
PointGroup

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PointGroup is a pure python library to determine the point symmetry group of molecules.

MAIN FEATURES

- Determine point symmetry group label
- Pure python implementation

1.1 Installation

PointGroup can be installed directly from the source code (python package) or via PyPI repository.

1.1.1 Requirements

- Python 2.7.x/3.5+
- numpy

1.1.2 Install

1) From source code

```
git clone https://github.com/abelcarreras/pointgroup.git pointgroup
cd pointgroup
python setup.py install --user
```

2) From PyPI repository

```
pip install pointgroup --user
```

1.2 Get started

PointGroup is a simple library based in a single class that is initialized from a set of atomic positions and atomic symbols.

1.2.1 Determine the point symmetry group

To determine the point symmetry group, first initialize a **PointGroup** object and then access to **get_point_group()** method. This returns a string containing the label of the determined point group for the given molecule. The following example shows the determination of the octahedral symmetry of SF₆ molecule:

```
from pointgroup import PointGroup

pg = PointGroup(positions=[[ 0.000000,  0.000000,  0.000000],
                           [ 0.000000,  0.000000,  1.561000],
                           [ 0.000000,  1.561000,  0.000000],
                           [ 0.000000,  0.000000, -1.561000],
                           [ 0.000000, -1.561000,  0.000000],
                           [ 1.561000,  0.000000,  0.000000],
                           [-1.561000,  0.000000,  0.000000]],
                 symbols=['S', 'F', 'F', 'F', 'F', 'F', 'F', 'F'])

print('Point group: ', pg.get_point_group())
```

1.3 Public API

class pointgroup.**PointGroup**(positions, symbols, tolerance_eig=0.01, tolerance_ang=4)

Point group main class

get_point_group()

get the point symmetry group symbol

Returns

the point symmetry group symbol

get_principal_axis_of_inertia()

get the principal axis of inertia in rows in increasing order of momenta of inertia

Returns

the principal axis of inertia

get_principal_moments_of_inertia()

get the principal momenta of inertia in increasing order

Returns

list of momenta of inertia

get_standard_coordinates()

get the coordinates centered in the center of mass and oriented along principal axis of inertia

Returns

the coordinates

PointGroup was originally developed by Efre Bernuz and currently maintained by Abel Carreras at Donostia International Physics Center (DIPC), Euskadi, Spain.

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