
opan Documentation

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Open Anharmonic is a Python wrapper for computational chemistry software packages intended to enable VPT2 computation of anharmonic vibrational constants. The code is still in the preliminary stages of development; no VPT2 functionality is yet available.

Other types of calculations are under consideration.

An adjunct goal of the project is to expose an API providing convenient access to various results of standalone calculations, as well as tools to manipulate those results. In particular, *OpenXYZ* and the subclasses of *SuperOpenGrad* and *SuperOpenHess* are anticipated to be particularly useful.

Due to the large number of possible variations of computational runs, parsing of output files is challenging, and only a small number of run types have been implemented to date. More are planned, but are currently low priority.

Open Anharmonic is available on PyPI as `opan`:

```
pip install opan
```

See the [dependencies page](#) for package dependencies and compatible versions. Note that due to common complications on Windows systems, dependencies are **NOT** set to automatically install.

The source repository for Open Anharmonic can be found at:

<https://www.github.com/bskinn/opan>

Bug reports and feature requests can be submitted as GitHub Issues. Other feedback is welcomed at:

```
bskinn at alum dot mit dot edu
```

Contents

Open Anharmonic User's Guide

Eventually there will be an introduction to the User's Guide here...

Contents:

1.1 Open Anharmonic - Usage & Examples

This will tell about how to actually use the package, with a focus on interactive usage.

Contents

1.1.1 const

The members of this module fall into three general categories:

- *Atomic number/symbol interconversion*
- *String and numerical constants*
- *Enumerations*

Atomic Numbers & Symbols

Conversions between atomic numbers and symbols is provided by two `dict` members.

`atom_num` provides the atomic number of an atomic symbol passed in **ALL CAPS**:

```
>>> open.const.atom_num['CU']  
29
```

`atom_sym` provides the atomic symbol corresponding to a given atomic number:

```
>>> open.const.atom_sym[96]  
'CM'
```

The elements hydrogen ($Z = 1$) through lawrencium ($Z = 103$) are currently supported.

String/Numerical Constants

The purpose of most of these classes and their member values is sufficiently explained in the respective *API entries*. The classes anticipated to be most useful to users are the physical constants of *PHYS*:

```
>>> from opan.const import PHYS
>>> PHYS.ANG_PER_BOHR
0.52917721067
>>> PHYS.LIGHT_SPEED           # Atomic units
137.036
```

as well as the string representations of engineering units of *UNITS*:

```
>>> from opan.const import UNITS
>>> from opan.const import EnumUnitsRotConst as EURC
>>> UNITS.rot_const[EURC.INV_INERTIA]
'1/(amu*B^2)'
>>> UNITS.rot_const[EURC.ANGFREQ_SECS]
'1/s'
```

Two of the remaining classes, *DEF* and *PRM*, define default values that are primarily relevant to programmatic use of opan. In unusual circumstances, though, they may be useful in console interactions.

CIC currently covers a very limited scope (the minimum and maximum atomic numbers implemented) and will likely not be useful at the console.

Enumerations

From the perspective of the end user, enumerations in opan are “functional types,” which don’t need instantiation before use:

```
>>> opan.const.EnumDispDirection.NO_DISP
'NO_DISP'
```

The enumeration values are simple strings:

```
>>> type(opan.const.EnumDispDirection.NO_DISP)
<class 'str'>
```

While this implementation is susceptible to accidental mixing of enumerated types, it has the advantage of allowing simple *str* inputs to functions expecting enumerated values. This is anticipated to be useful in console-level interactions with a variety of program elements. For example, the engineering units to be output from *opan.utils.inertia.rot_consts()* can be specified simply with the appropriate string, instead of the fully specified enumeration object:

```
>>> from opan.utils.inertia import rot_consts
>>> from opan.const import EnumUnitsRotConst as EURC
>>> rot_consts(some_geom, some_masses, 'INV_INERTIA')           # Works fine
array(...)
>>> rot_consts(some_geom, some_masses, EURC.INV_INERTIA)       # Also works
array(...)
```

As noted in the API documentation for *EnumIterMeta*, both iteration and membership testing with “in” are supported:

```
>>> 'NO_DISP' in opan.const.EnumDispDirection
True
>>> [e for e in sorted(opan.const.EnumDispDirection)]
['NEGATIVE', 'NO_DISP', 'POSITIVE']
```

1.1.2 error

Note: Most interactive use of `opan` will not require detailed knowledge of the custom errors in this module.

The custom exceptions in this module are all subclassed from `opan.error.OpenError`, which itself is a subclass of `Exception`. In addition to the typical error message included as part of initializing an `Exception`, the custom error subclasses of `OpenError` also define a `typecode` and a `source` attribute (typically a filename or other data source) to allow more finely-grained definition of error origins and types. In the below example, attempting to import the source file for this usage page as an OpenBabel XYZ file quite sensibly results in an error:

```
>>> x = opan.xyz.OpenXYZ(path='error.rst')
Traceback (most recent call last):
...
XYZError: (XYZFILE) No valid geometry found: XYZ file: error.rst
```

The custom exception `XYZError` is raised with `typecode` `XYZFILE`, indicating a problem with the indicated input file. The external data source causing the exception is included after the final colon (`error.rst`, this file). If no data source is relevant to a given exception, it is omitted.

The subclasses of `opan.const.OpenEnum` are equipped with membership testing of and iteration over their respective `typecodes`:

```
>>> 'XYZFILE' in XYZError
True
>>> [tc for tc in sorted(XYZError)]
['DIHED', 'NONPRL', 'OVERWRITE', 'XYZFILE']
```

Raising these exceptions follows standard syntax, save for the extra ‘`typecode`’ and ‘`source`’ parameters:

```
>>> raise XYZError(XYZError.OVERWRITE, "Spurious overwrite", "Console")
Traceback (most recent call last):
...
XYZError: (OVERWRITE) Spurious overwrite: Console
```

1.1.3 grad

Draft scratch content...

Gradient objects are a thing that have to be properly done in order for various of the automation functiony applications of the `opan` to work right, since different softwares make their things in different ways, but the core automating thingy has to not care what software made the data but the data has to be presented uniformly. Most console interactions with `opan` won’t care about this much, but it’s worth noting here the things that can be expected from ALL thingies, even though many other thingies will likely be available for any given other various software.

Firstly, the instance members specified as having to be there by `SuperOpanGrad`:

- `gradient` – 1-D `np.array` of `np.float` – Gradient data in $\left(\frac{E_h}{B}\right)$ *units*
- `geom` – 1-D `np.array` of `np.float` – Geometry data in `B` *units*
- `atom_syms` – list of `str` – Atomic symbols in **ALL CAPS**

There will need to be a private `_load` method, but that shouldn’t ever be useful or usable, interactively.

Other than that, the below subpages describe the software-specific data available in the specific subclass objects of `SuperOpanGrad`.

Implemented Subclasses

OrcaEngrad

Stuff

1.1.4 hess

Stuff

OrcaHess

Stuff

1.1.5 output

Stuff

OrcaOutput

Stuff

1.1.6 utils

Stuff

utils (base)

Stuff

utils.decorate

Stuff

utils.execute

Stuff

utils.inertia

Stuff

utils.symm

This module doesn't really work at present. It is planned to eventually attempt to fix it...

utils.vector

Stuff

1.1.7 vpt2

This module doesn't really exist yet. Sorry.

1.1.8 xyz

Stuff

1.2 Open Anharmonic - Theory

This will introduce the various calculations for which theory is provided here.

Contents:

1.2.1 Vector Operations

This will introduce the various vector operation sections.

1.2.2 Symmetry Operations

Introduction to discussion of implemented symmetry operations.

1.2.3 Inertial Properties

This will introduce the exposition of the inertial properties.

1.2.4 Harmonic Vibrational Frequencies

Intro about what's laid out about harmonic frequencies.

1.2.5 VPT2 Anharmonic Frequencies

Intro to everything described about VPT2.

1.2.6 Centrifugal Distortion

Intro to what's expositied about the centrifugal distortion calculations.

Open Anharmonic API

The full public API is delineated below. Cross-references to NumPy are displayed with the `np` package abbreviation.

Note: Documented or undocumented attributes, functions, methods, etc. named with a leading underscore are **NOT** formally part of the API. Their behavior may change without notice.

- *const*
- *error*
- *grad*
- *hess*
- *output*
- *utils*
 - *decorate*
 - *execute*
 - *inertia*
 - *symm*
 - *vector*
- *vpt2*
 - *repo*
- *xyz*

2.1 `opan.const`

Defines objects bearing assorted constants for Open Anharmonic.

2.1.1 Module-Level Members

`open.const.infty`
str – Unicode infinity symbol

`open.const.atom_num`
dict – Atomic number lookup from element symbol

Note: Keys for *atom_num* are **all uppercase** (e.g., ‘AR’ for argon)

`open.const.atom_sym`
dict – Element symbol lookup from atomic number, returned as **all uppercase**

2.1.2 Classes

Overview

Constants Classes

CIC – Application-internal code information constants

DEF – Default values for parameters intended to be user-adjustable

PHYS – Physical constants

PRM – Internal computation parameters, intended to be non-user-adjustable

UNITS – Functions returning text strings of units descriptions

Enumeration Classes

EnumIterMeta – Metaclass for iterable enumerations supporting membership testing with *in*

OpenEnum – Superclass for enumerations

Plain Enumerations

EnumCheckGeomMismatch – Mismatch type found during *check_geom()* comparison checks of two geometries.

EnumDispDirection – Displacement direction along a particular mode

EnumFileType – Various file types relevant to the software packages

EnumMassPertType – Type of atomic mass perturbation being applied

EnumSoftware – Implemented computational software packages

EnumTopType – Molecular top classification

Anharmonic (VPT2) HDF5 Repository Enumerations

EnumAnharmRepoData – Displacement-specific values

EnumAnharmRepoParam – Displacement-nonspecific values

Units Enumerations

Units implemented for numerical conversions for various physical quantities.

EnumUnitsRotConst – Rotational constants

API

class `open.const.CIC`

Bases: `object`

Container for application-internal code information constants

These may need expansion into dictionaries keyed by *EnumSoftware* enum values, depending on the atoms supported by various software packages. They may also require adjustment to accommodate ‘special’ atom types such as ghost atoms and point charges.

Members

MAX_ATOMIC_NUM = 103

`int` – Maximum atomic number supported

MIN_ATOMIC_NUM = 1

`int` – Minimum atomic number supported

class `open.const.DEF`

Bases: `object`

Container for default parameter values (possibly user-adjustable)

FILE_EXTS = {'ORCA': {'GRAD': 'engrad', 'INPUTFILE': 'txt', 'XYZ': 'XYZ', 'HESS': 'hess', 'OUTPUT': 'out'}}
`dict` of `dict` – Dictionary of dictionaries of file extensions for geometry, gradient, hessian, etc. files from the various software suites.

Access as `FILE_EXTS[EnumSoftware][EnumFileType]`

GRAD_COORD_MATCH_TOL = 1e-07

`float` – Max precision of GRAD geometries (currently *ORCA*-specific)

HESS_COORD_MATCH_TOL = 1e-06

`float` – Max precision of HESS geometries (currently *ORCA*-specific)

HESS_IR_MATCH_TOL = 0.01

`float` – Max precision of freqs in IR spectrum block (currently *ORCA*-specific)

MASS_PERT_MAG = 0.0001

`float` – Relative magnitude of atomic mass perturbations

ORTHONORM_TOL = 1e-08

`float` – Acceptable deviation from Kronecker delta for orthonormality testing

XYZ_COORD_MATCH_TOL = 1e-12

`float` – Max tolerable deviation between XYZ geoms (currently *ORCA*-specific)

class `open.const.EnumAnharmRepoData`

Bases: `open.const.OpenEnum`

Enumeration class for datatypes in VPT2 HDF5 repository.

Contains enumeration parameters to indicate the type of data to be retrieved from the on-disk HDF5 repository in the VPT2 anharmonic calculations of the *open.vpt2* submodule.

Enum Values

ENERGY = 'ENERGY'

Energy value at the given displacement

GEOM = 'GEOM'

Geometry at the given displacement (max precision available)

GRAD = 'GRAD'

Cartesian gradient vector

HESS = 'HESS'

Cartesian Hessian matrix

class `open.const.EnumAnharmRepoParam`

Bases: `open.const.OpenEnum`

Enumeration class for parameters in VPT2 HDF5 repository.

Contains enumeration parameters to indicate the parameter value to be retrieved from the on-disk HDF5 repository in the VPT2 anharmonic calculations of the `open.vpt2` submodule.

Enum Values

ATOMS = 'ATOMS'

Length- N vector of all-caps atomic symbols

CTR_MASS = 'CTR_MASS'

Cartesian center of mass of system, *with perturbations applied*, if any

INCREMENT = 'INCREMENT'

Displacement increment in $\text{B u}^{1/2}$. Note that these are *not* atomic *units*, which would instead be $\text{B m}_e^{1/2}$.

PERT_MODE = 'PERT_MODE'

`open.const.EnumMassPertType` indicating perturbation type

PERT_VEC = 'PERT_VEC'

Length- $3*N$ vector of perturbation factors (all should be ~ 1)

REF_MASSES = 'REF_MASSES'

Reference values of atomic masses (unperturbed)

class `open.const.EnumCheckGeomMismatch`

Bases: `open.const.OpenEnum`

Enumeration for mismatch types in `check_geom()`

Only mismatches of validly constructed coordinates and atoms vector combinations are represented here; other mismatches/misconfigurations result in raised Exceptions.

Enum Values

ATOMS = 'ATOMS'

Mismatch in individual atom(s)

COORDS = 'COORDS'

Mismatch in individual coordinate(s)

DIMENSION = 'DIMENSION'

Mismatch in dimensions of the two geometries

class `open.const.EnumDispDirection`

Bases: `open.const.OpenEnum`

Enumeration class for displacement directions.

Contains enumeration parameters to indicate the displacement of the molecular geometry associated with a gradient, hessian or other object.

Enum Values

NEGATIVE = 'NEGATIVE'

Negative displacement along a particular normal mode

NO_DISP = 'NO_DISP'

Non-displaced geometry

POSITIVE = 'POSITIVE'

Positive displacement along a particular normal mode

class `opan.const.EnumFileType`

Bases: `opan.const.OpenEnum`

Enumeration class for the file types generated by computational codes.

Enum Values

GRAD = 'GRAD'

Files containing nuclear gradient information

HESS = 'HESS'

Files containing nuclear Hessian information

INPUTFILE = 'INPUTFILE'

Input files for defining computations

OUTPUT = 'OUTPUT'

Files containing computational output

XYZ = 'XYZ'

XYZ atomic coordinates, assumed to follow the [Open Babel XYZ specification](#)

class `opan.const.EnumIterMeta`

Bases: `type`

Metaclass for enumeration types allowing *in* membership testing.

__iter__()

Iterate over all defined enumeration values.

Generator iterating over all class variables whose names match their contents. For a properly constructed `OpenEnum` subclass, these are identical to the enumeration values.

Example:

```
>>> [val for val in sorted(opan.const.EnumDispDirection)]
['NEGATIVE', 'NO_DISP', 'POSITIVE']
```

__contains__(value)

Returns `True` if *value* is a valid value for the enumeration type, else `False`.

Example:

```
>>> 'NO_DISP' in opan.const.EnumDispDirection
True
```

class `opan.const.EnumMassPertType`

Bases: `opan.const.OpenEnum`

Enumeration class for atom mass perturbation types.

Contains enumeration parameters to indicate the type of mass perturbation to be applied to the various atoms of a geometry, in order to: (a) break inertial degeneracy sufficiently to allow VPT2 computation using a lower-symmetry formalism; and (b), in the case of linear molecules, introduce an artificial ‘directional preference’ to the masses of the atoms (`BY_COORD` enum value) to break the intrinsic degeneracy of the bending modes.

Enum Values

BY_ATOM = 'BY_ATOM'

Atomic masses are perturbed atom-by-atom in an isotropic fashion

BY_COORD = 'BY_COORD'

Atomic masses are perturbed anisotropically, where the perturbation factor for each atom's mass varies slightly in the x-, y-, and z-directions

NO_PERTURB = 'NO_PERTURB'

Atomic masses are used without modification

class `opan.const.EnumSoftware`

Bases: `opan.const.OpenEnum`

Enumeration class for identifying computational chemistry packages.

This enum will be expanded if/when support for additional packages is implemented.

Enum Values

ORCA = 'ORCA'

The *ORCA* program package

class `opan.const.EnumTopType`

Bases: `opan.const.OpenEnum`

Enumeration class for classifying types of molecular tops.

Contains enumeration parameters to indicate the type of molecular top associated with a particular geometry.

Inertial moments with magnitudes less than `opan.const.PRM.ZERO_MOMENT_TOL` are taken as zero. Nonzero moments by this metric are considered to be equal if their ratio differs from unity by less than `opan.const.PRM.EQUAL_MOMENT_TOL`. See `opan.utils.inertia.principals()` and the other functions defined in `opan.utils.inertia` for more details.

Enum Values

ASYMM = 'ASYMM'

Three unique non-zero moments

ATOM = 'ATOM'

Three zero principal inertial moments

LINEAR = 'LINEAR'

One zero and two equal non-zero moments

SPHERICAL = 'SPHERICAL'

Three equal, non-zero moments

SYMM_OBL = 'SYMM_OBL'

Three non-zero moments; smallest two equal

SYMM_PROL = 'SYMM_PROL'

Three non-zero moments; largest two equal

class `opan.const.EnumUnitsRotConst`

Bases: `opan.const.OpenEnum`

Units Enumeration class for rotational constants.

Contains enumeration parameters to indicate the associated/desired units of interpretation/display of a rotational constant.

String expressions of these units are provided in `UNITS.rot_const`.

Enum Values

ANGFREQ_ATOMIC = 'ANGFREQ_ATOMIC'

Angular frequency in atomic *units*, $\frac{1}{T_a}$

ANGFREQ_SECS = 'ANGFREQ_SECS'

Angular frequency in SI units, $\frac{1}{s}$ (**NOT** Hz!)

CYCFREQ_ATOMIC = 'CYCFREQ_ATOMIC'

Cyclic frequency in atomic *units*, $\frac{cyc}{T_a}$

CYCFREQ_HZ = 'CYCFREQ_HZ'

Cyclic frequency in Hz, $\frac{cyc}{s}$

CYCFREQ_MHZ = 'CYCFREQ_MHZ'

Cyclic frequency in MHz, millions of $\frac{cyc}{s}$

INV_INERTIA = 'INV_INERTIA'

Inverse moment of inertia, $\frac{1}{u B^2}$. Note that the mass *units* here are *not* atomic units, which would require $\frac{1}{m_e B^2}$.

WAVENUM_ATOMIC = 'WAVENUM_ATOMIC'

Wavenumbers in atomic *units*, $\frac{cyc}{B}$

WAVENUM_CM = 'WAVENUM_CM'

Wavenumbers in conventional units, $\frac{cyc}{cm}$

class `opan.const.OpenEnum`

Bases: `object`

Superclass for enumeration objects.

Metaclassed with `EnumIterMeta` to allow direct iteration and membership testing of enumeration values on the subclass type.

class `opan.const.PHYS`

Bases: `object`

Container for physical constants

Members

ANG_PER_BOHR = 0.52917721067

`float` – Angstroms per Bohr radius (source: [NIST](#))

LIGHT_SPEED = 137.036

`float` – Speed of light in atomic *units*, $\frac{B}{T_a}$. Calculated from the [NIST](#) value for the speed of light in vacuum, $2.99792458e8 \frac{m}{s}$, using `ANG_PER_BOHR` and `SEC_PER_TA` as conversion factors

ME_PER_AMU = 1822.8885

`float` – Electron mass per unified atomic mass unit (source: [NIST](#))

PLANCK = 6.283185307179586

`float` – Standard Planck constant, equal to 2π in atomic *units* of $\frac{E_h T_a}{cyc}$

PLANCK_BAR = 1.0

`float` – Reduced Planck constant, unity by definition in the atomic *units* of $E_h T_a$

SEC_PER_TA = 2.4188843265e-17

`float` – Seconds per atomic time unit (source: [NIST](#))

class `opan.const.PRM`

Bases: `object`

Container for internal computation parameters (not user-adjustable)

Members

EQUAL MOMENT TOL = 0.001

float – Minimum deviation-ratio from unity below which two principal inertial moments are considered equal

MAX SANE DIPDER = 100.0

`float` – Trap value for aberrantly large dipole derivative values in *ORCA* if dipoles are not calculated in a NUMFREQ run

NON PARALLEL TOL = 0.001

`float` – Minimum angle deviation (degrees) required for two vectors to be considered non-parallel

ZERO MOMENT TOL = 0.001

`float` – Threshold value below which moments are considered equal to zero; *units* of u B^2

ZERO VEC TOL = 1e-06

float – Vector magnitude below which a vector is considered equal to the zero vector; dimensionless or *units* of B

```
class opam.const.UNITS
```

Bases: object

Container for dicts providing strings describing the various display units available for physical quantities.

Dictionary keys are the enum values provided in the corresponding `EnumUnits[...]` class in this module (`open.const`).

Dictionary	Enum	Physical Quantity
<code>rot_const</code>	<code>EnumUnitsRotConst</code>	Rotational constant

```
rot_const = {'WAVENUM_CM': 'cyc/cm', 'CYCFREQ_MHZ': 'MHz', 'INV_INERTIA': '1/(amu*B^2)', 'ANGFREQ'
```

2.2 `opan.error`

Defines custom errors for Open Anharmonic

Error classes are subclassed from `Exception` via an abstract superclass, *OpenError*, which defines several common features:

- Storage of a ‘typecode’ and a ‘source’ string along with the error message to allow passing of more fine-grained information to the exception stack
- Implementation of the *EnumIterMeta* metaclass on *OpenError*, enabling typecode validity checking with `in`
- Re-implementation of `__str__()` to enhance the usefulness of stack messages when one of these errors is raised

OpenError Subclasses

AnharmError – Raised as a result of *OpenVPT2* actions

GradError – Raised during parsing of or calculations using gradient data

HessError – Raised during parsing of or calculations using Hessian data

InertiaError – Raised by *opan.utils.inertia* submodule functions

OutputError – Raised during parsing of or calculations using output data

RepoError – Raised by HDF5 repository interactions

SymmError – Raised by *opan.utils.symm* submodule functions

VectorError – Raised by *opan.utils.vector* submodule functions

XYZError – Raised during parsing of or calculations using XYZ data

API

exception *opan.error.AnharmError* (*tc, msg, src*)

Bases: *opan.error.OpenError*

Error relating to *OpenVPT2* actions.

See the *OpenError* documentation for more information on attributes, methods, etc.

Typecodes

REPO = 'REPO'

OpenAnharmRepo conflict – no repo bound when assignment attempted, or attempt made to bind new repo when one already bound

STATUS = 'STATUS'

OpenVPT2 internal variables in inappropriate state for the requested operation

exception *opan.error.GradError* (*tc, msg, src*)

Bases: *opan.error.OpenError*

Error relating to parsing of or calculation from gradient data.

Not all typecodes may be relevant for all software packages.

See the *OpenError* documentation for more information on attributes, methods, etc.

Typecodes

BADATOM = 'BADATOM'

Missing or invalid atom symbols; SHOULD only be used by *SuperOpenGrad*

BADGEOM = 'BADGEOM'

Missing or invalid geometry data; SHOULD only be used by *SuperOpenGrad*

BADGRAD = 'BADGRAD'

Missing or invalid gradient data; SHOULD only be used by *SuperOpenGrad*

ENERGY = 'ENERGY'

Energy value not found

GEOMBLOCK = 'GEOMBLOCK'

Malformed or missing geometry block

GRADBLOCK = 'GRADBLOCK'

Malformed or missing gradient block

NUMATS = 'NUMATS'

Invalid number-of-atoms specification, or specification not found

OVERWRITE = 'OVERWRITE'

Object already initialized (overwrite not supported)

exception *opan.error.HessError* (*tc, msg, src*)

Bases: *opan.error.OpenError*

Error relating to parsing of or calculation from Hessian data.

Not all typecodes may be relevant for all software packages.

See the [OpanError](#) documentation for more information on attributes, methods, etc.

Typecodes

AT_BLOCK = 'AT_BLOCK'

Malformed or missing atom/geometry specification block

BADATOM = 'BADATOM'

Missing or invalid atom symbols; SHOULD only be used by [SuperOpanHess](#)

BADGEOM = 'BADGEOM'

Missing or invalid geometry data; SHOULD only be used by [SuperOpanHess](#)

BADHESS = 'BADHESS'

Missing or invalid Hessian data; SHOULD only be used by [SuperOpanHess](#)

DIPDER_BLOCK = 'DIPDER_BLOCK'

Malformed dipole derivatives block

EIGVAL_BLOCK = 'EIGVAL_BLOCK'

Malformed mass-weighted-Hessian eigenvalues block

EIGVEC_BLOCK = 'EIGVEC_BLOCK'

Malformed mass-weighted-Hessian eigenvectors block

ENERGY = 'ENERGY'

Malformed or missing energy value

FREQ_BLOCK = 'FREQ_BLOCK'

Malformed or missing frequencies block

HESS_BLOCK = 'HESS_BLOCK'

Malformed or missing Hessian block

IR_BLOCK = 'IR_BLOCK'

Malformed IR spectrum block

JOB_BLOCK = 'JOB_BLOCK'

Malformed job list block

MODES_BLOCK = 'MODES_BLOCK'

Malformed or missing normal modes block

OVERWRITE = 'OVERWRITE'

Object already initialized (overwrite not supported)

POLDER_BLOCK = 'POLDER_BLOCK'

Malformed polarizability derivatives block

RAMAN_BLOCK = 'RAMAN_BLOCK'

Malformed Raman spectrum block

TEMP = 'TEMP'

Malformed or missing temperature value

exception `opan.error.InertiaError (tc, msg, src)`

Bases: [opan.error.OpanError](#)

Error relating to [opan.utils.inertia](#) submodule functions.

See the [OpanError](#) documentation for more information on attributes, methods, etc.

Typecodes

BAD_GEOM = 'BAD_GEOM'

A geometry being parsed was unsuitable for a particular type of calculation/manipulation

NEG_MOMENT = 'NEG_MOMENT'

A negative principal inertial moment was computed

TOP_TYPE = 'TOP_TYPE'

No valid molecular top type was identified

exception `opan.error.OpenError` (*tc, msg, src*)

Bases: `Exception`

Base class for custom errors defined for Open Anharmonic

`OpenError` is an abstract superclass of any custom errors defined under the Open Anharmonic umbrella. It defines all common methods shared among the various subtype error classes, such that the only contents that must be declared by a subclass are `str` class variables with contents identical to their names. These are recognized by the `__iter__()` defined in `opan.const.EnumIterMeta` as being the set of valid typecodes.

Parameters

- **tc** – `str` – String representation of typecode to be associated with the `OpenError` subclass instance. *Must* be a validly constructed typecode defined for the relevant subclass.
- **msg** – `str` – Explanation of the nature of the error being reported
- **src** – `str` – Further detail of the code/file source of the error behavior, if relevant

Raises

- `NotImplementedError` – Upon attempt to instantiate abstract `OpenError` base class
- `KeyError` – Upon instantiation with an invalid typecode

msg

`str` – Explanation of the nature of the error being reported

src

`str` – Further detail of the code source of the error behavior

subclass_name

`str` – String representation of the `OpenError` subclass name

tc

`str` – String typecode associated with the instance

__str__()

String representation of an `OpenError` subclass instance.

Implemented primarily so that the error stack handling of the Python interpreter will provide useful information to the user.

Return value is constructed as:

(typecode string) Error message: Error source

Returns *retstr* – `str` – String representation of the instance.

exception `opan.error.OutputError` (*tc, msg, src*)

Bases: `opan.error.OpenError`

Error relating to parsing of or calculation from output data.

See the `OpenError` documentation for more information on attributes, methods, etc.

Typecodes

(none yet)

exception `opan.error.RepoError` (*tc, msg, src*)

Bases: `opan.error.OpenError`

Error relating to HDF5 repository interactions.

See the `OpenError` documentation for more information on attributes, methods, etc.

Typecodes

DATA = 'DATA'

Problem with a dataset in linked HDF5 `File`

GROUP = 'GROUP'

Problem with a group in linked HDF5 `File`

STATUS = 'STATUS'

HDF5 repo in improper status for requested operation

exception `opan.error.SymmError` (*tc, msg, src*)

Bases: `opan.error.OpenError`

Error relating to `opan.utils.symm` submodule functions.

See the `OpenError` documentation for more information on attributes, methods, etc.

Typecodes

NOTFOUND = 'NOTFOUND'

Symmetry element expected but not found

exception `opan.error.VectorError` (*tc, msg, src*)

Bases: `opan.error.OpenError`

Error relating to `opan.utils.vector` submodule functions.

See the `OpenError` documentation for more information on attributes, methods, etc.

Typecodes

NONPRL = 'NONPRL'

Insufficient non-parallel character in some manner of calculation

ORTHONORM = 'ORTHONORM'

Vectors which should have been orthonormal were determined not to be

exception `opan.error.XYZError` (*tc, msg, src*)

Bases: `opan.error.OpenError`

Error relating to parsing of or calculation using XYZ data.

See the `OpenError` documentation for more information on attributes, methods, etc.

Typecodes

DIHED = 'DIHED'

Dihedral angle calculation requested for a set of atoms containing an insufficiently nonlinear trio of atoms

NONPRL = 'NONPRL'

Insufficient non-parallel character in some manner of calculation

OVERWRITE = 'OVERWRITE'

Object already initialized (overwrite not supported)

XYZFILE = 'XYZFILE'

Inconsistent geometry in an OpenBabel XYZ file

• *ORCA* – .xyz or .trj

2.3 opan.grad

Module implementing imports of gradient data from external computations.

The abstract superclass *SuperOpenGrad* defines a common initializer and common method(s) that for use by subclasses importing gradient data from external computational packages.

Implemented Subclasses

OrcaEngrad – Imports ‘.engrad’ files from *ORCA*

Requirements

- The import for each external software package SHOULD have its own subclass.
- Each subclass MUST implement a `_load(self, **kwargs)` instance method as the entry point for import of gradient data.
- The gradient data MUST be stored:
 - In the instance member `self.gradient`
 - As a one-dimensional `np.array`
 - With *dtype* descended from `np.float`
 - In *units* of Hartrees per Bohr ($\frac{E_h}{B}$)
 - With elements ordered as:

$$\left[\frac{\partial E}{\partial x_1} \quad \frac{\partial E}{\partial y_1} \quad \frac{\partial E}{\partial z_1} \quad \frac{\partial E}{\partial x_2} \quad \frac{\partial E}{\partial y_2} \quad \cdots \quad \frac{\partial E}{\partial y_N} \quad \frac{\partial E}{\partial z_N} \right]$$

- The geometry data MUST be stored:
 - In the instance member `self.geom`
 - As a one-dimensional `np.array`
 - With *dtype* descended from `np.float`
 - In *units* of Bohrs (B)
 - With elements ordered as:

$$\left[x_1 \quad y_1 \quad z_1 \quad x_2 \quad y_2 \quad \cdots \quad y_N \quad z_N \right]$$

- The atoms list **MUST** be stored:
 - In the instance member `self.atom_syms`
 - As a `list` of `str`, with each atom specified by an **all-caps** atomic symbol (`opan.const.atom_sym` may be helpful)
- Subclasses **MAY** define an unlimited number of methods, class variables, and/or instance variables of unrestricted type, in addition to those defined above.

Superclass

`class opan.grad.SuperOpanGrad (**kwargs)`

Abstract superclass of gradient import classes.

Performs the following actions:

- 1.Ensures that the abstract superclass is not being instantiated, but instead a subclass.
- 2.Calls the `_load()` method on the subclass, passing all *kwargs* through unmodified.
- 3.Typechecks the `self.gradient`, `self.geom`, and `self.atom_syms` required members for existence, proper data type, and properly matched lengths.

The checks performed in step 3 are primarily for design-time member- and type-enforcement during development of subclasses for newly implemented external software packages, rather than run-time data checking. It is **RECOMMENDED** to include robust data validity checking inside each subclass, rather than relying on these tests.

Methods

`check_geom(coords, atoms[, tol])`

Check for consistency of gradient geometry with input coords/atoms.

The cartesian coordinates associated with a gradient object are considered consistent with the input *coords* if each component matches to within *tol*. If *coords* or *atoms* vectors are passed that are of different length than those stored in the instance, a `False` value is returned, rather than an exception raised.

Parameters

- **coords** – length-3N `np.float_` – Vector of stacked ‘lab-frame’ Cartesian coordinates
- **atoms** – length-N `str` or `int` – Vector of atom symbols or atomic numbers
- **tol** – `float`, optional Tolerance for acceptable deviation of each passed geometry coordinate from that in the instance to still be considered matching. Default value is `DEF.GRAD_COORD_MATCH_TOL`

See `opan.utils.check_geom` for details on return values and exceptions raised.

Subclasses

class `open.grad.OrcaEngrad` (*path*='...')

Container for gradient data generated by *ORCA*.

Initialize by passing the path to the file to be loaded as the *path* keyword argument.

Key information contained includes the gradient, the energy, the number of atoms, the geometry, and the atom IDs. For *ORCA*, the precision of the geometry is inferior to that in an XYZ file.

Methods

`_load` (***kwargs*)

Initialize *OrcaEngrad* object from .engrad file

Searches indicated file for energy, geometry, gradient, and number of atoms and stores in the corresponding instance variables.

Parameters *path* – *str* – Complete path to the .engrad file to be read.

Raises

- *GradError*

Typecode *OVERWRITE* – If *OrcaEngrad* instance has already been instantiated.

Various typecodes – If indicated gradient file is malformed in some fashion

- *IOError* – If the indicated file does not exist or cannot be read

Class Variables

class *Pat*

re.compile() patterns for data parsing.

atblock

Captures the entire block of atom ID & geometry data.

atline

Extracts single lines from the atom ID / geometry block.

energy

Captures the electronic energy.

gradblock

Captures the gradient data block.

numats

Retrieves the stand-alone ‘number of atoms’ field.

Instance Variables

`OrcaEngrad.atom_syms`
length-N `list` of `str` – Uppercased atomic symbols for the atoms in the system.

`OrcaEngrad.energy`
`float` – Single-point energy for the geometry.

`OrcaEngrad.geom`
length-3N `np.float_` – Vector of the atom coordinates in B.

`OrcaEngrad.gradient`
length-3N `np.float_` – Vector of the Cartesian gradient in $\frac{E_h}{B}$.

`OrcaEngrad.in_str`
`str` – Complete text of the ENGRAD file read in to generate the *OrcaEngrad* instance.

`OrcaEngrad.num_ats`
`int` – Number of atoms in the geometry ('N')

2.4 opan.hess

Module implementing imports of Hessian data from external computations.

The abstract superclass *SuperOpenHess* defines a common initializer and common method(s) for use by subclasses importing Hessian data from external computational packages.

Implemented Subclasses

OrcaHess – Imports '.hess' files from *ORCA*

Requirements

- The import for each external software package SHOULD have its own subclass.
- Each subclass MUST implement a `_load(**kwargs)` method as the entry point for import of Hessian data.
- The Hessian data MUST be stored:
 - In the instance member `self.hess`
 - As a two-dimensional `np.array`
 - With `dtype` descended from `np.float`
 - In *units* of Hartrees per Bohr-squared ($\frac{E_h}{B^2}$)
 - With elements arranged as:

$$\begin{bmatrix} \frac{\partial^2 E}{\partial x_1^2} & \frac{\partial^2 E}{\partial x_1 \partial y_1} & \frac{\partial^2 E}{\partial x_1 \partial z_1} & \frac{\partial^2 E}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 E}{\partial x_1 \partial y_N} & \frac{\partial^2 E}{\partial x_1 \partial z_N} \\ \frac{\partial^2 E}{\partial y_1 \partial x_1} & \frac{\partial^2 E}{\partial y_1^2} & \frac{\partial^2 E}{\partial y_1 \partial z_1} & \frac{\partial^2 E}{\partial y_1 \partial x_2} & \cdots & \frac{\partial^2 E}{\partial y_1 \partial y_N} & \frac{\partial^2 E}{\partial y_1 \partial z_N} \\ \frac{\partial^2 E}{\partial z_1 \partial x_1} & \frac{\partial^2 E}{\partial z_1 \partial y_1} & \frac{\partial^2 E}{\partial z_1^2} & \frac{\partial^2 E}{\partial z_1 \partial x_2} & \cdots & \frac{\partial^2 E}{\partial z_1 \partial y_N} & \frac{\partial^2 E}{\partial z_1 \partial z_N} \\ \frac{\partial^2 E}{\partial x_2 \partial x_1} & \frac{\partial^2 E}{\partial x_2 \partial y_1} & \frac{\partial^2 E}{\partial x_2 \partial z_1} & \frac{\partial^2 E}{\partial x_2^2} & \cdots & \frac{\partial^2 E}{\partial x_2 \partial y_N} & \frac{\partial^2 E}{\partial x_2 \partial z_N} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{\partial^2 E}{\partial y_N \partial x_1} & \frac{\partial^2 E}{\partial y_N \partial y_1} & \frac{\partial^2 E}{\partial y_N \partial z_1} & \frac{\partial^2 E}{\partial y_N \partial x_2} & \cdots & \frac{\partial^2 E}{\partial y_N^2} & \frac{\partial^2 E}{\partial y_N \partial z_N} \\ \frac{\partial^2 E}{\partial z_N \partial x_1} & \frac{\partial^2 E}{\partial z_N \partial y_1} & \frac{\partial^2 E}{\partial z_N \partial z_1} & \frac{\partial^2 E}{\partial z_N \partial x_2} & \cdots & \frac{\partial^2 E}{\partial z_N \partial y_N} & \frac{\partial^2 E}{\partial z_N^2} \end{bmatrix}$$

Note: The Hessian is elsewhere assumed to be symmetric (real-Hermitian), and thus MUST be returned as such here. Symmetric character is **NOT** explicitly checked, however!

- The geometry data MUST be stored:
 - In the instance member `self.geom`
 - As a one-dimensional `np.array`
 - With `dtype` descended from `np.float`
 - In `units` of Bohrs (B)
 - With elements ordered as:

$$\begin{bmatrix} x_1 & y_1 & z_1 & x_2 & y_2 & \cdots & y_N & z_N \end{bmatrix}$$

- The atoms list MUST be stored:
 - In the instance member `self.atom_syms`
 - As a `list` of `str`, with each atom specified by an **all-caps** atomic symbol (`opan.const.atom_sym` may be helpful)
- Subclasses MAY define an unlimited number of methods, class variables, and/or instance variables in addition to those defined above, of unrestricted type.

Superclass

class `opan.hess.SuperOpanHess` (***kwargs*)

Abstract superclass of Hessian import classes.

Performs the following actions:

- 1.Ensures that the abstract superclass is not being instantiated, but instead a subclass.
- 2.Calls the `_load()` method on the subclass, passing all `kwargs` through unmodified.
- 3.Typechecks the `self.hess`, `self.geom`, and `self.atom_syms` required members for existence, proper data type, and properly matched lengths/dimensions.

The checks performed in step 3 are primarily for design-time member and type enforcement during development of subclasses for new external software packages, rather than run-time data checking. It is RECOMMENDED to include robust data validity checking inside each subclass, rather than relying on these tests.

Methods

check_geom (*coords*, *atoms*[, *tol*])

Check for consistency of Hessian geometry with input coords/atoms.

The cartesian coordinates associated with a Hessian object are considered consistent with the input *coords* and *atoms* if each component matches to within *tol* and all atoms are identical. If *coords* or *atoms* vectors are passed that are of different length than those stored in the instance, a `False` value is returned, rather than an exception raised.

Parameters

- **coords** – length-3N `np.float_` – Vector of stacked ‘lab-frame’ Cartesian coordinates
- **atoms** – length-N `str` or `int` – Vector of atom symbols or atomic numbers
- **tol** – `float`, optional – Tolerance for acceptable deviation of each passed geometry coordinate from that in the instance to still be considered matching. Default value is `DEF.HESS_COORD_MATCH_TOL`

See `open.utils.check_geom` for details on return values and exceptions raised.

Subclasses

class `open.hess.OrcaHess` (*path*=‘...’)

Container for HESS data generated by *ORCA*.

Initialize by passing the path to the file to be loaded as the *path* keyword argument.

Information contained includes the Hessian matrix, the number of atoms, the atomic symbols, the atomic weights, and the geometry, as reported in the .hess file. See ‘Instance Variables’ below for a full list. For variables marked “required”, a `HessError` is raised if the block is not found, whereas for variables marked “optional” a `None` value is stored. For either type, if the data is malformed or invalid in some fashion, a `HessError` is raised with an appropriate typecode.

Zero frequencies corresponding to translation/rotation are **not** excised from the frequencies list, normal modes, IR spectrum, Raman spectrum, etc.

The precision of the geometry is less than that reported in an .xyz file, and thus should **not** be used for generation of subsequent computations.

Output *units*:

- Hessian : Hartrees per Bohr-squared ($\frac{E_h}{B^2}$)
- Frequencies : Wavenumbers ($\frac{cyc}{cm}$)
- IR intensities (T^2 values) : $\frac{km}{mol}$
- Raman activities : $\frac{\text{\AA}^4}{u}$
- Dipole derivatives : (???)
- Polarizability derivatives : (???)
- Eigenvalues of the mass-weighted Hessian : $\frac{E_h}{u B^2}$

- Eigenvectors of the mass-weighted Hessian : (dimensionless)

Methods

`_load(kwargs)`**

Initialize OrcaHess Hessian object from .hess file

Searches indicated file for data blocks within the .hess file. The geometry, Hessian block, frequencies, and normal modes must be present and will be retrieved; other blocks will be imported if present, or ignored if absent (stored as `None` in the resulting object). If malformed/inaccurate data is found in any block that is present, some flavor of `HessError` will be raised.

Parameters `path` – `str` – `kwargs` parameter specifying complete path to the .hess file to be read.

Raises

- `HessError` – (various typecodes) If indicated Hessian file is malformed in some fashion.
- `KeyError` – If invalid atomic symbol appears in .hess file.
- `IOError` – If the indicated file does not exist or cannot be read.

Class Variables

class `Pat`

`re.compile()` patterns for data parsing.

`at_block`

Captures the entire block of atom IDs & weights, as well as the geometry data.

`at_line`

Retrieves individual lines within the atom / geometry specification block.

`dipder_block`

Captures the entire dipole derivatives block.

`dipder_line`

Retrieves individual lines in the dipole derivatives block.

`eigvals_block`

Captures the entire mass-weighted Hessian eigenvalues block.

`eigvals_line`

Retrieves individual lines of the mass-weighted hessian eigenvalues block.

`eigvecs_block`

Captures the entire set of mass-weighted Hessian eigenvectors blocks.

eigvecs_sec

Extracts sections (individual blocks) of the mass-weighted Hessian eigenvectors blocks.

eigvecs_line

Retrieves individual lines of a mass-weighted Hessian eigenvectors block.

energy

Retrieves the energy reported in the .hess file.

freq_block

Captures the entire vibrational frequencies block.

freq_line

Retrieves individual lines of the frequencies block.

hess_block

Captures the entire set of Hessian blocks.

hess_sec

Extracts full-height, 3- or 6-column sections (individual blocks) of the set of Hessian blocks.

hess_line

Retrieves individual lines within a Hessian block.

jobs_block

Captures the entire job list block.

jobs_line

Retrieves individual lines of the job list block.

ir_block

Captures the entire IR spectrum block

ir_line

Retrieves individual lines of the IR spectrum block

modes_block

Captures the entire set of (weighted, column-normalized) normal modes blocks

modes_sec

Extracts full-height, 3- or 6-column sections (individual blocks) of the set of normal modes blocks

modes_line

Retrieves individual lines within a normal modes block

polder_block

Captures the polarizability derivatives block

polder_line

Retrieves individual lines in the polarizability derivatives block

raman_block

Captures the Raman spectrum block

raman_line

Retrieves individual lines in the Raman spectrum block

temp

Retrieves the ‘actual temperature’ field (sometimes is spuriously zero)

Instance Variables

OrcaHess.atom_masses
length-N `list` of `np.float_` – List of atom masses as reported in the .hess file

OrcaHess.atom_syms
length-N `list` of `str` – List of uppercase atomic symbols

OrcaHess.dipders
3N x 3 `np.float_` – Matrix of dipole derivatives

OrcaHess.energy
`float` – Electronic energy reported in the Hessian file

OrcaHess.freqs
length-3N `np.float_` – Vibrational frequencies in $\frac{\text{cyc}}{\text{cm}}$, as reported in the Hessian file

OrcaHess.geom
length-3N `np.float_` – Geometry vector

OrcaHess.hess
3N x 3N `np.float_` – Cartesian Hessian matrix

OrcaHess.hess_path
`str` – Complete path/filename from which the Hessian data was retrieved

OrcaHess.in_str
`str` – Complete contents of the imported .hess file

OrcaHess.ir_comps
3N x 3 `np.float_` – (T_x, T_y, T_z) components of the transition dipole for each normal mode

OrcaHess.ir_mags
length-3N `np.float_` – T^2 values (squared-magnitudes) of the transition dipole for each mode

OrcaHess.joblist
N x 3 `bool` – Completion status for each displacement in calculation of the Hessian

OrcaHess.modes
3N x 3N `np.float_` – Rotation- and translation-purified, mass-weighted vibrational normal modes, with each mode (column vector) separately normalized by *ORCA*.

OrcaHess.mwh_eigvals
length-3N `np.float_` – Eigenvalues of the mass-weighted Hessian, in $\frac{E_h}{u B^2}$

OrcaHess.mwh_eigvecs
3N x 3N `np.float_` – Eigenvectors of the mass-weighted Hessian, as column vectors: the eigenvector of eigenvalue i would be retrieved with `mwh_eigvecs[:, i]`

OrcaHess.num_ats
`int` – Number of atoms in the system

OrcaHess.polders
3N x 6 `np.float_` – Matrix of Cartesian polarizability derivatives

OrcaHess.raman_acts
length-3N `np.float_` – Vector of Raman activities

OrcaHess.raman_depols
length-3N `np.float_` – Vector of Raman depolarization factors

OrcaHess.temp
`float` – “Actual temperature” reported in the .hess file. Occasionally stored by *ORCA* as a meaningless zero value instead of the temperature used.

2.5 open.output

Module implementing parsing of output data from external computations.

Warning: This module **will** be refactored at some point, to introduce a superclass in the same vein as *SuperOpenGrad* and *SuperOpenHess*. This is necessary because automated execution of external computation softwares will require some unified mechanism for indicating whether a particular computation completed successfully, independent of the identify of the software package that was executed.

Warning: Further refactoring is also planned for *OrcaOutput* generally. Beware relying heavily on the behavior of this class & module.

Superclass

To be implemented

Implemented Subclasses

Note: Not yet actually a subclass of anything

OrcaOutput – Imports output files from *ORCA*

Subclasses

class open.output.**OrcaOutput** (*file_path*)

Container for parsed textual output generated by *ORCA*.

All implemented results that are found in the indicated output are stored in the *OrcaOutput* instance. If a given quantity was not detectable, it is stored as *None* in the corresponding instance variable.

Note: In particular, thermochemistry from single atom/ion computations **should work**, with *None* or zero/negligible values returned for rotational and vibrational quantities.

The verbose contents of the output file are not generally retained within the *OrcaOutput* instance due to the potential for such to involve a tremendously large string. Exceptions include, if present:

- THERMOCHEMISTRY section

Contents

- Methods*

`__init__()`

`en_last()`

•Class Variables

–Enumerations

**EN*

**SPINCONT*

**THERMO*

–Regular Expression Patterns

**p_en*

**p_spincont*

**p_thermo*

•Instance Variables

Methods

`__init__(file_path)`

Initialize *OrcaOutput* object.

Imports the data found in the output file found at *file_path*.

Warning: THIS CLASS PRESENTLY ONLY WORKS ON A **VERY SMALL** SUBSET OF COMPUTATION TYPES, currently HF, LDA-DFT, GGA-DFT, and mGGA-DFT. *MAY* work on some double-hybrid or range-separated DFT.

Available data includes:

- SCF energies (incl D3BJ, gCP, COSMO outlying charge corrections)
- Thermochemistry
- Spin expectation values (actual, ideal, and deviation)

Success indicators include:

•*completed*

Checks for the ‘ORCA TERMINATED NORMALLY’ report at the end of the file

•*converged*

Checks for any occurrence of successful SCF convergence in the file (questionable for anything but single-point calculations)

•*optimized*

Checks for any occurrence of “OPTIMIZATION HAS CONVERGED” in the file (questionable for anything but a standalone OPT – i.e., not useful for a mode or internal coordinate scan)

Parameters `file_path` – *str* – Full path to the output file to be parsed.

Raises *OutputError* – (various typecodes) If indicated output is un-parseably malformed in some fashion

en_last()

Report the energies from the last SCF present in the output.

Returns a `dict` providing the various energy values from the last SCF cycle performed in the output. Keys are those of `p_en`. Any energy value not relevant to the parsed output is assigned as `None`.

Returns `last_ens` – `dict` of `np.float_` – Energies from the last SCF present in the output.

Class Variables Enumerations

class EN

OpenEnum for the energies reported at the end of SCF cycles.

D3

Grimme’s D3BJ dispersion correction [Gri10]. May or may not play nicely with D3ZERO. Likely non-functional with DFT-NL dispersion.

GCP

Grimme’s geometric counterpose (gCP) correction [Kru12]

OCC

COSMO outlying charge correction

SCFFINAL

SCF energy including gCP and D3 corrections

SCFFINALOCC

SCFFINAL energy, but also with COSMO outlying charge correction

SCFOCC

SCF energy with only the COSMO outlying charge correction (no dispersion or gCP corrections)

class OrcaOutput . SPINCONT

OpenEnum for the spin contamination values reported after each unrestricted SCF cycle.

ACTUAL

Calculated $\langle S^2 \rangle$ expectation value

DEV

Deviation of $\langle S^2 \rangle$ (calculated minus ideal)

IDEAL

Ideal $\langle S^2 \rangle$ expectation value

class OrcaOutput . THERMO

OpenEnum for the quantities reported in the THERMOCHEMISTRY block.

BLOCK

Entire THERMOCHEMISTRY block (as `str`)

E_EL

Electronic energy from the thermochemistry block, often slightly different than the last `EN.SCFFINAL` value (E_h)

E_ROT

Thermal rotational internal energy correction (E_h)

E_TRANS

Thermal translational internal energy correction (E_h)

E_VIB

Thermal vibrational internal energy correction (E_h)

E_ZPE

Zero-point energy correction (E_h)

H_IG

Ideal-gas ($k_B T$) enthalpy contribution (E_h)

PRESS

Simulated pressure (atm)

QROT

Rotational partition function (unitless)

TEMP

Simulated temperature (K)

TS_EL

Electronic TS entropy contribution (E_h)

TS_TRANS

Translational TS entropy contribution (E_h)

TS_VIB

Vibrational TS entropy contribution (E_h)

Regular Expression Patterns

`OrcaOutput.p_en`

`dict` of `re.compile()` for the energies reported at the end of SCF cycles. Keys are in `EN`.

`OrcaOutput.p_spincont`

`dict` of `re.compile()` for the spin contamination block values. Keys are in `SPINCONT`.

`OrcaOutput.p_thermo`

`dict` of `re.compile()` for the quantities extracted from the THERMOCHEMISTRY block. Keys are in `THERMO`.

Instance Variables

`OrcaOutput.completed`
 bool – True if *ORCA* output reports normal termination, False otherwise.

`OrcaOutput.converged`
 bool – True if SCF converged ANYWHERE in run.

`OrcaOutput.en`
 dict of list of `np.float_` – Lists of the various energy values from the parsed output. Dict keys are those of *EN*, above. Any energy type not found in the output is assigned as an empty list.

`OrcaOutput.optimized`
 bool – True if any OPT converged ANYWHERE in run. Fine for OPT, but ambiguous for scans.

`OrcaOutput.spincont`
 dict of list of `np.float_` – Lists of the various values from the spin contamination calculations in the output, if present. Empty lists if absent. Dict keys are those of *SPINCONT*, above.

`OrcaOutput.src_path`
 str – Full path to the associated output file

`OrcaOutput.thermo`
 dict of `np.float_` – Values from the thermochemistry block of the parsed output. Dict keys are those of *THERMO*, above.

`OrcaOutput.thermo_block`
 str – Full text of the thermochemistry block, if found.

2.6 opan.utils

Utility functions for Open Anharmonic, including execution automation.

Sub-Modules

decorate – Custom Open Anharmonic decorators

execute – Functions for execution of external computational software packages

inertia – Inertia-related tools (center of mass, rotational constants, principal moments/axes, etc.)

symm – Molecular symmetry utility functions (**INCOMPLETE**)

vector – Vector utility functions

Functions

`opan.utils.base.assert_npfloatarray` (*obj*, *varname*, *desc*, *exc*, *tc*, *errsrc*)
 Assert a value is an `np.array` of NumPy floats.

Pass *None* to *varname* if *obj* itself is to be checked. Otherwise, *varname* is the string name of the attribute of *obj* to check. In either case, *desc* is a string description of the object to be checked, for use in raising of exceptions.

Raises the exception *exc* with typecode *tc* if the indicated object is determined not to be an `np.array`, with a NumPy float dtype.

Intended primarily to serve as an early check for proper implementation of subclasses of *SuperOpanGrad* and *SuperOpanHess*. Early type-checking of key attributes will hopefully avoid confusing bugs downstream.

Parameters

- **obj** – (arbitrary) – Object to be checked, or object with attribute to be checked.
- **varname** – str or None – Name of the attribute of *obj* to be type-checked. *None* indicates to check *obj* itself.

- **desc** – *str* – Description of the object being checked to be used in any raised exceptions.
- **exc** – Subclass of *OpanError* to be raised on a failed typecheck.
- **tc** – Typecode of *exc* to be raised on a failed typecheck.
- **errsrc** – *str* – String description of the source of the data leading to a failed typecheck.

`opan.utils.base.check_geom(c1, a1, c2, a2[, tol])`

Check for consistency of two geometries and atom symbol lists

Cartesian coordinates are considered consistent with the input coords if each component matches to within *tol*. If coords or atoms vectors are passed that are of mismatched lengths, a *False* value is returned.

Both coords vectors must be three times the length of the atoms vectors or a *ValueError* is raised.

Parameters

- **c1** – length-3N *np.float_* – Vector of first set of stacked ‘lab-frame’ Cartesian coordinates
- **a1** – length-N *str* or *int* – Vector of first set of atom symbols or atomic numbers
- **c2** – length-3N *np.float_* – Vector of second set of stacked ‘lab-frame’ Cartesian coordinates
- **a2** – length-N *str* or *int* – Vector of second set of atom symbols or atomic numbers
- **tol** – *float*, optional – Tolerance for acceptable deviation of each geometry coordinate from that in the reference instance to still be considered matching. Default value is specified by `opan.const.DEF.XYZ_COORD_MATCH_TOL`

Returns

- *match* – *bool* – Whether input coords and atoms match (*True*) or not (*False*)
- *fail_type* – *EnumCheckGeomMismatch* or *None* – Type of check failure

If *match* == *True*:

Returns as *None*

If *match* == *False*:

An *EnumCheckGeomMismatch* value indicating the reason for the failed match:

DIMENSION – Mismatch in geometry size (number of atoms)

COORDS – Mismatch in one or more coordinates

ATOMS – Mismatch in one or more atoms

- *fail_loc* – length-3N *bool* or length-N *bool* or *None* – Mismatched elements

If *match* == *True*:

Returns as *None*

If *match* == *False*:

For “array-level” problems such as a dimension mismatch, a *None* value is returned.

For “element-level” problems, a vector is returned indicating positions of mismatch in either *coords* or *atoms*, depending on the value of *fail_type*.

True elements indicate **MATCHING** values

False elements mark **MISMATCHES**

Raises `ValueError` – If a pair of coords & atoms array lengths is inconsistent:

```
if len(c1) != 3 * len(a1) or len(c2) != 3 * len(a2):
    raise ValueError(...)
```

`opan.utils.base.delta_fxn(a, b)`
Kronecker delta for objects *a* and *b*.

Parameters

- **a** – First object
- **b** – Second object

Returns `delta` – `int` – Value of Kronecker delta for provided indices, as tested by Python ==

`opan.utils.base.iterable(y)`
Check whether or not an object supports iteration.

Adapted directly from NumPy ~1.10 at commit 46d2e83.

Parameters **y** – (arbitrary) – Object to be tested.

Returns `test` – `bool` – Returns `False` if `iter()` raises an exception when *y* is passed to it; `True` otherwise.

Examples

```
>>> opan.utils.iterable([1, 2, 3])
True
>>> opan.utils.iterable(2)
False
```

`opan.utils.base.make_timestamp(el_time)`
Generate an hour-minutes-seconds timestamp from an interval in seconds.

Assumes numeric input of a time interval in seconds. Converts this interval to a string of the format “#h #m #s”, indicating the number of hours, minutes, and seconds in the interval. Intervals greater than 24h are unproblematic.

Parameters **el_time** – `int` or `float` – Time interval in seconds to be converted to h/m/s format

Returns `stamp` – `str` – String timestamp in #h #m #s format

`opan.utils.base.pack_tups(*args)`
Pack an arbitrary set of iterables and non-iterables into tuples.

Function packs a set of inputs with arbitrary iterability into tuples. Iterability is tested with `iterable()`. Non-iterable inputs are repeated in each output tuple. Iterable inputs are expanded uniformly across the output tuples. For consistency, all iterables must be the same length.

The input arguments are parsed such that bare strings are treated as **NON-ITERABLE**, through the use of a local subclass of `str` that cripples the `__iter__()` method. Any strings passed are returned in the packed tuples as standard, **ITERABLE** instances of `str`, however.

The order of the input arguments is retained within each output tuple.

No structural conversion is attempted on the arguments.

If all inputs are non-iterable, a list containing a single `tuple` will be returned.

Parameters ***args** – Arbitrary number of arbitrary mix of iterable and non-iterable objects to be packed into tuples.

Returns *tups* – list of *tuple* – Number of tuples returned is equal to the length of the iterables passed in **args*

Raises *ValueError* – If any iterable objects are of different lengths

`opan.utils.base.safe_cast(invar, totype)`

Performs a “safe” typecast.

Ensures that *invar* properly casts to *totype*. Checks after casting that the result is actually of type *totype*. Any exceptions raised by the typecast itself are unhandled.

Parameters

- **invar** – (arbitrary) – Value to be typecast.
- **totype** – *type* – Type to which *invar* is to be cast.

Returns *outvar* – type ‘*totype*’ – Typecast version of *invar*

Raises *TypeError* – If result of typecast is not of type *totype*

`opan.utils.base.template_subst(template, subs[, delims=['<', '>']])`

Perform substitution of content into tagged string.

For substitutions into template input files for external computational packages, no checks for valid syntax are performed.

Each key in *subs* corresponds to a delimited substitution tag to be replaced in *template* by the entire text of the value of that key. For example, the dict `{"ABC": "text"}` would convert `The <ABC> is working to The text is working`, using the default delimiters of ‘<’ and ‘>’. Substitutions are performed in iteration order from *subs*; recursive substitution as the tag parsing proceeds is thus feasible if an `OrderedDict` is used and substitution key/value pairs are added in the proper order.

Start and end delimiters for the tags are modified by *delims*. For example, to substitute a tag of the form `{|TAG|}`, the tuple `("{|", "|}")` should be passed to *subs_delims*. Any elements in *delims* past the second are ignored. No checking is performed for whether the delimiters are “sensible” or not.

Parameters

- **template** – *str* – Template containing tags delimited by *subs_delims*, with tag names and substitution contents provided in *subs*
- **subs** – dict of *str* – Each item’s key and value are the tag name and corresponding content to be substituted into the provided template.
- **delims** – iterable of *str* – Iterable containing the ‘open’ and ‘close’ strings used to mark tags in the template, which are drawn from elements zero and one, respectively. Any elements beyond these are ignored.

Returns *subst_text* – *str* – String generated from the parsed template, with all tag substitutions performed.

2.6.1 opan.utils.decorate

Custom decorators defined for Open Anharmonic.

Decorators

`class opan.utils.decorate.arraysqueeze(*args)`

Converts selected arguments to squeezed np.arrays

Pre-applies an `np.array(...).squeeze()` conversion to all positional arguments according to integer indices passed, and to any keyword arguments according to any strings passed.

Each `int` argument passed instructs the decorator to convert the corresponding positional argument in the function definition.

Each `str` argument passed instructs the decorator to convert the corresponding keyword argument.

`str` parameters corresponding to keyword arguments absent in a particular function call and positional/optional argument indices beyond the range of the actual `*args` of the decorated function are ignored.

Warning: Likely fragile with optional arguments; needs to be tested.

Parameters `*args` (`int` or `str`) – Arguments to convert to squeezed `np.array`.

2.6.2 opan.utils.execute

Functions to enable Open Anharmonic to execute external software packages.

Functions

`opan.utils.execute.execute_orca` (`inp_tp`, `work_dir`, `exec_cmd`, `subs=None`, `subs_delims`=('<', '>'), `sim_name`='orcarun', `inp_ext`='txt', `out_ext`='out', `wait_to_complete`=True, `bohrs`=False)

Executes *ORCA* on a dynamically constructed input file.

Warning: Function is still under active development! Execution with `wait_to_complete == True` should be robust, however.

Execution

Generates an *ORCA* input file dynamically from information passed into the various arguments, performs the run, and returns with exit info and computation results (*in some fashion; still under development*). Any required resources (.gbw, .xyz, etc.) MUST already be present in `work_dir`. No check for pre-existing files of the same base name is made; any such will be overwritten.

ORCA MUST be called using a wrapper script; this function does not implement the redirection necessary to send output from a direct *ORCA* call to a file on disk.

If `wait_to_complete` is `True`, the `subprocess.call()` syntax will be used and the function will not return until execution of the wrapper script completes. If `False`, *indicate what will be returned if not waiting*.

The command to call *ORCA* must be specified in the parameter list syntax of the `args` argument to the `subprocess.Popen` constructor. The implementation is flexible and general, to allow interface with local scripts for, e.g., submission to a job queue in a shared-resource environment.

Valid *ORCA* input syntax of the resulting text is NOT checked before calling *ORCA*.

No mechanism is implemented to detect hangs of *ORCA*. Periodic manual oversight is recommended.

Template Substitution

See `utils.template_subst` for implementation details of the tag substitution mechanism.

Here, in addition to performing any substitutions on the input file template as indicated by `subs`, the special tags **INP** and **OUT**, enclosed with the `subs_delims` delimiters, will be replaced with `sim_name + '.' + inp_ext` and `sim_name + '.' + out_ext`, respectively, in the input template and in all elements of `exec_cmd` before executing the call. In the special case of `inp_ext == None`, the **INP** tag will be replaced with just `sim_name` (no extension), and similarly for **OUT** if `out_ext == None`. The tag **NAME** will be replaced just with `sim_name` in all cases.

`inp_ext` and `out_ext` must be different, to avoid collisions.

Return Values

The information returned depends on the value of `wait_to_complete`:

If `wait_to_complete == True`:

A `tuple` of objects is returned, with elements of type

(OrcaOutput, OpanXYZ, OrcaEngrad, OrcaHess)

These objects contain the corresponding results from the computation, if the latter exist, or `None` if they are missing.

If `wait_to_complete == False`:

TBD, but current intention is to return the PID of the spawned subprocess.

Signature

Parameters

- **inp_tp** – `str` – Template text for the input file to be generated.
- **work_dir** – `str` – Path to base working directory. Must already exist and contain any resource files (.gbw, .xyz, etc.) required for the calculation.
- **exec_cmd** – `list` of `str` – Sequence of strings defining the *ORCA* execution call in the syntax of the `Popen` constructor. This call must be to a local script; stream redirection of the forked process is not supported in this function.
- **subs** – `dict` of `str`, optional – Substitutions to be performed in the template (see *Template Substitution*, above).
- **subs_delims** – 2-`tuple` of `str`, optional – Tag delimiters passed directly to `template_subst()`. Defaults to ('<', '>').
- **sim_name** – `str`, optional – Basename to use for the input/output/working files. If omitted, “orcarun” will be used.
- **inp_ext** – `str`, optional – Extension to be used for the input file generated (default is ‘txt’).
- **out_ext** – `str`, optional – Extension to be used for the output file generated (default is ‘out’).
- **wait_to_complete** – `bool`, optional – Whether to wait within this function for *ORCA* execution to complete (`True`), or to spawn/fork a child process and return (`False`). Default is `True`. `False` **IS NOT YET IMPLEMENTED**.
- **bohrs** – `bool`, optional – Flag to indicate the units (Bohrs or Angstroms) of the coordinates in .xyz and .trj files.

Returns [*varies*] – `tuple` of objects or `int` PID. Varies depending on `wait_to_complete`; see *Return Values* above

Raises

- `ValueError` – If `inp_ext` and `out_ext` are identical.
- `KeyError` – If special tag names **INP**, **OUT**, or **NAME** are defined in `subs`
- `TypeError` – If any elements in `subs` are not tuples

2.6.3 opan.utils.inertia

Utilities for calculation of inertia tensor, principal axes/moments, and rotational constants.

These functions are housed separately from the `opan.vpt2` VPT2 module since they may have broader applicability to other envisioned capabilities of Open Anharmonic.

Functions

`opan.utils.inertia.ctr_geom(geom, masses)`

Returns geometry shifted to center of mass.

Helper function to automate / encapsulate translation of a geometry to its center of mass.

Parameters

- **geom** – length-3N `np.float_` – Original coordinates of the atoms
- **masses** – length-N OR length-3N `np.float_` – Atomic masses of the atoms. Length-3N option is to allow calculation of a per-coordinate perturbed value.

Returns *ctr_geom* – length-3N `np.float_` – Atomic coordinates after shift to center of mass

Raises `ValueError` – If shapes of *geom* & *masses* are inconsistent

`opan.utils.inertia.ctr_mass(geom, masses)`

Calculate the center of mass of the indicated geometry.

Take a geometry and atom masses and compute the location of the center of mass.

Parameters

- **geom** – length-3N `np.float_` – Coordinates of the atoms
- **masses** – length-N OR length-3N `np.float_` – Atomic masses of the atoms. Length-3N option is to allow calculation of a per-coordinate perturbed value.

Returns *ctr* – length-3 `np.float_` – Vector location of center of mass

Raises `ValueError` – If *geom* & *masses* shapes are inconsistent

`opan.utils.inertia.inertia_tensor(geom, masses)`

Generate the 3x3 moment-of-inertia tensor.

Compute the 3x3 moment-of-inertia tensor for the provided geometry and atomic masses. Always recenters the geometry to the center of mass as the first step.

Reference for inertia tensor: [\[Kro92\]](#), Eq. (2.26)

Parameters

- **geom** – length-3N `np.float_` – Coordinates of the atoms
- **masses** – length-N OR length-3N `np.float_` – Atomic masses of the atoms. Length-3N option is to allow calculation of a per-coordinate perturbed value.

Returns *tensor* – 3 x 3 `np.float_` – Moment of inertia tensor for the system

Raises `ValueError` – If shapes of *geom* & *masses* are inconsistent

`opan.utils.inertia.principals(geom, masses[, on_tol])`

Principal axes and moments of inertia for the indicated geometry.

Calculated by `scipy.linalg.eigh()`, since the moment of inertia tensor is symmetric (real-Hermitian) by construction. More convenient to compute both the axes and moments at the same time since the eigenvectors must be processed to ensure repeatable results.

The principal axes (inertia tensor eigenvectors) are processed in a fashion to ensure repeatable, **identical** generation, including orientation AND directionality.

Parameters

- **geom** – length-3N `np.float_` – Coordinates of the atoms
- **masses** – length-N OR length-3N `np.float_` – Atomic masses of the atoms. Length-3N option is to allow calculation of a per-coordinate perturbed value.
- **on_tol** – `np.float_`, optional – Tolerance for deviation from unity/zero for principal axis dot products within which axes are considered orthonormal. Default is `opan.const.DEF.ORTHONORM_TOL`.

Returns

- **moments** – length-3 `np.float_` – Principal inertial moments, sorted in increasing order ($0 \leq I_A \leq I_B \leq I_C$)
- **axes** – 3 x 3 `np.float_` – Principal axes, as column vectors, sorted with the principal moments and processed for repeatability. The axis corresponding to `moments[i]` is retrieved as `axes[:, i]`
- **top** – `EnumTopType` – Detected molecular top type

`opan.utils.inertia.rot_consts(geom, masses[, units[, on_tol]])`

Rotational constants for a given molecular system.

Calculates the rotational constants for the provided system with numerical value given in the units provided in *units*. The orthonormality tolerance *on_tol* is required in order to be passed through to the `principals()` function.

If the system is linear or a single atom, the effectively-zero principal moments of inertia will be assigned values of `opan.const.PRM.ZERO_MOMENT_TOL` before transformation into the appropriate rotational constant units.

The moments of inertia are always sorted in increasing order as $0 \leq I_A \leq I_B \leq I_C$; the rotational constants calculated from these will thus always be in **decreasing** order as $B_A \geq B_B \geq B_C$, retaining the ordering and association with the three principal axes `[:, i]` generated by `principals()`.

Parameters

- **geom** – length-3N `np.float_` – Coordinates of the atoms
- **masses** – length-N OR length-3N `np.float_` – Atomic masses of the atoms. Length-3N option is to allow calculation of a per-coordinate perturbed value.
- **units** – `EnumUnitsRotConst`, optional – Enum value indicating the desired units of the output rotational constants. Default is `INV_INERTIA` ($\frac{1}{\text{uB}^2}$)
- **on_tol** – `np.float_`, optional – Tolerance for deviation from unity/zero for principal axis dot products, within which axes are considered orthonormal. Default is `opan.const.DEF.ORTHONORM_TOL`

Returns *rc* – length-3 `np.float_` – Vector of rotational constants in the indicated units

2.6.4 opan.utils.symm

Utilities submodule for molecular symmetry operations and detection.

Warning: Module is **NON-FUNCTIONAL**

[Assumes molecule has already been translated to center-of-mass.]

[Molecular geometry is a vector, in order of x1, y1, z1, x2, y2, z2, ...]

[Will need to harmonize the matrix typing; currently things are just passed around as np.array for the most part.]

2.6.5 opan.utils.vector

Submodule for miscellaneous vector operations

Functions implemented here are (to the best of this author's knowledge) not available in NumPy or SciPy.

Functions

`opan.utils.vector.ortho_basis(normal[, ref_vec])`

Generates an orthonormal basis in the plane perpendicular to *normal*

The orthonormal basis generated spans the plane defined with *normal* as its normal vector. The handedness of *on1* and *on2* in the returned basis is such that:

$$\text{on1} \times \text{on2} = \frac{\text{normal}}{\|\text{normal}\|}$$

normal must be expressible as a one-dimensional `np.array` of length 3.

Parameters

- **normal** – length-3 `np.float_` – The orthonormal basis output will span the plane perpendicular to *normal*.
- **ref_vec** – length-3 `np.float_`, optional – If specified, *on1* will be the normalized projection of *ref_vec* onto the plane perpendicular to *normal*. Default is `None`.

Returns

- *on1* – length-3 `np.float_` – First vector defining the orthonormal basis in the plane normal to *normal*
- *on2* – length-3 `np.float_` – Second vector defining the orthonormal basis in the plane normal to *normal*

Raises

- `ValueError` – If *normal* or *ref_vec* is not expressible as a 1-D vector with 3 elements
- `VectorError` – (typecode `NONPRL`) If *ref_vec* is specified and it is insufficiently non-parallel with respect to *normal*

`opan.utils.vector.orthonorm_check(a[, tol[, report]])`

Checks orthonormality of the column vectors of a matrix.

If a one-dimensional `np.array` is passed to *a*, it is treated as a single column vector, rather than a row matrix of length-one column vectors.

The matrix *a* does not need to be square, though it must have at least as many rows as columns, since orthonormality is only possible in N-space with a set of no more than N vectors. (This condition is not directly checked.)

Parameters

- **a** – R x S `np.float_` – 2-D array of column vectors to be checked for orthonormality.
- **tol** – `np.float_`, optional – Tolerance for deviation of dot products from one or zero. Default value is `opan.const.DEF.ORTHONORM_TOL`.

- **report** – `bool`, optional – Whether to record and return vectors / vector pairs failing the orthonormality condition. Default is `False`.

Returns

- `o` – `bool` – Indicates whether column vectors of `a` are orthonormal to within tolerance `tol`.
- `n_fail` – `list` of `int`, or `None` –

If `report == True`:

A list of indices of column vectors failing the normality condition, or an empty list if all vectors are normalized.

If `report == False`:

`None`

- `o_fail` – `list` of 2-tuples of `int`, or `None` –

If `report == True`:

A list of 2-tuples of indices of column vectors failing the orthogonality condition, or an empty list if all vectors are orthogonal.

If `report == False`:

`None`

`opan.utils.vector.parallel_check(vec1, vec2)`

Checks whether two vectors are parallel OR anti-parallel.

Vectors must be of the same dimension.

Parameters

- **vec1** – length-R `np.float_` – First vector to compare
- **vec2** – length-R `np.float_` – Second vector to compare

Returns `par` – `bool` – `True` if (anti-)parallel to within `opan.const.PRM.NON_PARALLEL_TOL` degrees. `False` otherwise.

`opan.utils.vector.proj(vec, vec_onto)`

Vector projection.

Calculated as:

$$\text{vec_onto} * \frac{\text{vec} \cdot \text{vec_onto}}{\text{vec_onto} \cdot \text{vec_onto}}$$

Parameters

- **vec** – length-R `np.float_` – Vector to project
- **vec_onto** – length-R `np.float_` – Vector onto which `vec` is to be projected

Returns `proj_vec` – length-R `np.float_` – Projection of `vec` onto `vec_onto`

`opan.utils.vector.rej(vec, vec_onto)`

Vector rejection.

Calculated by subtracting from `vec` the projection of `vec` onto `vec_onto`:

$$\text{vec} - \text{proj}(\text{vec}, \text{vec_onto})$$

Parameters

- **vec** – length-R `np.float_` – Vector to reject
- **vec_onto** – length-R `np.float_` – Vector onto which *vec* is to be rejected

Returns *rej_vec* – length-R `np.float_` – Rejection of *vec* onto *vec_onto*

`opan.utils.vector.vec_angle(vec1, vec2)`

Angle between two R-dimensional vectors.

Angle calculated as:

$$\arccos \left[\frac{\text{vec1} \cdot \text{vec2}}{\|\text{vec1}\| \|\text{vec2}\|} \right]$$

Parameters

- **vec1** – length-R `np.float_` – First vector
- **vec2** – length-R `np.float_` – Second vector

Returns *angle* – `np.float_` – Angle between the two vectors in degrees

2.7 opan.vpt2

Submodule implementing VPT2 anharmonic computations.

Warning: This module is under active development. API &c. may change with little notice.

Sub-Modules

repo – HDF5 repository for OpanVPT2

Classes

OpanVPT2 – Core driver class for VPT2 anharmonic calculations.

API

class `opan.vpt2.base.OpanVPT2`

Container for data from VPT2 anharmonic calculations.

To be added...

2.7.1 opan.vpt2.repo

Sub-module for HDF5 repo interactions for VPT2 anharmonic calculations.

Warning: Module is under active development. API &c. may change with little notice.

Classes

class `opan.vpt2.repo.OpanAnharmRepo(fname=None)`

HDF5 repo interface for VPT2 anharmonic calculations.

Operations here **DO NOT** ensure consistency with the surrounding data. Such consistency must be checked/handled at a higher level. This is just a wrapper class to facilitate I/O interactions!

Currently no chunking or any filters are used. May or may not be worth robustification. Things stored are not likely to be huge....

Instantiation

`__init__` (...)

Class Variables

To be documented

Instance Variables

To be documented

Methods

To be documented

2.8 opan.xyz

Module implementing OpenBabel XYZ parsing and interpretation.

The single class `OpanXYZ` imports molecular geometries in the OpenBabel XYZ format , with the following variations:

- Coordinates of any precision will be read, not just the 10.5 specified by OpenBabel
- Both atomic symbols and atomic numbers are valid
- Multiple geometries/frames are supported, but the number of atoms and their sequence in the atoms list must be maintained in all geometries.

Contents

Class Variables

Instance Variables

Methods

All return values from a single indicated geometry.

`geom_single()` – Entire geometry vector

`displ_single()` – Displacement between two atoms

`dist_single()` – Euclidean distance between two atoms

`angle_single()` – Spanned angle of three atoms (one central and two distal atoms)

`dihed_single()` – Dihedral angle among four atoms

Generators

All yielded values are composited from an arbitrary set of geometry and/or atom indices; indexing with negative values is supported.

Each parameter can either be a single index, or an iterable of indices. If any iterables are passed, all must be the same length R, and a total of R values will be returned, one for each set of elements across the iterables. (This behavior is loosely similar to Python's `zip()` builtin.) Single values are used as provided for all values returned.

As an additional option, a `None` value can be passed to exactly one parameter, which will then be assigned the full 'natural' range of that parameter (`range(G)` for `g_nums` and `range(N)` for `ats_#`).

If the optional parameter *invalid_error* is `False` (the default), if `IndexError` or `ValueError` is raised in the course of calculating a given value, it is ignored and a `None` value is returned. If `True`, then the errors are raised as-is.

Note: For *angle_iter()* and *dihed_iter()*, using a `None` parameter with *invalid_error* == `True` is **guaranteed** to raise an error.

geom_iter() – Geometries

displ_iter() – Displacement vectors

dist_iter() – Euclidean distances

angle_iter() – Span angles

dihed_iter() – Dihedral angles

Class Definition

class `opan.xyz.OpenXYZ` (***kwargs*)
 Container for OpenBabel XYZ data.

Initializer can be called in one of two forms:

```
OpenXYZ(path='path/to/file')
OpenXYZ(atom_syms=[{array of atoms}], coords=[{array of coordinates}])
```

If *path* is specified, *atom_syms* and *coords* are ignored, and the instance will contain all validly formatted geometries present in the OpenBabel file at the indicated path.

Note: Certain types of improperly formatted geometry blocks, such as one with alphabetic characters on the ‘number-of-atoms’ line, may not raise errors during loading, but instead just result in import of fewer geometries/frames than expected.

If initialized with the *atom_syms* and *coords* keyword arguments, the instance will contain the single geometry represented by the provided inputs.

In both forms, the optional keyword argument *bohrs* can be specified, to indicate the units of the coordinates as Bohrs (`True`) or Angstroms (`False`). Angstrom and Bohr units are the default for the *path* and *atom_syms/coords* forms, respectively. The units of all coordinates stored in the instance are **Bohrs**.

‘N’ and ‘G’ in the below documentation refer to the number of atoms per geometry and the number of geometries present in the file, respectively. Note that **ALL** geometries present **MUST** contain the same number of atoms, and the elements must all **FALL IN THE SAME SEQUENCE** in each geometry/frame. No error will be raised if positions of like atoms are swapped, but for obvious reasons this will almost certainly cause semantic difficulties in downstream computations.

Note: In *ORCA* ‘.xyz’ files contain the highest precision geometry information of any output (save perhaps the textual output generated by the program), and are stored in Angstrom units.

Class Variables

p_coords

`re.compile()` pattern – Retrieves individual lines from coordinate blocks matched by *p_geom*

p_geom

`re.compile()` pattern – Retrieves full OpenBabel XYZ geometry frames/blocks

LOAD_DATA_FLAG = 'NOT FILE'

str – Flag for irrelevant data in *atom_syms/coords* initialization mode.

Instance Variables

Except where indicated, all *str* and *list*-of-*str* values are stored as *LOAD_DATA_FLAG* when initialized with *atom_syms/coords* arguments.

atom_syms

length-N *str* – Atomic symbols for the atoms (all uppercase)

descs

length-G *str* – Text descriptions for each geometry included in a loaded file

geoms

length-G *list* of length-3N *np.float_* – Molecular geometry/geometries read from file or passed to *coords* argument

in_str

str – Complete contents of the input file

num_atoms

int – Number of atoms per geometry, N

num_geoms

int – Number of geometries, G

XYZ_path

str – Full path to imported OpenBabel file

Methods

geom_single(g_num)

Retrieve a single geometry.

The atom coordinates are returned with each atom's x/y/z coordinates grouped together:

[A1x, A1y, A1z, A2x, A2y, A2z, ...]

An alternate method to achieve the same effect as this function is by simply indexing into *geoms*:

```
>>> x = opan.xyz.OpanXYZ(path='...')
>>> x.geom_single(g_num)      # One way to do it
>>> x.geoms[g_num]           # Another way
```

Parameters `g_num` – `int` – Index of the desired geometry

Returns `geom` – length-3N `np.float_` – Vector of the atomic coordinates for the geometry indicated by `g_num`

Raises `IndexError` – If an invalid (out-of-range) `g_num` is provided

displ_single (`g_num`, `at_1`, `at_2`)

Displacement vector between two atoms.

Returns the displacement vector pointing from `at_1` toward `at_2` from geometry `g_num`. If `at_1 == at_2` a strict zero vector is returned.

Displacement vector is returned in units of Bohrs.

Parameters

- `g_num` – `int` – Index of the desired geometry
- `at_1` – `int` – Index of the first atom
- `at_2` – `int` – Index of the second atom

Returns `displ` – length-3 `np.float_` – Displacement vector from `at_1` to `at_2`

Raises `IndexError` – If an invalid (out-of-range) `g_num` or `at_#` is provided

dist_single (`g_num`, `at_1`, `at_2`)

Distance between two atoms.

Parameters

- `g_num` – `int` – Index of the desired geometry
- `at_1` – `int` – Index of the first atom
- `at_2` – `int` – Index of the second atom

Returns `dist` – `np.float_` – Distance in Bohrs between `at_1` and `at_2` from geometry `g_num`

Raises `IndexError` – If an invalid (out-of-range) `g_num` or `at_#` is provided

angle_single (`g_num`, `at_1`, `at_2`, `at_3`)

Spanning angle among three atoms.

The indices `at_1` and `at_3` can be the same (yielding a trivial zero angle), but `at_2` must be different from both `at_1` and `at_3`.

Parameters

- `g_num` – `int` – Index of the desired geometry
- `at_1` – `int` – Index of the first atom
- `at_2` – `int` – Index of the second atom
- `at_3` – `int` – Index of the third atom

Returns `angle` – `np.float_` – Spanning angle in degrees between `at_1-at_2-at_3`, from geometry `g_num`

Raises

- `IndexError` – If an invalid (out-of-range) `g_num` or `at_#` is provided
- `ValueError` – If `at_2` is equal to either `at_1` or `at_3`

dihed_single (`g_num`, `at_1`, `at_2`, `at_3`, `at_4`)

Dihedral/out-of-plane angle among four atoms.

Returns the out-of-plane angle among four atoms from geometry `g_num`, in degrees. The reference plane is spanned by `at_1`, `at_2` and `at_3`. The out-of-plane angle is defined such that a positive angle represents a counter-clockwise rotation of the projected `at_3`→`at_4` vector with respect to the reference plane when looking from `at_3` toward `at_2`. Zero rotation corresponds to occlusion of `at_1` and `at_4`; that is, the case where the respective rejections of `at_1`→`at_2` and `at_3`→`at_4` onto `at_2`→`at_3` are ANTI-PARALLEL.

All four atom indices must be distinct. Both of the atom trios 1-2-3 and 2-3-4 must be sufficiently nonlinear, as diagnosed by a bend angle different from 0 or 180 degrees by at least `PRM.NON_PARALLEL_TOL`.

Parameters

- `g_num` – `int` – Index of the desired geometry
- `at_1` – `int` – Index of the first atom
- `at_2` – `int` – Index of the second atom
- `at_3` – `int` – Index of the third atom
- `at_4` – `int` – Index of the fourth atom

Returns `dihed` – `np.float_` – Out-of-plane/dihedral angle in degrees for the indicated `at_#`, drawn from geometry `g_num`

Raises

- `IndexError` – If an invalid (out-of-range) `g_num` or `at_#` is provided
- `ValueError` – If any indices `at_#` are equal
- `XYZError` – (typecode `DIHED`) If either of the atom trios (1-2-3 or 2-3-4) is too close to linearity

Generators

geom_iter (`g_nums`)

Iterator over a subset of geometries.

The indices of the geometries to be returned are indicated by an iterable of `ints` passed as `g_nums`.

As with `geom_single()`, each geometry is returned as a length-3N `np.float_` with each atom's x/y/z coordinates grouped together:

```
[A1x, A1y, A1z, A2x, A2y, A2z, ...]
```

In order to use NumPy [slicing](#) or [advanced indexing](#), `geoms` must first be explicitly converted to `np.array`, e.g.:

```
>>> x = opan.xyz.OpanXYZ(path='...')
>>> np.array(x.geoms)[[2,6,9]]
```

Parameters `g_nums` – length-R iterable of `int` – Indices of the desired geometries

Yields *geom* – length-3N `np.float_` – Vectors of the atomic coordinates for each geometry indicated in *g_nums*

Raises `IndexError` – If an item in *g_nums* is invalid (out of range)

`displ_iter` (*g_nums*, *ats_1*, *ats_2*)

Iterator over indicated displacement vectors.

Displacements are in Bohrs as with `displ_single()`.

See [above](#) for more information on calling options.

Parameters

- **`g_nums`** – `int` or length-R iterable `int` or `None` – Index/indices of the desired geometry/geometries
- **`ats_1`** – `int` or length-R iterable `int` or `None` – Index/indices of the first atom(s)
- **`ats_2`** – `int` or length-R iterable `int` or `None` – Index/indices of the second atom(s)
- **`invalid_error`** – `bool`, optional – If `False` (the default), `None` values are returned for results corresponding to invalid indices. If `True`, exceptions are raised per normal.

Yields *displ* – `np.float_` – Displacement vector in Bohrs between each atom pair of *ats_1* → *ats_2* from the corresponding geometries of *g_nums*.

Raises

- `IndexError` – If an invalid (out-of-range) *g_num* or *at_#* is provided.
- `ValueError` – If all iterable objects are not the same length.

`dist_iter` (*g_nums*, *ats_1*, *ats_2*)

Iterator over selected interatomic distances.

Distances are in Bohrs as with `dist_single()`.

See [above](#) for more information on calling options.

Parameters

- **`g_nums`** – `int` or length-R iterable `int` or `None` – Index/indices of the desired geometry/geometries
- **`ats_1`** – `int` or iterable `int` or `None` – Index/indices of the first atom(s)
- **`ats_2`** – `int` or iterable `int` or `None` – Index/indices of the second atom(s)
- **`invalid_error`** – `bool`, optional – If `False` (the default), `None` values are returned for results corresponding to invalid indices. If `True`, exceptions are raised per normal.

Yields *dist* – `np.float_` – Interatomic distance in Bohrs between each atom pair of *ats_1* and *ats_2* from the corresponding geometries of *g_nums*.

Raises

- `IndexError` – If an invalid (out-of-range) *g_num* or *at_#* is provided.
- `ValueError` – If all iterable objects are not the same length.

`angle_iter` (*g_nums*, *ats_1*, *ats_2*, *ats_3*)

Iterator over selected atomic angles.

Angles are in degrees as with `angle_single()`.

See [above](#) for more information on calling options.

Parameters

- **g_nums** – `int` or iterable `int` or `None` – Index of the desired geometry
- **ats_1** – `int` or iterable `int` or `None` – Index of the first atom
- **ats_2** – `int` or iterable `int` or `None` – Index of the second atom
- **ats_3** – `int` or iterable `int` or `None` – Index of the third atom
- **invalid_error** – `bool`, optional – If `False` (the default), `None` values are returned for results corresponding to invalid indices. If `True`, exceptions are raised per normal.

Yields *angle* – `np.float_` – Spanning angles in degrees between corresponding *ats_1-ats_2-ats_3*, from geometry/geometries *g_nums*

Raises

- `IndexError` – If an invalid (out-of-range) *g_num* or *at_#* is provided.
- `ValueError` – If all iterable objects are not the same length.
- `ValueError` – If any *ats_2* element is equal to either the corresponding *ats_1* or *ats_3* element.

dihed_iter (*g_nums*, *ats_1*, *ats_2*, *ats_3*, *ats_4*)

Iterator over selected dihedral angles.

Angles are in degrees as with *dihed_single()*.

See *above* for more information on calling options.

Parameters

- **g_nums** – `int` or iterable `int` or `None` – Indices of the desired geometry
- **ats_1** – `int` or iterable `int` or `None` – Indices of the first atoms
- **ats_2** – `int` or iterable `int` or `None` – Indices of the second atoms
- **ats_3** – `int` or iterable `int` or `None` – Indices of the third atoms
- **ats_4** – `int` or iterable `int` or `None` – Indices of the fourth atoms
- **invalid_error** – `bool`, optional – If `False` (the default), `None` values are returned for results corresponding to invalid indices. If `True`, exceptions are raised per normal.

Yields *dihed* – `np.float_` – Out-of-plane/dihedral angles in degrees for the indicated atom sets *ats_1-ats_2-ats_3-ats_4*, drawn from the respective *g_nums*.

Raises

- `IndexError` – If an invalid (out-of-range) *g_num* or *at_#* is provided.
- `ValueError` – If all iterable objects are not the same length.
- `ValueError` – If any corresponding *ats_#* indices are equal.
- `XYZError` – (typecode *DIHED*) If either of the atom trios (1-2-3 or 2-3-4) is too close to linearity for any group of *ats_#*

Notational and Algebraic Conventions

In order to aid comprehension, this documentation strives to obey the following formatting/notation conventions.

In text:

- Function/method parameters are set in *italics*.
- When not used for emphasis, **bold** text is used to set apart words/phrases with specific contextual meaning.
- Code snippets are set in fixed font, colored red, and boxed: `[v for v in range(6)]`.
- References to Python objects are set in fixed font, colored black (in most cases), and boxed: `OpenXYZ`. Where practical, they will be linked to the relevant documentation (via `intersphinx`).
- Code examples are set in fixed font and boxed the full width of the page:

```
from open.utils.vector import proj
pvec = proj(vec1, vec2)
```

Interactive usage examples are formatted like a Python console session, as per `doctest`:

```
>>> 1 + 2 + 3
6
```

- Where included, the key words “MUST”, “MUST NOT”, “REQUIRED”, “SHALL”, “SHALL NOT”, “SHOULD”, “SHOULD NOT”, “RECOMMENDED”, “MAY”, and “OPTIONAL” in this documentation are to be interpreted as described in **RFC 2119**.
- Mathematical symbols and engineering units are set as in equations, below.

In equations:

- Roman variables are set in serif italics: $x + C$
- Lowercase Greek variables are set in italics: $\frac{\theta + \pi}{\gamma}$
- Uppercase Greek variables are set in upright serif: $\Phi + \Theta$
- Vectors are set in bold, upright, serif Roman symbols: $\mathbf{r}_2 - \mathbf{r}_1$
- Matrices are set as bold, uppercase, serif Roman or Greek symbols: $\mathbf{M}^{-1/2} \mathbf{F} \mathbf{M}^{-1/2}$
- Engineering units are set in upright Roman (serif) equation type: $\left(\frac{E_h}{B^2}\right)$

Common symbols:

- N – the number of atoms in the system of interest
- G – the number of geometries in an OpenBabel XYZ file

- R, S, \dots – Arbitrary integers

Supported Software Packages

At this development stage, Open Anharmonic is being built with support only for ORCA. Pending community response, support for other packages may be added. In anticipation of such interest, the Open Anharmonic framework is being designed to facilitate extensibility to other computational packages to the extent possible.

Proper installation/configuration of external software packages and construction of suitable input templates, execution scripts, etc. are entirely the responsibility of the user. **It is the responsibility of the user to ascertain whether usage of these software packages in concert with Open Anharmonic is in accord with their respective licenses!!**

Descriptions are quoted from the respective software websites. [ORCA](#)

The program ORCA is a modern electronic structure program package written by F. Neese, with contributions from many current and former coworkers and several collaborating groups. ... ORCA is a flexible, efficient and easy-to-use general purpose tool for quantum chemistry with specific emphasis on spectroscopic properties of open-shell molecules. It features a wide variety of standard quantum chemical methods ranging from semiempirical methods to DFT to single- and multireference correlated ab initio methods. It can also treat environmental and relativistic effects.

Open Anharmonic Dependencies

Open Anharmonic is compatible only with Python ≥ 3.4 . Open Anharmonic depends on the following Python libraries and has been tested to work on the versions indicated:

- `numpy` ($\geq 1.10, < 1.12$)
- `scipy` ($\geq 0.12, < 0.18$)
- `h5py` ($\geq 2.4, < 2.7$)

Unix/Linux and MacOS users should likely be able to obtain suitable versions of these packages either through `pip` or the respective OS package managers. Windows users should obtain these packages either via [anaconda](#) (or a similar prepackaged environment) or from Christoph Gohlke's [‘aftermarket’ repository](#).

Units of Measure

6.1 Atomic Units

- B – Bohr radius, atomic unit of length, equal to $0.52917721067 \text{ \AA}$ or $0.52917721067 \times 10^{-10} \text{ m}$ – [\[NISTCUU_B\]](#)
- E_h – Hartree, atomic unit of energy, equal to 4.35974465 J – [\[NISTCUU_Eh\]](#)
- m_e – Electron mass, atomic unit of mass, equal to $9.10938356 \times 10^{-31} \text{ kg}$ – [\[NISTCUU_me\]](#)
- T_a – Atomic time unit, equal to $2.4188843265 \times 10^{-17} \text{ s}$ – [\[NISTCUU-Ta\]](#)

6.2 Other Units

- cyc – Numerical value of 2π ($\frac{\text{cyc}}{2\pi} = 1$), serving to convert angular frequencies into cyclic frequencies.
- u – unified atomic mass unit; equal to $1822.8885 m_e$ [\[NISTCUU_me_u\]](#) or $1.660539040 \times 10^{-27} \text{ kg}$ [\[NISTCUU_u_kg\]](#).

References

From the [NIST Reference on Constants, Units and Uncertainty](#)

Indices and Tables

- [genindex](#)
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- [search](#)

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