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# spyrmsd Documentation

**spyrmsd**

**Apr 05, 2024**



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`spyrmsd` is a Python tool for symmetry-corrected RMSD calculations.



## INSTALLATION

spyrmsd is available on [PyPI](#) and [conda-forge](#) and can be easily installed from source.

### 1.1 Installation

Installing spyrmsd with `pip`, `conda` or from source will install the package as a library. In order to install the package as a standalone tool, [Open Babel](#) or [RDKit](#) need to be installed as well (see [Dependencies](#)).

#### 1.1.1 pip

```
pip install spyrmsd
```

#### 1.1.2 conda

```
conda install spyrmsd -c conda-forge
```

#### 1.1.3 GitHub

```
git clone https://github.com/RMeli/spyrmsd.git
cd spyrmsd
pip install .
```

### 1.2 Dependencies

spyrmsd can be used both as a module or as a standalone tool.

### 1.2.1 Module

The following packages are required to use `spyrmsd` as a module:

- `graph-tool` or `NetworkX`
- `numpy`
- `scipy`

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**Note:** `spyrmsd` uses `graph-tool` by default but will fall back to `NetworkX` if the former is not installed (e.g. on Windows).

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### 1.2.2 Standalone Tool

Additionally, one of the following packages is required to use `spyrmsd` as a standalone tool:

- `Open Babel`
- `RDKit`



## TUTORIAL

```
import spyrmsd
from spyrmsd import io, rmsd
```

### 2.1 OpenBabel or RDKit

spyrmsd natively supports [OpenBabel](#) and [RDKit](#) to load molecules in order to work as a standalone tool. However, the API for RMSD calculations is extremely minimal and only needs the following information:

- Atomic coordinates
- Atomic numbers
- Molecular adjacency matrix (for symmetry)

This means that spyrmsd can be used in combination with any library that can provide such information.

### 2.2 Loading Molecules

The `spyrmsd.io` module provides functions to easily load molecules from a file and to transform them into a `spyrmsd.molecule.Molecule` object:

```
ref = io.loadmol("molecules/1a4k_ligand.sdf")
```

`io.loadmol` load a single molecule from a file. In order to load all molecules we need to use `io.loadallmols`:

```
mols = io.loadallmols("molecules/1a4k_dock.sdf")
```

### 2.3 Loading RDKit or OpenBabel Molecules

spyrmsd natively supports Open Babel and RDKit (if installed). The `Molecule` class provides `from_openbabel()` and `from_rdkit()` constructors.

```
from rdkit import Chem
from rdkit.Chem import AllChem

rdmol1 = Chem.MolFromSmiles("c1ccccc1")
```

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```
rdmol2 = Chem.MolFromSmiles("c1ccccc1")
AllChem.EmbedMolecule(rdmol1)
AllChem.EmbedMolecule(rdmol2)

from spyrmsd.molecule import Molecule
from spyrmsd.rmsd import rmsdwrapper

mol1 = Molecule.from_rdkit(rdmol1)
mol2 = Molecule.from_rdkit(rdmol2)

rmsdwrapper(mol1, mol2)
```

```
<frozen importlib._bootstrap>:241: RuntimeWarning: to-Python converter for std::__1::pair
↳<double, double> already registered; second conversion method ignored.
[21:58:01] Molecule does not have explicit Hs. Consider calling AddHs()
[21:58:01] Molecule does not have explicit Hs. Consider calling AddHs()
```

```
[0.019162902039384797]
```

## 2.4 Removing Hydrogen Atoms

Hydrogen atoms can be removed with the `strip()` function:

```
ref.strip()
```

```
for mol in mols:
    mol.strip()
```

## 2.5 Symmetry-Corrected RMSD

spyrmsd only needs atomic coordinates, atomic number and the molecular adjacency matrix to compute the standard RMSD with `spyrmsd.rmsd.symmrmsd`. The `spyrmsd.molecule.Molecule` class provides easy access to such information:

```
coords_ref = ref.coordinates
anum_ref = ref.atomicnums
adj_ref = ref.adjacency_matrix
```

```
coords = [mol.coordinates for mol in mols]
anum = mols[0].atomicnums
adj = mols[0].adjacency_matrix
```

With this information we can easily compute the RMSD between the reference molecule and all other molecules:

```
RMSD = rmsd.symmrmsd(
    coords_ref,
    coords,
```

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```

    anum_ref,
    anum,
    adj_ref,
    adj,
)

print(RMSD)

```

```

[2.0246085732404446, 1.4951562971486378, 10.028009301306854, 7.900570020309068, 7.
↪578344354783399, 9.52999506817054, 4.952371789159667, 7.762808670066815, 9.
↪996922964463582, 7.1732072690335755]

```

## 2.5.1 Minimum RMSD

We can also compute the minimum RMSD obtained by superimposing the molecular structures:

```

RMSD = rmsd.symmrmsd(
    coords_ref,
    coords,
    anum_ref,
    anum,
    adj_ref,
    adj,
    minimize=True,
)

print(RMSD)

```

```

[1.2012368667355435, 1.0533413220699535, 1.153253104575529, 1.036542688936588, 0.
↪8407673221224187, 1.1758143217869736, 0.7817315189656655, 1.0933314311267845, 1.
↪0260767175206462, 0.9586369647000478]

```

## 2.6 Change Backend

spyrmsd supports multiple backends. You see which backends are available by looking at the `available_backends` attribute:

```
spyrmsd.available_backends
```

```
['graph_tool', 'networkx']
```

The available backends are a subset of the supported backends. Only the backends that are installed will be available.

You can check the current backend with

```
spyrmsd.get_backend()
```

```
'graph_tool'
```

You can switch the backend using

```
spyrmsd.set_backend("networkx")  
spyrmsd.get_backend()
```

```
'networkx'
```

## 3.1 spyrmsd package

Python RMSD tool with symmetry correction.

### 3.1.1 Subpackages

**spyrmsd.graphs package**

**Submodules**

**spyrmsd.graphs.gt module**

`spyrmsd.graphs.gt.cycle(n)`

Build cycle graph

**Parameters**

**n** (*int*) – Number of nodes

**Returns**

Cycle graph

**Return type**

Graph

`spyrmsd.graphs.gt.graph_from_adjacency_matrix(adjacency_matrix: Union[ndarray, List[List[int]]],  
aprops: Optional[Union[ndarray, List[Any]]] = None)`

Graph from adjacency matrix.

**Parameters**

- **adjacency\_matrix** (Union[*np.ndarray*, List[List[int]]]) – Adjacency matrix
- **aprops** (Union[*np.ndarray*, List[Any]], *optional*) – Atomic properties

**Returns**

Molecular graph

**Return type**

Graph

## Notes

If the atomic numbers are passed, they are used as node attributes.

`spyrmsd.graphs.gt.lattice(n1: int, n2: int)`

Build 2D lattice graph

### Parameters

- **n1** (*int*) – Number of nodes in dimension 1
- **n2** (*int*) – Number of nodes in dimension 2

### Returns

Lattice graph

### Return type

Graph

`spyrmsd.graphs.gt.match_graphs(G1, G2) → List[Tuple[List[int], List[int]]]`

Compute graph isomorphisms.

### Parameters

- **G1** – Graph 1
- **G2** – Graph 2

### Returns

All possible mappings between nodes of graph 1 and graph 2 (isomorphisms)

### Return type

List[Tuple[List[int], List[int]]]

### Raises

**NonIsomorphicGraphs** – If the graphs *G1* and *G2* are not isomorphic

`spyrmsd.graphs.gt.num_edges(G) → int`

Number of edges

### Parameters

**G** – Graph

### Returns

Number of edges

### Return type

int

`spyrmsd.graphs.gt.num_vertices(G) → int`

Number of vertices

### Parameters

**G** – Graph

### Returns

Number of vertices (nodes)

### Return type

int

`spyrmsd.graphs.gt.vertex_property(G, vproperty: str, idx: int) → Any`

Get vertex (node) property from graph

**Parameters**

- **G** – Graph
- **vproperty** (*str*) – Vertex property name
- **idx** (*int*) – Vertex index

**Returns**

Vertex property value

**Return type**

Any

## spyrmsd.graphs.nx module

`spyrmsd.graphs.nx.cycle(n)`

Build cycle graph

**Parameters**

**n** (*int*) – Number of nodes

**Returns**

Cycle graph

**Return type**

Graph

`spyrmsd.graphs.nx.graph_from_adjacency_matrix(adjacency_matrix: Union[ndarray, List[List[int]]],  
aprops: Optional[Union[ndarray, List[Any]]] = None)  
→ Graph`

Graph from adjacency matrix.

**Parameters**

- **adjacency\_matrix** (*Union[np.ndarray, List[List[int]]*) – Adjacency matrix
- **aprops** (*Union[np.ndarray, List[Any]], optional*) – Atomic properties

**Returns**

Molecular graph

**Return type**

Graph

## Notes

If the atomic numbers are passed, they are used as node attributes.

`spyrmsd.graphs.nx.lattice(n1, n2)`

Build 2D lattice graph

**Parameters**

- **n1** (*int*) – Number of nodes in dimension 1
- **n2** (*int*) – Number of nodes in dimension 2

**Returns**

Lattice graph

**Return type**

Graph

`spyrmsd.graphs.nx.match_graphs(G1, G2) → List[Tuple[List[int], List[int]]]`

Compute graph isomorphisms.

**Parameters**

- **G1** – Graph 1
- **G2** – Graph 2

**Returns**

All possible mappings between nodes of graph 1 and graph 2 (isomorphisms)

**Return type**

List[Tuple[List[int],List[int]]]

**Raises**

*NonIsomorphicGraphs* – If the graphs *G1* and *G2* are not isomorphic

`spyrmsd.graphs.nx.num_edges(G) → int`

Number of edges

**Parameters**

**G** – Graph

**Returns**

Number of edges

**Return type**

int

`spyrmsd.graphs.nx.num_vertices(G) → int`

Number of vertices

**Parameters**

**G** – Graph

**Returns**

Number of vertices (nodes)

**Return type**

int

`spyrmsd.graphs.nx.vertex_property(G, vproperty: str, idx: int) → Any`

Get vertex (node) property from graph

**Parameters**

- **G** – Graph
- **vproperty** (*str*) – Vertex property name
- **idx** (*int*) – Vertex index

**Returns**

Vertex property value

**Return type**

Any



## spyrmsd.optional package

### Submodules

#### spyrmsd.optional.obabel module

`spyrmsd.optional.obabel.adjacency_matrix(mol) → ndarray`

Adjacency matrix from OpenBabel molecule.

**Parameters**

**mol** – Molecule

**Returns**

Adjacency matrix of the molecule

**Return type**

np.ndarray

`spyrmsd.optional.obabel.bonds(mol) → List[Tuple[int, int]]`

List of bonds

**Parameters**

**mol** – Molecule

**Returns**

List of bonds

**Return type**

List[Tuple[int, int]]

### Notes

A bond is defined by a tuple of (0-based) indices of two atoms.

`spyrmsd.optional.obabel.load(fname: str)`

Load molecule from file.

**Parameters**

**fname** (*str*) – File name

**Return type**

*Molecule*

`spyrmsd.optional.obabel.loadall(fname: str)`

Load molecules from file.

**Parameters**

**fname** (*str*) – File name

**Return type**

List of molecules

`spyrmsd.optional.obabel.numatoms(mol) → int`

Number of atoms.

**Parameters**

**mol** – Molecule

**Returns**

Number of atoms

**Return type**

int

`spyrmsd.optional.obabel.numbonds(mol) → int`

Number of bonds.

**Parameters**

**mol** – Molecule

**Returns**

Number of bonds

**Return type**

int

`spyrmsd.optional.obabel.to_molecule(mol, adjacency: bool = True)`

Transform molecule to *pyrmsd* molecule.

**Parameters**

- **mol** – Molecule
- **adjacency** (*boolean, optional*) – Flag to decide wether to build the adjacency matrix from molecule

**Returns**

*pyrmsd* molecule

**Return type**

`pyrmsd.molecule.Molecule`

## spyrmsd.optional.rdkit module

`spyrmsd.optional.rdkit.adjacency_matrix(mol) → ndarray`

Adjacency matrix from OpenBabel molecule.

**Parameters**

**mol** – Molecule

**Returns**

Adjacency matrix of the molecule

**Return type**

`np.ndarray`

`spyrmsd.optional.rdkit.bonds(mol) → List[Tuple[int, int]]`

List of bonds.

**Parameters**

**mol** – Molecule

**Returns**

List of bonds

**Return type**

`List[Tuple[int, int]]`

## Notes

A bond is defined by a tuple of (0-based) indices of two atoms.

`spyrmsd.optional.rdkit.load(fname: str)`

Load molecule from file.

**Parameters**

**fname** (*str*) – File name

**Return type**

*Molecule*

`spyrmsd.optional.rdkit.loadall(fname: str)`

Load molecules from file.

**Parameters**

**fname** (*str*) – File name

**Return type**

List of molecules

`spyrmsd.optional.rdkit.numatoms(mol) → int`

Number of atoms.

**Parameters**

**mol** – Molecule

**Returns**

Number of atoms

**Return type**

int

`spyrmsd.optional.rdkit.numbonds(mol) → int`

Number of bonds.

**Parameters**

**mol** – Molecule

**Returns**

Number of bonds

**Return type**

int

`spyrmsd.optional.rdkit.to_molecule(mol, adjacency: bool = True)`

Transform molecule to *pyrmsd* molecule.

**Parameters**

- **mol** – Molecule
- **adjacency** (*boolean, optional*) – Flag to decide whether to build the adjacency matrix from molecule

**Returns**

*spyrmsd* molecule

**Return type**

*spyrmsd.molecule.Molecule*

### 3.1.2 Submodules

#### spyrmsd.constants module

Useful constants.

#### Notes

Periodic table data (atomic masses and covalent radii) are extracted from [QCElemental](#)

#### spyrmsd.due module

Stub file for a guaranteed safe import of duecredit constructs: if duecredit is not available.

To use it, place it into your project codebase to be imported, e.g. copy as

```
cp stub.py /path/to/module/module/due.py
```

Note that it might be better to avoid naming it duecredit.py to avoid shadowing installed duecredit.

Then use in your code as

```
from .due import due, Doi, BibTeX, Text
```

See <https://github.com/duecredit/duecredit/blob/master/README.md> for examples.

Origin: Originally a part of the duecredit Copyright: 2015-2019 DueCredit developers License: BSD-2

**spyrmsd.due.BibTeX(\*args, \*\*kwargs)**

Perform no good and no bad

**spyrmsd.due.Doi(\*args, \*\*kwargs)**

Perform no good and no bad

**class spyrmsd.due.InactiveDueCreditCollector**

Bases: object

Just a stub at the Collector which would not do anything

**activate(\*args, \*\*kwargs)**

Perform no good and no bad

**active = False**

**add(\*args, \*\*kwargs)**

Perform no good and no bad

**cite(\*args, \*\*kwargs)**

Perform no good and no bad

**dcite(\*args, \*\*kwargs)**

If I could cite I would

**dump(\*args, \*\*kwargs)**

Perform no good and no bad

**load(\*args, \*\*kwargs)**

Perform no good and no bad

`spyrmsd.due.Text(*args, **kwargs)`

Perform no good and no bad

`spyrmsd.due.Url(*args, **kwargs)`

Perform no good and no bad

## spyrmsd.exceptions module

**exception** `spyrmsd.exceptions.NonIsomorphicGraphs`

Bases: `ValueError`

Raised when graphs are not isomorphic

## spyrmsd.graph module

`spyrmsd.graph.adjacency_matrix_from_atomic_coordinates(aprops: ndarray, coordinates: ndarray) → ndarray`

Compute adjacency matrix from atomic coordinates.

### Parameters

- **aprops** (*numpy.ndarray*) – Atomic properties
- **coordinates** (*numpy.ndarray*) – Atomic coordinates

### Returns

Adjacency matrix

### Return type

*numpy.ndarray*

## Notes

This function is based on an automatic bond perception algorithm: two atoms are considered to be bonded when their distance is smaller than the sum of their covalent radii plus a tolerance value.<sup>3</sup>

**Warning:** The automatic bond perception rule implemented in this functions is very simple and only depends on atomic coordinates. Use with care!

## spyrmsd.hungarian module

`spyrmsd.hungarian.cost_mtx(A: ndarray, B: ndarray)`

Compute the cost matrix for atom-atom assignment.

### Parameters

- **A** (*numpy.ndarray*) – Atomic coordinates of molecule A
- **B** (*numpy.ndarray*) – Atomic coordinates of molecule B

### Returns

Cost matrix of squared atomic distances between atoms of molecules A and B

<sup>3</sup> E. C. Meng and R. A. Lewis, *Determination of molecular topology and atomic hybridization states from heavy atom coordinates*, J. Comp. Chem. **12**, 891-898 (1991).

**Return type**

np.ndarray

`spyrmsd.hungarian.hungarian_rmsd(A: ndarray, B: ndarray, apropsA: ndarray, apropsB: ndarray) → float`

Solve the optimal assignment problems between atomic coordinates of molecules A and B.

**Parameters**

- **A** (*numpy.ndarray*) – Atomic coordinates of molecule A
- **B** (*numpy.ndarray*) – Atomic coordinates of molecule B
- **apropsA** (*numpy.ndarray*) – Atomic properties of molecule A
- **apropsB** (*numpy.ndarray*) – Atomic properties of molecule B

**Returns**

RMSD computed with the Hungarian method

**Return type**

float

**Notes**

The Hungarian algorithm is used to solve the linear assignment problem, which is a minimum weight matching of the molecular graphs (bipartite).

The linear assignment problem is solved for every element separately.<sup>1</sup>

`spyrmsd.hungarian.optimal_assignment(A: ndarray, B: ndarray)`

Solve the optimal assignment problems between atomic coordinates of molecules A and B.

**Parameters**

- **A** (*numpy.ndarray*) – Atomic coordinates of molecule A
- **B** (*numpy.ndarray*) – Atomic coordinates of molecule B

**Returns**

Cost of the optimal assignment, together with the row and column indices of said assignment

**Return type**

Tuple[float, nd.array, nd.array]

**spyrmsd.io module**

`spyrmsd.io.adjacency_matrix(mol) → ndarray`

Adjacency matrix from OpenBabel molecule.

**Parameters**

**mol** – Molecule

**Returns**

Adjacency matrix of the molecule

**Return type**

np.ndarray

---

<sup>1</sup> W. J. Allen and R. C. Rizzo, *Implementation of the Hungarian Algorithm to Account for Ligand Symmetry and Similarity in Structure-Based Design*, J. Chem. Inf. Model. **54**, 518-529 (2014)

`spyrmsd.io.bonds(mol) → List[Tuple[int, int]]`

List of bonds

**Parameters**

**mol** – Molecule

**Returns**

List of bonds

**Return type**

List[Tuple[int, int]]

## Notes

A bond is defined by a tuple of (0-based) indices of two atoms.

`spyrmsd.io.load(fname: str)`

Load molecule from file.

**Parameters**

**fname** (*str*) – File name

**Return type**

*Molecule*

`spyrmsd.io.loadall(fname: str)`

Load molecules from file.

**Parameters**

**fname** (*str*) – File name

**Return type**

List of molecules

`spyrmsd.io.numatoms(mol) → int`

Number of atoms.

**Parameters**

**mol** – Molecule

**Returns**

Number of atoms

**Return type**

int

`spyrmsd.io.numbonds(mol) → int`

Number of bonds.

**Parameters**

**mol** – Molecule

**Returns**

Number of bonds

**Return type**

int

`spyrmsd.io.to_molecule(mol, adjacency: bool = True)`

Transform molecule to *pyrmsd* molecule.

#### Parameters

- **mol** – Molecule
- **adjacency** (*boolean, optional*) – Flag to decide whether to build the adjacency matrix from molecule

#### Returns

*pyrmsd* molecule

#### Return type

`pyrmsd.molecule.Molecule`

### spyrmsd.molecule module

```
class spyrmsd.molecule.Molecule(atomicnums: Union[ndarray, List[int]], coordinates: Union[ndarray, List[List[float]]], adjacency_matrix: Optional[Union[ndarray, List[List[int]]] = None)
```

Bases: `object`

**center\_of\_geometry()** → `ndarray`

Center of geometry.

#### Returns

Center of geometry

#### Return type

`np.ndarray`

**center\_of\_mass()** → `ndarray`

Center of mass.

#### Returns

Center of mass

#### Return type

`np.ndarray`

### Notes

Atomic masses are cached.

```
classmethod from_obabel(obmol, adjacency: bool = True)
```

Constructor from OpenBabel molecule.

#### Parameters

- **obmol** – OpenBabel molecule
- **adjacency** – Flag to compute the adjacency matrix

#### Returns

*spyrmsd* Molecule

#### Return type

*spyrmsd.molecule.Molecule*



**classmethod** `from_rdkit`(*rdmol*, *adjacency*: *bool* = *True*)

Constructor from RDKit molecule.

**Parameters**

- **rdmol** – RDKit molecule
- **adjacency** – Flag to compute the adjacency matrix

**Returns**

spyrmsd Molecule

**Return type**

*spyrmsd.molecule.Molecule*

**rotate**(*angle*: *float*, *axis*: *Union*[*ndarray*, *List*[*float*]], *units*: *str* = 'rad') → *None*

Rotate molecule.

**Parameters**

- **angle** (*float*) – Rotation angle
- **axis** (*np.ndarray*) – Axis of rotation (in 3D)
- **units** (*{“rad”, “deg”}*) – Units of the angle (radians *rad* or degrees *deg*)

**strip**() → *None*

Strip hydrogen atoms.

**to\_graph**()

Convert molecule to graph.

**Returns**

Molecular graph.

**Return type**

Graph

## Notes

If the molecule does not have an associated adjacency matrix, a simple bond perception is used.

The molecular graph is cached per backend.

**translate**(*vector*: *Union*[*ndarray*, *List*[*float*]]) → *None*

Translate molecule.

**Parameters**

- **vector** (*np.ndarray*) – Translation vector (in 3D)

`spyrmsd.molecule.coords_from_molecule`(*mol*: *Molecule*, *center*: *bool* = *False*) → *ndarray*

Atomic coordinates from molecule.

**Parameters**

- **mol** (*molecule.Molecule*) – Molecule
- **center** (*bool*) – Center flag

**Returns**

Atomic coordinates (possibly centred)

**Return type**

*np.ndarray*

## Notes

Atomic coordinates are centred according to the center of geometry, not the center of mass.

## spyrmsd.qcp module

`spyrmsd.qcp.K_mtx(M)`

Compute symmetric key matrix.

### Parameters

**M** (*numpy.ndarray*) – Inner product between coordinate matrices

### Returns

Symmetric key matrix

### Return type

*numpy.ndarray*

## Notes

The symmetric key matrix corresponds to the matrix **K**.<sup>2</sup>

If  $S_{xy}$  is defined as

$$S_{xy} = \sum_i^N x_{B,i} y_{A,i}$$

then **K** is the  $4 \times 4$  symmetric matrix given by

$$\begin{pmatrix} S_{xx} + S_{yy} + S_{zz} & S_{yz} - S_{zy} & S_{zx} - S_{xz} & S_{xy} - S_{yx} \\ S_{xx} - S_{yy} - S_{zz} & S_{xy} + S_{yx} & S_{zy} - S_{yz} & S_{zx} + S_{xz} \\ -S_{xx} + S_{yy} - S_{zz} & S_{yz} - S_{zy} & S_{xy} - S_{yx} & S_{zx} + S_{xz} \\ -S_{xx} - S_{yy} + S_{zz} & S_{zx} + S_{xz} & S_{xy} - S_{yx} & S_{yz} - S_{zy} \end{pmatrix}$$

`spyrmsd.qcp.M_mtx(A: ndarray, B: ndarray) → ndarray`

Compute inner product between coordinate matrices.

### Parameters

- **A** (*numpy.ndarray*) – Coordinates A
- **B** (*numpy.ndarray*) – Coordinates B

### Returns

Inner product of the coordinate matrices A and B

### Return type

*numpy.ndarray*

---

<sup>2</sup> D. L. Theobald, *Rapid calculation of RMSDs using a quaternion-based characteristic polynomial*, Acta Cryst. A **61**, 478-480 (2005).

## Notes

The inner product of the coordinate matrices  $A$  and  $B$  corresponds to the matrix  $\mathbf{M}$ .<sup>1</sup>

If  $S_{xy}$  is defined as

$$S_{xy} = \sum_i^N x_{B,i} y_{A,i}$$

then  $\mathbf{M}$  is the  $3 \times 3$  matrix given by

$$\begin{pmatrix} S_{xx} & S_{xy} & S_{xz} \\ S_{yx} & S_{yy} & S_{yz} \\ S_{zx} & S_{zy} & S_{zz} \end{pmatrix}$$

`spyrmsd.qcp.coefficients(M: ndarray, K: ndarray) → Tuple[float, float, float]`

Compute quaternion polynomial coefficients.

### Parameters

- **M** (*numpy.ndarray*) – Inner product between coordinate matrices
- **K** (*numpy.ndarray*) – Symmetric key matrix

### Returns

Quaternion polynomial coefficients

### Return type

Tuple[float, float, float]

## Notes

Returns only  $\mathbf{M}$ - and  $\mathbf{K}$ -dependent coefficients are returned.  $c_4 = 1$  and  $c_3 = 0$  are not returned.

The  $\mathbf{M}$ - and  $\mathbf{K}$ -dependent quaternion polynomial coefficients are given by

$$c_2 = -2 \operatorname{tr}(\mathbf{M}^T \mathbf{M})$$

$$c_1 = -8 \det(\mathbf{M})$$

$$c_0 = \det(\mathbf{K})$$

`spyrmsd.qcp.lambda_max(Ga: float, Gb: float, c2: float, c1: float, c0: float) → float`

Find largest root of the quaternion polynomial.

### Parameters

- **Ga** (*float*) – Inner product of structure A
- **Gb** – Inner product of structure B
- **c2** – Coefficient  $c_2$  of the quaternion polynomial
- **c1** – Coefficient  $c_1$  of the quaternion polynomial
- **c0** – Coefficient  $c_0$  of the quaternion polynomial

### Returns

Largest root of the quaternion polynomial ( $\lambda_{\max}$ )

<sup>1</sup> D. L. Theobald, *Rapid calculation of RMSDs using a quaternion-based characteristic polynomial*, Acta Cryst. A **61**, 478–480 (2005).

**Return type**

float

`spyrmsd.qcp.qcp_rmsd(A: ndarray, B: ndarray, atol: float = 1e-09) → float`

Compute RMSD using the quaternion polynomial method.

**Parameters**

- **A** (*numpy.ndarray*) – Coordinates of structure A
- **B** (*numpy.ndarray*) – Coordinates of structure B
- **atol** (*float*) – Absolute tolerance parameter (see notes)

**Returns**

RMSD between structures A and B

**Return type**

float

**Raises**

**AssertionError** – If the shape of structures A and B is different

**Notes**

If the structures A and B can be superimposed exactly (i.e. they differ only by center-of-mass translations and rotations), we have

$$G_a + G_b = 2\lambda_{\max}$$

This means that  $s = G_a + G_b - 2 * \lambda_{\max}$  can become negative because of numerical errors and therefore  $\sqrt{s}$  fails. In order to avoid this problem, the final RMSD is set to 0 if  $|s| < atol$ .

**spyrmsd.rmsd module**

`spyrmsd.rmsd.hrmsd(coords1: ndarray, coords2: ndarray, atomicn1: ndarray, atomicn2: ndarray, center=False)`

Compute minimum RMSD using the Hungarian method.

**Parameters**

- **coords1** (*np.ndarray*) – Coordinate of molecule 1
- **coords2** (*np.ndarray*) – Coordinates of molecule 2
- **atomicn1** (*np.ndarray*) – Atomic numbers for molecule 1
- **atomicn2** (*np.ndarray*) – Atomic numbers for molecule 2

**Returns**

Minimum RMSD (after assignment)

**Return type**

float

## Notes

The Hungarian algorithm is used to solve the linear assignment problem, which is a minimum weight matching of the molecular graphs (bipartite).<sup>2</sup>

The linear assignment problem is solved for every element separately.

`spyrmsd.rmsd.rmsd(coords1: ndarray, coords2: ndarray, atomicn1: ndarray, atomicn2: ndarray, center: bool = False, minimize: bool = False, atol: float = 1e-09) → float`

Compute RMSD

### Parameters

- **coords1** (*np.ndarray*) – Coordinate of molecule 1
- **coords2** (*np.ndarray*) – Coordinates of molecule 2
- **atomicn1** (*np.ndarray*) – Atomic numbers for molecule 1
- **atomicn2** (*np.ndarray*) – Atomic numbers for molecule 2
- **center** (*bool*) – Center molecules at origin
- **minimize** (*bool*) – Compute minimum RMSD (with QCP method)
- **atol** (*float*) – Absolute tolerance parameter for QCP method (see `qcp_rmsd()`)

### Returns

RMSD

### Return type

float

## Notes

When *minimize=True*, the QCP method is used.<sup>1</sup> The molecules are centred at the origin according to the center of geometry and superimposed in order to minimize the RMSD.

`spyrmsd.rmsd.rmsdwrapper(molref: Molecule, mols: Union[Molecule, List[Molecule]], symmetry: bool = True, center: bool = False, minimize: bool = False, strip: bool = True, cache: bool = True) → Any`

Compute RMSD between two molecule.

### Parameters

- **molref** (*molecule.Molecule*) – Reference molecule
- **mols** (*Union[molecule.Molecule, List[molecule.Molecule]]*) – Molecules to compare to reference molecule
- **symmetry** (*bool, optional*) – Symmetry-corrected RMSD (using graph isomorphism)
- **center** (*bool, optional*) – Center molecules at origin
- **minimize** (*bool, optional*) – Minimised RMSD (using the quaternion polynomial method)
- **strip** (*bool, optional*) – Strip hydrogen atoms

### Returns

RMSDs

<sup>2</sup> W. J. Allen and R. C. Rizzo, *Implementation of the Hungarian Algorithm to Account for Ligand Symmetry and Similarity in Structure-Based Design*, J. Chem. Inf. Model. **54**, 518-529 (2014)

<sup>1</sup> D. L. Theobald, *Rapid calculation of RMSDs using a quaternion-based characteristic polynomial*, Acta Cryst. A **61**, 478-480 (2005).

**Return type**

List[float]

`spyrmsd.rmsd.symmrmsd(coordsref: ndarray, coords: Union[ndarray, List[ndarray]], apropsref: ndarray, aprops: ndarray, amref: ndarray, am: ndarray, center: bool = False, minimize: bool = False, cache: bool = True, atol: float = 1e-09) → Any`

Compute RMSD using graph isomorphism for multiple coordinates.

**Parameters**

- **coordsref** (*np.ndarray*) – Coordinate of reference molecule
- **coords** (*List[np.ndarray]*) – Coordinates of other molecule
- **apropsref** (*np.ndarray*) – Atomic properties for reference
- **aprops** (*np.ndarray*) – Atomic properties for other molecule
- **amref** (*np.ndarray*) – Adjacency matrix for reference molecule
- **am** (*np.ndarray*) – Adjacency matrix for other molecule
- **center** (*bool*) – Centering flag
- **minimize** (*bool*) – Minimum RMSD
- **cache** (*bool*) – Cache graph isomorphisms
- **atol** (*float*) – Absolute tolerance parameter for QCP (see `qcp_rmsd()`)

**Returns**

**float** – Symmetry-corrected RMSD(s) and graph isomorphisms

**Return type**

Union[float, List[float]]

**Notes**

Graph isomorphism is introduced for symmetry corrections. However, it is also useful when two molecules do not have the atoms in the same order since atom matching according to atomic numbers and the molecular connectivity is performed. If atoms are in the same order and there is no symmetry, use the *rmsd* function.

**spyrmsd.utils module**

`spyrmsd.utils.center(coordinates: ndarray) → ndarray`

Center coordinates.

**Parameters**

**coordinates** (*np.ndarray*) – Coordinates

**Returns**

Centred coordinates

**Return type**

*np.ndarray*

`spyrmsd.utils.center_of_geometry(coordinates: ndarray) → ndarray`

Center of geometry.

**Parameters**

**coordinates** (*np.ndarray*) – Coordinates

### Returns

Center of geometry

### Return type

np.ndarray

`spyrmsd.utils.deg_to_rad(angle: float) → float`

Convert angle in degrees to angle in radians.

### Parameters

**angle** (*float*) – Angle (in degrees)

### Returns

Angle (in radians)

### Return type

float

`spyrmsd.utils.format(fname: str) → str`

Extract format extension from file name.

### Parameters

**fname** (*str*) – File name

### Returns

File extension

### Return type

str

## Notes

The file extension is returned without the `.` character, i.e. for the file *path/filename.ext* the string *ext* is returned.

If a file is compressed, the `.gz` extension is ignored.

`spyrmsd.utils.molformat(fname: str) → str`

Extract an OpenBabel-friendly format from file name.

### Parameters

**fname** (*str*) – File name

### Returns

File extension in an OpenBabel-friendly format

### Return type

str

## Notes

File types in OpenBabel do not always correspond to the file extension. This function converts the file extension to an OpenBabel file type.

The following table shows the different conversions performed by this function:

Extension	File Type
xyz	XYZ

`spyrmsd.utils.rotate(v: ndarray, angle: float, axis: ndarray, units: str = 'rad') → ndarray`

Rotate vector.

### Parameters

- **v** (*numpy.array*) – 3D vector to be rotated
- **angle** (*float*) – Angle of rotation (in *units*)
- **axis** (*numpy.array*) – 3D axis of rotation
- **units** (*{“rad”, “deg”}*) – Units of *angle* (in radians *rad* or degrees *deg*)

### Returns

Rotated vector

### Return type

*numpy.array*

### Raises

- **AssertionError** – If the axis of rotation is not a 3D vector
- **ValueError** – If *units* is not *rad* or *deg*



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