-
proper=False)
```

```
    Bases: intermol.forces.abstract_type.AbstractType
```

```
    bondingtype1
```

```
    bondingtype2
```

```
    bondingtype3
```

```
    bondingtype4
```

```
    improper
```

intermol.forces.abstract_nonbonded_type module

```
class intermol.forces.abstract_nonbonded_type.AbstractNonbondedType (atom1,
atom2,
type)
```

```
    Bases: intermol.forces.abstract_type.AbstractType
```

```

atom1
atom2
type

```

intermol.forces.abstract_pair_type module

```

class intermol.forces.abstract_pair_type.AbstractPairType(bondingtype1, bonding-
type2, scaleLJ=None,
scaleQQ=None,
long=False)

Bases: intermol.forces.abstract_type.AbstractType

bondingtype1
bondingtype2
long
scaleLJ
scaleQQ

```

intermol.forces.abstract_type module

```

class intermol.forces.abstract_type.AbstractType
Bases: object

__repr__()
    Print the object and all of its non-magic attributes.

```

intermol.forces.atom_c_type module

```

class intermol.forces.atom_c_type.AtomCType(*args, **kws)
Bases: intermol.forces.abstract_atom_type.AbstractAtomType

```

intermol.forces.atom_sigeps_type module

```

class intermol.forces.atom_sigeps_type.AtomSigepsType(*args, **kws)
Bases: intermol.forces.abstract_atom_type.AbstractAtomType

```

intermol.forces.buckingham_nonbonded_type module

```
class intermol.forces.buckingham_nonbonded_type.BuckinghamNonbonded (atom1,  
atom2,  
bonding-  
type1=None,  
bonding-  
type2=None,  
a=Quantity(value=0.0,  
unit=kilojoule/mole),  
b=Quantity(value=0.0,  
unit=nanometer),  
C6=Quantity(value=0.0,  
unit=nanometer**6*kilojoule/mole),  
type=False)
```

Bases: `intermol.forces.buckingham_nonbonded_type.BuckinghamNonbondedType`

stub documentation

```
class intermol.forces.buckingham_nonbonded_type.BuckinghamNonbondedType (*args,  
**kwds)
```

Bases: `intermol.forces.abstract_nonbonded_type.AbstractNonbondedType`

C6

a

b

type

intermol.forces.connection_bond_type module

```
class intermol.forces.connection_bond_type.ConnectionBond (atom1, atom2, bonding-  
type1=None, bonding-  
type2=None, order=1,  
c=False)
```

Bases: `intermol.forces.connection_bond_type.ConnectionBondType`

stub documentation

```
class intermol.forces.connection_bond_type.ConnectionBondType (*args, **kwds)
```

Bases: `intermol.forces.abstract_bond_type.AbstractBondType`

c

order

intermol.forces.convert_dihedrals module

`intermol.forces.convert_dihedrals.convert_dihedral_from_OPLS_to_RB` (*f*)

`intermol.forces.convert_dihedrals.convert_dihedral_from_RB_to_OPLS` (*c*)

`intermol.forces.convert_dihedrals.convert_dihedral_from_RB_to_trig` (*c*)

`intermol.forces.convert_dihedrals.convert_dihedral_from_fourier_to_trig` (*f*)

`intermol.forces.convert_dihedrals.convert_dihedral_from_proper_to_trig` (*p*)

`intermol.forces.convert_dihedrals.convert_dihedral_from_trig_to_RB` (*fcs*)


```
intermol.forces.convert_dihedrals.convert_dihedral_from_trig_to_fourier (fcs)
intermol.forces.convert_dihedrals.convert_dihedral_from_trig_to_proper (fcs,
                                                                    con-
                                                                    ven-
                                                                    tion='0')

intermol.forces.convert_dihedrals.convert_nothing (x)
    useful utility for not converting anything
```

intermol.forces.cosine_angle_type module

```
class intermol.forces.cosine_angle_type.CosineAngle (atom1, atom2, atom3, bond-
                                                                    ingtype1=None,
                                                                    bonding-
                                                                    type2=None, bondingtype3=None,
                                                                    k=Quantity(value=0.0,
                                                                    unit=kilojoule/mole), c=False)

    Bases: intermol.forces.cosine_angle_type.CosineAngleType
```

http://lammps.sandia.gov/doc/angle_cosine.html

```
class intermol.forces.cosine_angle_type.CosineAngleType (*args, **kwargs)
    Bases: intermol.forces.abstract_angle_type.AbstractAngleType

    c

    k
```

intermol.forces.cosine_squared_angle_type module

```
class intermol.forces.cosine_squared_angle_type.CosineSquaredAngle (atom1,
                                                                    atom2,
                                                                    atom3,
                                                                    bonding-
                                                                    type1=None,
                                                                    bonding-
                                                                    type2=None,
                                                                    bonding-
                                                                    type3=None,
                                                                    theta=Quantity(value=0.0,
                                                                    unit=degree),
                                                                    k=Quantity(value=0.0,
                                                                    unit=kilojoule/mole),
                                                                    c=False)

    Bases: intermol.forces.cosine_squared_angle_type.CosineSquaredAngleType

    stub documentation
```

```
class intermol.forces.cosine_squared_angle_type.CosineSquaredAngleType (*args,
                                                                    **kwargs)
    Bases: intermol.forces.abstract_angle_type.AbstractAngleType

    c

    k

    theta
```

intermol.forces.cross_bond_angle_angle_type module

```
class intermol.forces.cross_bond_angle_angle_type.CrossBondAngleAngle (atom1,  
                                atom2,  
                                atom3,  
                                bonding-  
                                type1=None,  
                                bonding-  
                                type2=None,  
                                bonding-  
                                type3=None,  
                                r1=Quantity(value=0.0,  
                                unit=nanometer),  
                                r2=Quantity(value=0.0,  
                                unit=nanometer),  
                                r3=Quantity(value=0.0,  
                                unit=nanometer),  
                                k=Quantity(value=0.0,  
                                unit=kilojoule/(nanometer**2*mole),  
                                c=False)  
  
    Bases: intermol.forces.cross_bond_angle_angle_type.CrossBondAngleAngleType  
    stub documentation
```

```
class intermol.forces.cross_bond_angle_angle_type.CrossBondAngleAngleType (*args,  
                                                                           **kwargs)  
  
    Bases: intermol.forces.abstract_angle_type.AbstractAngleType  
  
    c  
  
    k  
  
    r1  
  
    r2  
  
    r3
```

intermol.forces.cross_bond_bond_angle_type module

```
class intermol.forces.cross_bond_bond_angle_type.CrossBondBondAngle (atom1,  
                                atom2,  
                                atom3,  
                                bonding-  
                                type1=None,  
                                bonding-  
                                type2=None,  
                                bonding-  
                                type3=None,  
                                r1=Quantity(value=0.0,  
                                unit=nanometer),  
                                r2=Quantity(value=0.0,  
                                unit=nanometer),  
                                k=Quantity(value=0.0,  
                                unit=kilojoule/(nanometer**2*mole),  
                                c=False)  
  
    Bases: intermol.forces.cross_bond_bond_angle_type.CrossBondBondAngleType
```

stub documentation

```
class intermol.forces.cross_bond_bond_angle_type.CrossBondBondAngleType (*args,
                                                                    **kwds)
    Bases: intermol.forces.abstract_angle_type.AbstractAngleType
    c
    k
    r1
    r2
```

intermol.forces.cubic_bond_type module

```
class intermol.forces.cubic_bond_type.CubicBond (atom1,          atom2,          bonding-
                                                type1=None,          bondingtype2=None,
                                                length=Quantity(value=0.0,
                                                            unit=nanometer),
                                                C2=Quantity(value=0.0,
                                                            unit=kilojoule/(nanometer**2*mole)),
                                                C3=Quantity(value=0.0,
                                                            unit=kilojoule/(nanometer**3*mole)),
                                                order=1, c=False)
    Bases: intermol.forces.cubic_bond_type.CubicBondType
```

stub documentation

```
class intermol.forces.cubic_bond_type.CubicBondType (*args, **kwds)
    Bases: intermol.forces.abstract_bond_type.AbstractBondType
    C2
    C3
    c
    length
    order
```

intermol.forces.fene_bond_type module

```
class intermol.forces.fene_bond_type.FeneBond (atom1, atom2, bondingtype1=None, bond-
                                                ingtype2=None, length=Quantity(value=0.0,
                                                            unit=nanometer), kb=Quantity(value=0.0,
                                                            unit=kilojoule/(nanometer**2*mole)),
                                                order=1, c=False)
    Bases: intermol.forces.fene_bond_type.FeneBondType
```

stub documentation

```
class intermol.forces.fene_bond_type.FeneBondType (*args, **kwds)
    Bases: intermol.forces.abstract_bond_type.AbstractBondType
    c
    kb
    length
```

order

intermol.forces.fene_expandable_bond_type module

```
class intermol.forces.fene_expandable_bond_type.FeneExpandableBond (atom1,
                                                                    atom2,
                                                                    bonding-
                                                                    type1=None,
                                                                    bonding-
                                                                    type2=None,
                                                                    k=Quantity(value=0.0,
                                                                    unit=kilojoule/(nanometer**2*mole)),
                                                                    length=Quantity(value=0.0,
                                                                    unit=nanometer),
                                                                    ep-
                                                                    silon=Quantity(value=0.0,
                                                                    unit=kilojoule/mole),
                                                                    sigma=Quantity(value=0.0,
                                                                    unit=nanometer),
                                                                    delta=Quantity(value=0.0,
                                                                    unit=nanometer),
                                                                    order=1,
                                                                    c=False)
```

Bases: `intermol.forces.fene_expandable_bond_type.FeneExpandableBondType`

stub documentation

```
class intermol.forces.fene_expandable_bond_type.FeneExpandableBondType (*args,
                                                                    **kwds)
```

Bases: `intermol.forces.abstract_bond_type.AbstractBondType`

c

delta

epsilon

k

length

order

sigma

intermol.forces.forcedata module

intermol.forces.forcefunctions module

`intermol.forces.forcefunctions.build_paramlist` (*program*)

Create a paramlist specific for a given program.

`intermol.forces.forcefunctions.build_unitvars` (*program, paramlist, dumself=None*)

Takes a string program name (one of the supported programs), and a 'self' object it looks like the keyword is not being used, but it is used in the line `eval(unit)`. The test name 'dumself' needs to match what is in the force data arrays. Currently only used for lammmps.

`intermol.forces.forcefunctions.capiifyname` (*forcename*)

Return name of the class in camelCase.

`intermol.forces.forcefunctions.create_kwd_dict` (*unitvars*, *paramlist*, *force_type_object*, *values*, *optvalues=None*)

`intermol.forces.forcefunctions.create_kwds_from_entries` (*unitvars*, *paramlist*, *entries*, *force_type*, *offset=0*)

Create a keyword dictionary given an array of information from a file format

requires the master set of units, the master set of parameter lists, an object (either a `force_class` or `force_type`), the list of information to be converted into a keyword, and an offset.

Parameters `offset` (*int*) – how far over from the first entry we translate

`intermol.forces.forcefunctions.get_parameter_kwds_from_force` (*force*, *forceparams*, *paramlist*)

`intermol.forces.forcefunctions.get_parameter_list_from_force` (*force*, *paramlist*)

Create a function that returns the paramters of a function type.

First, we need make some additions to the parameter list dictionary, which we do once when the `forcedata` script is imported. Useful to put the forces here as well. We won't make this a function for now since it's needed in this module.

`intermol.forces.forcefunctions.get_parameter_list_from_kwds` (*force*, *kwds*, *paramlist*)

`intermol.forces.forcefunctions.optforceparams` (*force_type*, *forcetype_object=None*)

Return the dictionary of optional paramters of an abstract force type.

If no object is given, we fill with blanks.

`intermol.forces.forcefunctions.optparamkeylookup` (*force_type*)

Given a `force_type` object, determine the key associated with the optional parameters.

`intermol.forces.forcefunctions.optparamlookup` (*force_type_object*, *object_default=False*)

A wrapper for `optforceparams` that takes a `force_type` object and returns the optional parameter dictionary.

`intermol.forces.forcefunctions.specify` (*program_units*, *unitset*, *dumself=None*, *shouldEval=True*)

Takes the dict of units, and a set of dimensions and replaces the dimensions with the appropriate units.

`intermol.forces.four_fdn_virtual_type` module

```
class intermol.forces.four_fdn_virtual_type.FourFdnVirtual (atom1, atom2, atom3,
atom4, atom5, bondingtype1=None,
bondingtype2=None,
bondingtype3=None,
bondingtype4=None,
bondingtype5=None,
a=Quantity(value=0.0, unit=dimensionless),
b=Quantity(value=0.0, unit=dimensionless),
c=Quantity(value=0.0, unit=nanometer), placeholder=False)
```

Bases: `intermol.forces.four_fdn_virtual_type.FourFdnVirtualType`

stub documentation

```
class intermol.forces.four_fdn_virtual_type.FourFdnVirtualType (*args, **kwds)
```

Bases: `intermol.forces.abstract_4_virtual_type.Abstract4VirtualType`

a
b
c
placeholder

intermol.forces.fourier_dihedral_type module

```
class intermol.forces.fourier_dihedral_type.FourierDihedral (atom1, atom2, atom3,  
atom4, bonding-  
type1=None, bond-  
ingtype2=None,  
bondingtype3=None,  
bondingtype4=None,  
c1=Quantity(value=0.0,  
unit=kilojoule/mole),  
c2=Quantity(value=0.0,  
unit=kilojoule/mole),  
c3=Quantity(value=0.0,  
unit=kilojoule/mole),  
c4=Quantity(value=0.0,  
unit=kilojoule/mole),  
c5=Quantity(value=0.0,  
unit=kilojoule/mole),  
improper=False)
```

Bases: `intermol.forces.fourier_dihedral_type.FourierDihedralType`

stub documentation

```
class intermol.forces.fourier_dihedral_type.FourierDihedralType (*args, **kwds)  
Bases: intermol.forces.abstract_dihedral_type.AbstractDihedralType
```

c1

c2

c3

c4

c5

improper

intermol.forces.g96_bond_type module

```
class intermol.forces.g96_bond_type.G96Bond (atom1, atom2, bondingtype1=None, bond-  
ingtype2=None, length=Quantity(value=0.0,  
unit=nanometer), k=Quantity(value=0.0,  
unit=kilojoule/(nanometer**4*mole)), order=1,  
c=False)
```

Bases: `intermol.forces.g96_bond_type.G96BondType`

stub documentation

```
class intermol.forces.g96_bond_type.G96BondType (*args, **kwds)  
Bases: intermol.forces.abstract_bond_type.AbstractBondType
```

c
k
length
order

intermol.forces.harmonic_angle_type module

```
class intermol.forces.harmonic_angle_type.HarmonicAngle(atom1, atom2, atom3,
    bondingtype1=None,
    bondingtype2=None,
    bondingtype3=None,
    theta=Quantity(value=0.0,
    unit=degree),
    k=Quantity(value=0.0,
    unit=kilojoule/(mole*radian**2)),
    c=False)
```

Bases: `intermol.forces.harmonic_angle_type.HarmonicAngleType`

stub documentation

```
class intermol.forces.harmonic_angle_type.HarmonicAngleType(*args, **kwargs)
    Bases: intermol.forces.abstract_angle_type.AbstractAngleType
```

c
k
theta

intermol.forces.harmonic_bond_type module

```
class intermol.forces.harmonic_bond_type.HarmonicBond(atom1, atom2, bond-
    ingtype1=None, bond-
    ingtype2=None,
    length=Quantity(value=0.0,
    unit=nanometer),
    k=Quantity(value=0.0,
    unit=kilojoule/(nanometer**2*mole)),
    order=1, c=False)
```

Bases: `intermol.forces.harmonic_bond_type.HarmonicBondType`

stub documentation

```
class intermol.forces.harmonic_bond_type.HarmonicBondType(*args, **kwargs)
    Bases: intermol.forces.abstract_bond_type.AbstractBondType
```

c
k
length
order

intermol.forces.harmonic_potential_bond_type module

```
class intermol.forces.harmonic_potential_bond_type.HarmonicPotentialBond (atom1,  
atom2,  
bond-  
ing-  
type1=None,  
bond-  
ing-  
type2=None,  
length=Quantity(value=0.0,  
unit=nanometer),  
k=Quantity(value=0.0,  
unit=kilojoule/(nanometer**2),  
or-  
der=1,  
c=False)
```

```
Bases: intermol.forces.harmonic_potential_bond_type.HarmonicPotentialBondType  
stub documentation
```

```
class intermol.forces.harmonic_potential_bond_type.HarmonicPotentialBondType (*args,  
**kwds)
```

```
Bases: intermol.forces.abstract_bond_type.AbstractBondType
```

```
c
```

```
k
```

```
length
```

```
order
```


intermol.forces.improper_harmonic_dihedral_type module

```
class intermol.forces.improper_harmonic_dihedral_type.ImproperHarmonicDihedral (atom1,
                                                                                   atom2,
                                                                                   atom3,
                                                                                   atom4,
                                                                                   bond-
                                                                                   ing-
                                                                                   type1=None,
                                                                                   bond-
                                                                                   ing-
                                                                                   type2=None,
                                                                                   bond-
                                                                                   ing-
                                                                                   type3=None,
                                                                                   bond-
                                                                                   ing-
                                                                                   type4=None,
                                                                                   xi=Quantity(value=0,
                                                                                   unit=degree),
                                                                                   k=Quantity(value=0,
                                                                                   unit=kilojoule/mole),
                                                                                   im-
                                                                                   proper=False)
```

Bases: `intermol.forces.improper_harmonic_dihedral_type.ImproperHarmonicDihedralType`

stub documentation

```
class intermol.forces.improper_harmonic_dihedral_type.ImproperHarmonicDihedralType (*args,
                                                                                       **kwds)
```

Bases: `intermol.forces.abstract_dihedral_type.AbstractDihedralType`

improper

k

xi

intermol.forces.lj_c_nonbonded_type module

```
class intermol.forces.lj_c_nonbonded_type.LjCNonbonded (atom1,      atom2,      bond-
                                                                                   ingtype1=None,      bond-
                                                                                   ingtype2=None,
                                                                                   C6=Quantity(value=0.0,
                                                                                   unit=nanometer**6*kilojoule/mole),
                                                                                   C12=Quantity(value=0.0,
                                                                                   unit=nanometer**12*kilojoule/mole),
                                                                                   type=False)
```

Bases: `intermol.forces.lj_c_nonbonded_type.LjCNonbondedType`

stub documentation

```
class intermol.forces.lj_c_nonbonded_type.LjCNonbondedType (*args, **kwds)
```

Bases: `intermol.forces.abstract_nonbonded_type.AbstractNonbondedType`

C12

C6

type

intermol.forces.lj_c_pair_type module

```
class intermol.forces.lj_c_pair_type.LjCPair(atom1, atom2, bondingtype1=None, bondingtype2=None, C6=Quantity(value=0.0, unit=nanometer**6*kilojoule/mole), C12=Quantity(value=0.0, unit=nanometer**12*kilojoule/mole), scaleLJ=None, scaleQQ=None, long=False)
```

Bases: `intermol.forces.lj_c_pair_type.LjCPairType`

stub documentation

```
class intermol.forces.lj_c_pair_type.LjCPairType(*args, **kwds)
Bases: intermol.forces.abstract_pair_type.AbstractPairType
```

C12

C6

long

scaleLJ

scaleQQ

intermol.forces.lj_default_pair_type module

```
class intermol.forces.lj_default_pair_type.LjDefaultPair(atom1, atom2, bondingtype1=None, bondingtype2=None, scaleLJ=None, scaleQQ=None, long=False)
```

Bases: `intermol.forces.lj_default_pair_type.LjDefaultPairType`

stub documentation

```
class intermol.forces.lj_default_pair_type.LjDefaultPairType(*args, **kwds)
Bases: intermol.forces.abstract_pair_type.AbstractPairType
```

long

scaleLJ

scaleQQ

intermol.forces.lj_sigeps_nonbonded_type module

```
class intermol.forces.lj_sigeps_nonbonded_type.LjSigepsNonbonded (atom1, atom2,
                                                                    bonding-
                                                                    type1=None,
                                                                    bonding-
                                                                    type2=None,
                                                                    sigma=Quantity(value=0.0,
                                                                    unit=nanometer),
                                                                    ep-
                                                                    silon=Quantity(value=0.0,
                                                                    unit=kilojoule/mole),
                                                                    type=False)
```

Bases: `intermol.forces.lj_sigeps_nonbonded_type.LjSigepsNonbondedType`

stub documentation

```
class intermol.forces.lj_sigeps_nonbonded_type.LjSigepsNonbondedType (*args,
                                                                    **kwds)
```

Bases: `intermol.forces.abstract_nonbonded_type.AbstractNonbondedType`

epsilon

sigma

type

intermol.forces.lj_sigeps_pair_type module

```
class intermol.forces.lj_sigeps_pair_type.LjSigepsPair (atom1, atom2, bond-
                                                                    ingtype1=None, bond-
                                                                    ingtype2=None,
                                                                    sigma=Quantity(value=0.0,
                                                                    unit=nanometer), ep-
                                                                    silon=Quantity(value=0.0,
                                                                    unit=kilojoule/mole),
                                                                    scaleLJ=None,
                                                                    scaleQQ=None, long=False)
```

Bases: `intermol.forces.lj_sigeps_pair_type.LjSigepsPairType`

stub documentation

```
class intermol.forces.lj_sigeps_pair_type.LjSigepsPairType (*args, **kwds)
```

Bases: `intermol.forces.abstract_pair_type.AbstractPairType`

epsilon

long

scaleLJ

scaleQQ

sigma

intermol.forces.ljq_c_pair_type module

```
class intermol.forces.ljq_c_pair_type.LjqCPair (atom1, atom2, bondingtype1=None, bondingtype2=None, qi=Quantity(value=0.0, unit=elementary charge), qj=Quantity(value=0.0, unit=elementary charge), C6=Quantity(value=0.0, unit=nanometer**6*kilojoule/mole), C12=Quantity(value=0.0, unit=nanometer**12*kilojoule/mole), scaleLJ=None, scaleQQ=None, long=False)
```

Bases: [intermol.forces.ljq_c_pair_type.LjqCPairType](#)

stub documentation

```
class intermol.forces.ljq_c_pair_type.LjqCPairType (*args, **kws)  
Bases: intermol.forces.abstract\_pair\_type.AbstractPairType
```

C12

C6

long

qi

qj

scaleLJ

scaleQQ

intermol.forces.ljq_default_pair_type module

```
class intermol.forces.ljq_default_pair_type.LjqDefaultPair (atom1, atom2, bondingtype1=None, bondingtype2=None, scaleLJ=None, scaleQQ=None, long=False)
```

Bases: [intermol.forces.ljq_default_pair_type.LjqDefaultPairType](#)

stub documentation

```
class intermol.forces.ljq_default_pair_type.LjqDefaultPairType (*args, **kws)  
Bases: intermol.forces.abstract\_pair\_type.AbstractPairType
```

long

scaleLJ

scaleQQ

intermol.forces.ljq_sigeps_pair_type module

```
class intermol.forces.ljq_sigeps_pair_type.LjqSigepsPair (atom1, atom2, bondingtype1=None,
bondingtype2=None,
qi=Quantity(value=0.0,
unit=elementary charge),
qj=Quantity(value=0.0,
unit=elementary charge),
sigma=Quantity(value=0.0,
unit=nanometer), epsilon=Quantity(value=0.0,
unit=kilojoule/mole),
scaleLJ=None,
scaleQQ=None,
long=False)
```

Bases: `intermol.forces.ljq_sigeps_pair_type.LjqSigepsPairType`

stub documentation

```
class intermol.forces.ljq_sigeps_pair_type.LjqSigepsPairType (*args, **kwds)
```

Bases: `intermol.forces.abstract_pair_type.AbstractPairType`

epsilon

long

qi

qj

scaleLJ

scaleQQ

sigma

intermol.forces.make_forces module**intermol.forces.morse_bond_type** module

```
class intermol.forces.morse_bond_type.MorseBond (atom1, atom2, bondingtype1=None,
bondingtype2=None,
length=Quantity(value=0.0,
unit=nanometer), D=Quantity(value=0.0,
unit=kilojoule/mole),
beta=Quantity(value=0.0,
unit=nanometer), order=1, c=False)
```

Bases: `intermol.forces.morse_bond_type.MorseBondType`

stub documentation

```
class intermol.forces.morse_bond_type.MorseBondType (*args, **kwds)
```

Bases: `intermol.forces.abstract_bond_type.AbstractBondType`

D

beta

c

length

order

intermol.forces.nonlinear_bond_type module

```
class intermol.forces.nonlinear_bond_type.NonlinearBond(atom1, atom2, bond-  
ingtype1=None, bond-  
ingtype2=None, ep-  
silon=Quantity(value=0.0,  
unit=kilojoule/mole),  
r0=Quantity(value=0.0,  
unit=nanometer),  
lamda=Quantity(value=0.0,  
unit=nanometer), order=1,  
c=False)
```

Bases: `intermol.forces.nonlinear_bond_type.NonlinearBondType`

http://lammps.sandia.gov/doc/bond_nonlinear.html

```
class intermol.forces.nonlinear_bond_type.NonlinearBondType(*args, **kwds)
```

Bases: `intermol.forces.abstract_bond_type.AbstractBondType`

c

epsilon

lamda

order

r0

intermol.forces.proper_periodic_dihedral_type module

```

class intermol.forces.proper_periodic_dihedral_type.ProperPeriodicDihedral (atom1,
                                                                    atom2,
                                                                    atom3,
                                                                    atom4,
                                                                    bond-
                                                                    ing-
                                                                    type1=None,
                                                                    bond-
                                                                    ing-
                                                                    type2=None,
                                                                    bond-
                                                                    ing-
                                                                    type3=None,
                                                                    bond-
                                                                    ing-
                                                                    type4=None,
                                                                    phi=Quantity(value=0.0,
                                                                    unit=degree),
                                                                    k=Quantity(value=0.0,
                                                                    unit=kilojoule/mole),
                                                                    mul-
                                                                    ti-
                                                                    plic-
                                                                    ity=Quantity(value=0.0,
                                                                    unit=dimensionless),
                                                                    weight=Quantity(value=0,
                                                                    unit=dimensionless),
                                                                    im-
                                                                    proper=False)

```

Bases: `intermol.forces.proper_periodic_dihedral_type.ProperPeriodicDihedralType`
 stub documentation

```

class intermol.forces.proper_periodic_dihedral_type.ProperPeriodicDihedralType (*args,
                                                                    **kwds)

```

Bases: `intermol.forces.abstract_dihedral_type.AbstractDihedralType`

improper

k

multiplicity

phi

weight

intermol.forces.quartic_angle_type module

```
class intermol.forces.quartic_angle_type.QuarticAngle (atom1, atom2, atom3,  
            bondingtype1=None,  
            bondingtype2=None,  
            bondingtype3=None,  
            theta=Quantity(value=0.0,  
                           unit=degree),  
            C0=Quantity(value=0.0,  
                        unit=kilojoule/mole),  
            C1=Quantity(value=0.0,  
                        unit=kilojoule/(mole*radian)),  
            C2=Quantity(value=0.0,  
                        unit=kilojoule/(mole*radian**2)),  
            C3=Quantity(value=0.0,  
                        unit=kilojoule/(mole*radian**3)),  
            C4=Quantity(value=0.0,  
                        unit=kilojoule/(mole*radian**4)),  
            c=False)
```

Bases: `intermol.forces.quartic_angle_type.QuarticAngleType`

stub documentation

```
class intermol.forces.quartic_angle_type.QuarticAngleType (*args, **kwargs)
```

Bases: `intermol.forces.abstract_angle_type.AbstractAngleType`

C0

C1

C2

C3

C4

c

theta

intermol.forces.quartic_bond_type module

```
class intermol.forces.quartic_bond_type.QuarticBond (atom1, atom2, bonding-  
            type1=None, bondingtype2=None,  
            length=Quantity(value=0.0,  
                             unit=nanometer),  
            C2=Quantity(value=0.0,  
                        unit=kilojoule/(nanometer**2*mole)),  
            C3=Quantity(value=0.0,  
                        unit=kilojoule/(nanometer**3*mole)),  
            C4=Quantity(value=0.0,  
                        unit=kilojoule/(nanometer**4*mole)),  
            order=1, c=False)
```

Bases: `intermol.forces.quartic_bond_type.QuarticBondType`

stub documentation

```
class intermol.forces.quartic_bond_type.QuarticBondType (*args, **kwargs)
```

Bases: `intermol.forces.abstract_bond_type.AbstractBondType`

C2
C3
C4
c
length
order

intermol.forces.quartic_breakable_bond_type module

```

class intermol.forces.quartic_breakable_bond_type.QuarticBreakableBond(atom1,
                                                                    atom2,
                                                                    bond-
                                                                    ing-
                                                                    type1=None,
                                                                    bond-
                                                                    ing-
                                                                    type2=None,
                                                                    k=Quantity(value=0.0,
                                                                    unit=kilojoule/(nanometer**4)*r
                                                                    B1=Quantity(value=0.0,
                                                                    unit=nanometer),
                                                                    B2=Quantity(value=0.0,
                                                                    unit=nanometer),
                                                                    Rc=Quantity(value=0.0,
                                                                    unit=nanometer),
                                                                    U0=Quantity(value=0.0,
                                                                    unit=kilojoule/mole),
                                                                    or-
                                                                    der=1,
                                                                    c=False)

```

Bases: `intermol.forces.quartic_breakable_bond_type.QuarticBreakableBondType`

http://lammps.sandia.gov/doc/bond_quartic.html

```

class intermol.forces.quartic_breakable_bond_type.QuarticBreakableBondType(*args,
                                                                              **kwds)

```

Bases: `intermol.forces.abstract_bond_type.AbstractBondType`

B1
B2
Rc
U0
c
k
order

intermol.forces.rb_dihedral_type module

```
class intermol.forces.rb_dihedral_type.RbDihedral (atom1, atom2, atom3, atom4, bonding-  
type1=None, bondingtype2=None,  
bondingtype3=None, bonding-  
type4=None, C0=Quantity(value=0.0,  
unit=kilojoule/mole),  
C1=Quantity(value=0.0,  
unit=kilojoule/mole),  
C2=Quantity(value=0.0,  
unit=kilojoule/mole),  
C3=Quantity(value=0.0,  
unit=kilojoule/mole),  
C4=Quantity(value=0.0,  
unit=kilojoule/mole),  
C5=Quantity(value=0.0,  
unit=kilojoule/mole),  
C6=Quantity(value=0.0,  
unit=kilojoule/mole), im-  
proper=False)  
Bases: intermol.forces.rb_dihedral_type.RbDihedralType
```

stub documentation

```
class intermol.forces.rb_dihedral_type.RbDihedralType (*args, **kws)  
Bases: intermol.forces.abstract_dihedral_type.AbstractDihedralType  
C0  
C1  
C2  
C3  
C4  
C5  
C6  
improper
```

intermol.forces.settles module

```
class intermol.forces.settles.Settles (*args, **kws)  
Bases: intermol.forces.abstract_type.AbstractType
```

intermol.forces.three_fad_virtual_type module

```
class intermol.forces.three_fad_virtual_type.ThreeFadVirtual (atom1, atom2, atom3,
                                                             atom4,      bonding-
                                                             type1=None,  bond-
                                                             ingtype2=None,
                                                             bondingtype3=None,
                                                             bondingtype4=None,
                                                             theta=Quantity(value=0.0,
                                                             unit=degree),
                                                             d=Quantity(value=0.0,
                                                             unit=nanometer),
                                                             placeholder=False)
```

Bases: `intermol.forces.three_fad_virtual_type.ThreeFadVirtualType`

stub documentation

```
class intermol.forces.three_fad_virtual_type.ThreeFadVirtualType (*args, **kwds)
```

Bases: `intermol.forces.abstract_3_virtual_type.Abstract3VirtualType`

d

placeholder

theta

intermol.forces.three_fd_virtual_type module

```
class intermol.forces.three_fd_virtual_type.ThreeFdVirtual (atom1, atom2, atom3,
                                                             atom4,      bonding-
                                                             type1=None,  bond-
                                                             ingtype2=None,
                                                             bondingtype3=None,
                                                             bondingtype4=None,
                                                             a=Quantity(value=0.0,
                                                             unit=dimensionless),
                                                             d=Quantity(value=0.0,
                                                             unit=nanometer), placeholder=False)
```

Bases: `intermol.forces.three_fd_virtual_type.ThreeFdVirtualType`

stub documentation

```
class intermol.forces.three_fd_virtual_type.ThreeFdVirtualType (*args, **kwds)
```

Bases: `intermol.forces.abstract_3_virtual_type.Abstract3VirtualType`

a

d

placeholder

intermol.forces.three_linear_virtual_type module

```
class intermol.forces.three_linear_virtual_type.ThreeLinearVirtual (atom1,  
atom2,  
atom3,  
atom4,  
bonding-  
type1=None,  
bonding-  
type2=None,  
bonding-  
type3=None,  
bonding-  
type4=None,  
a=Quantity(value=0.0,  
unit=dimensionless),  
b=Quantity(value=0.0,  
unit=dimensionless),  
place-  
holder=False)  
  
Bases: intermol.forces.three_linear_virtual_type.ThreeLinearVirtualType  
stub documentation
```

```
class intermol.forces.three_linear_virtual_type.ThreeLinearVirtualType (*args,  
**kwds)  
Bases: intermol.forces.abstract_3_virtual_type.Abstract3VirtualType  
  
a  
  
b  
  
placeholder
```

intermol.forces.three_out_virtual_type module

```
class intermol.forces.three_out_virtual_type.ThreeOutVirtual (atom1, atom2, atom3,  
atom4, bonding-  
type1=None, bond-  
ingtype2=None,  
bondingtype3=None,  
bondingtype4=None,  
a=Quantity(value=0.0,  
unit=dimensionless),  
b=Quantity(value=0.0,  
unit=dimensionless),  
c=Quantity(value=0.0,  
unit=/nanometer),  
placeholder=False)  
  
Bases: intermol.forces.three_out_virtual_type.ThreeOutVirtualType  
stub documentation
```

```
class intermol.forces.three_out_virtual_type.ThreeOutVirtualType (*args, **kwds)  
Bases: intermol.forces.abstract_3_virtual_type.Abstract3VirtualType  
  
a
```

b
c
placeholder

intermol.forces.trig_dihedral_type module

```
class intermol.forces.trig_dihedral_type.TrigDihedral (atom1,      atom2,      atom3,
                                                    atom4,      bondingtype1=None,
                                                    bondingtype2=None,
                                                    bondingtype3=None,
                                                    bondingtype4=None,
                                                    phi=Quantity(value=0.0,
                                                         unit=degree),
                                                    fc0=Quantity(value=0.0,
                                                         unit=kilojoule/mole),
                                                    fc1=Quantity(value=0.0,
                                                         unit=kilojoule/mole),
                                                    fc2=Quantity(value=0.0,
                                                         unit=kilojoule/mole),
                                                    fc3=Quantity(value=0.0,
                                                         unit=kilojoule/mole),
                                                    fc4=Quantity(value=0.0,
                                                         unit=kilojoule/mole),
                                                    fc5=Quantity(value=0.0,
                                                         unit=kilojoule/mole),
                                                    fc6=Quantity(value=0.0,
                                                         unit=kilojoule/mole),
                                                    proper=False)           im-
```

Bases: `intermol.forces.trig_dihedral_type.TrigDihedralType`

stub documentation

```
class intermol.forces.trig_dihedral_type.TrigDihedralType (*args, **kwds)
Bases: intermol.forces.abstract_dihedral_type.AbstractDihedralType
fc0
fc1
fc2
fc3
fc4
fc5
fc6
improper
phi
```

intermol.forces.two_virtual_type module

```
class intermol.forces.two_virtual_type.TwoVirtual (atom1, atom2, atom3,  
                                             bondingtype1=None, bond-  
                                             ingtype2=None, bonding-  
                                             type3=None, a=Quantity(value=0.0,  
                                             unit=dimensionless), place-  
                                             holder=False)
```

Bases: `intermol.forces.two_virtual_type.TwoVirtualType`

stub documentation

```
class intermol.forces.two_virtual_type.TwoVirtualType (*args, **kws)
```

Bases: `intermol.forces.abstract_2_virtual_type.Abstract2VirtualType`

a

placeholder

intermol.forces.urey_bradley_angle_type module

```
class intermol.forces.urey_bradley_angle_type.UreyBradleyAngle (atom1, atom2,  
                                             atom3, bonding-  
                                             type1=None, bond-  
                                             ingtype2=None,  
                                             bonding-  
                                             type3=None,  
                                             theta=Quantity(value=0.0,  
                                             unit=degree),  
                                             k=Quantity(value=0.0,  
                                             unit=kilojoule/(mole*radian**2)),  
                                             r=Quantity(value=0.0,  
                                             unit=nanometer),  
                                             kUB=Quantity(value=0.0,  
                                             unit=kilojoule/(nanometer**2*mole)),  
                                             c=False)
```

Bases: `intermol.forces.urey_bradley_angle_type.UreyBradleyAngleType`

stub documentation

```
class intermol.forces.urey_bradley_angle_type.UreyBradleyAngleType (*args,  
                                                                     **kws)
```

Bases: `intermol.forces.abstract_angle_type.AbstractAngleType`

c

k

kUB

r

theta

3.4.2 Module contents

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