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# **cosymlib Documentation**

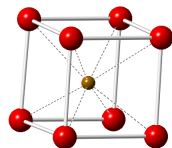
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**Jun 09, 2023**



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**Cosymlib** is a python library for computing continuous symmetry & shape measures (CSMs & CShMs). Although its main aim is to provide simple and ready-to-use tools for the analysis of the symmetry & shape of molecules, many of the procedures contained in **cosymlib** can be easily applied to any finite geometrical object defined by a set of vertices or a by mass distribution function.

The basic tasks included in the current version of **cosymlib** are:

1. **Molecular structure analysis**

- Calculation of Continuous Shape Measures (CShMs)
- Calculation of Continuous Symmetry Measures (CSMs)
- Calculation of Continuous Chirality Measures (CCMs)

2. **Electronic structure analysis**

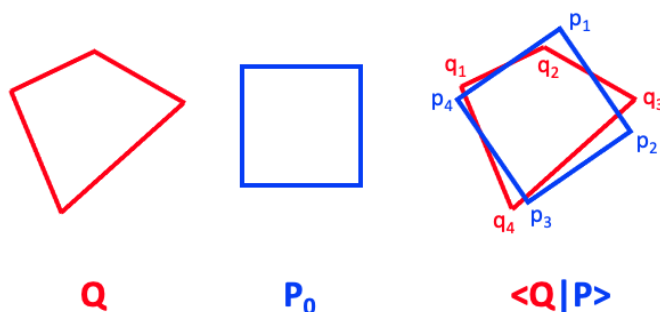
- Pseudosymmetry analysis of molecular orbitals & wavefunctions
- Continuous Symmetry & Chirality Measures for the molecular electron density



**Cosymlib** is a python library for computing continuous symmetry & shape measures (CSMs & CShMs). Although most of the tools included in **cosymlib** have been devised especially with the purpose of analyzing the symmetry & shape of molecules as proposed initially by D. Avnir and coworkers [AVN], many of the procedures contained in **cosymlib** can be easily applied to any finite geometrical object defined by a set of vertices or a by mass distribution function.

## 1.1 Continuous Shape Measures (CShMs)

In a nutshell, the continuous shape measure  $S_p(Q)$  of object  $Q$  with respect to the reference shape  $P$  is an indicator of how much  $Q$  resembles another object  $P_0$  with a given ideal shape, for instance a square as in the figure below.



Given that the shape is invariant upon translations, rotations, and scaling, the most evident way to compare the two objects is to translate, rotate and scale one of them, for instance  $P_0$ , until we maximize the overlap  $\langle Q|P \rangle$  between  $Q$  and  $P$ , where  $P$  is the image of  $P_0$  after these transformations.

If both the problem and the reference structures  $Q$  and  $P$  are defined as a set of vertices, we can define the shape measure simply as:

$$S_P(Q) = \min \frac{\sum_{i=1}^N |q_i - p_i|^2}{\sum_{i=1}^N |q_i - q_0|^2} \times 100$$

where  $N$  is the number of vertices in the structures we are comparing,  $q_i$  and  $p_i$  are the position vectors of the vertices of  $Q$  and  $P$ , respectively, and  $q_0$  the geometric center of the problem structure  $Q$ . The minimization in this equation refers to the relative position, orientation, and scaling that must be applied to  $P_0$  to minimize the sum of squares of distances between their respective vertices, which is equivalent to maximizing the overlap  $\langle Q|P \rangle$ . If the mismatch of the two shapes is described, as in the equation above by the distance between vertices of the two objects, a further minimization with respect to all possible ways to label the  $N$  vertices in the reference structure  $P_0$  is also needed.

From the definition of  $S_P(Q)$  it follows that if  $Q$  and  $P$  have exactly the same shape, then  $S_P(Q) = 0$ . Since  $S_P(Q)$  is always positive, the larger its value, the less similar is  $Q$  to the ideal shape  $P$ . It can be shown that the maximum value for  $S_P(Q)$  is 100, corresponding to the unphysical situation for which all vertices of  $Q$  collapse into a single point. A more detailed description of continuous shape measures and some of their applications in chemistry may be found in the following references [CShM]:

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## 1.2 Continuous Symmetry Measures (CSMs)

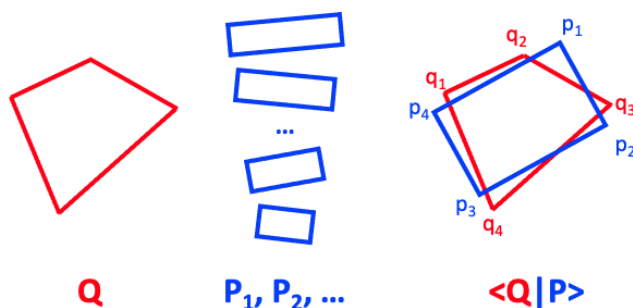
To define a continuous measure for the degree of symmetry of an object one may proceed in the same way as for the definition of CShMs. The final result for the symmetry measure with respect to a given point symmetry group  $G$ , denoted as  $S_G(Q)$ , yields an expression totally analogous to the equation above, in which  $Q$  refers again to the problem structure, but where  $P$  is now the  $G$ -symmetric structure closest to  $Q$ :

$$S_G(Q) = \min \frac{\sum_{i=1}^N |q_i - p_i|^2}{\sum_{i=1}^N |q_i - q_0|^2} \times 100$$

The minimization process in this case refers to the relative position of the two structures (translation), the orientation of the symmetry elements for the reference  $G$ -symmetric structure  $P$ , the scale factor, and again, the labeling of vertices of the symmetric structure. Note that although the same equation may be used both to define shape and symmetry measures, there is a fundamental difference between the two procedures: while in computing a shape measure we know in advance the reference object  $P_0$ , in the case of symmetry measures the shape of the closest  $G$ -symmetric structure is, in principle, previously unknown and must be found in the procedure of computing  $S_G(Q)$ .

Consider, for instance that we would like to measure the rectangular symmetry for a given general quadrangle. Besides optimizing to seek for the translation, rotation, and scaling that leads to the optimal overlap of our quadrangle  $Q$  with a particular rectangle  $P$  as in a shape measure, we will need to consider also which is the ratio between the side lengths of the best matching rectangle and optimize also with respect to this parameter.



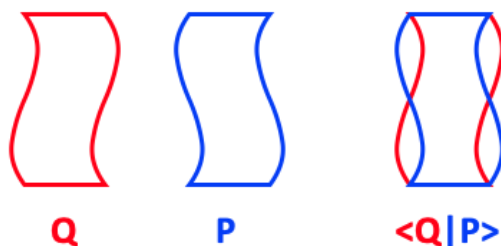


Although this additional optimization process may seem difficult to generalize for any given symmetry group, it has been shown that it is possible to do it efficiently using either the folding–unfolding algorithm or via the calculation of intermediate symmetry operation measures.

As in the case of shape measures, the values of CSMs are also limited between 0 and 100, with  $S_G(Q) = 0$ , meaning that  $Q$  is a  $G$ -symmetric shape. A more detailed description of continuous shape measures and some of their applications in chemistry may be found in the following references [CSM]:

### 1.3 Continuous Chirality Measures (CCMs)

A special mention should be made to chirality, a specific type of symmetry that has a prominent role in chemistry. A chiral object is usually described as an object that cannot be superposed with its mirror image. In this sense, we could obtain a continuous chirality measure by using the same equation as for shape measures just by replacing  $P$  by the mirror image of  $Q$ .



Technically speaking chirality is somewhat more complex since it implies the lack of any improper rotation symmetry and its CCM can be based on estimating how close a given object is from having this symmetry. Using the CSMs defined above, the continuous chirality measure can be defined as the minimal of all  $S_G(Q)$  values for  $S_n(Q)$  with  $n=1,2,4, \dots$ . In most cases it will be either for  $G = S_1 = C_s$  or  $G = S_2 = C_i$ , whereas in a few cases we will have to look for  $G = S_4$  or higher-order even improper rotation axes. Since in most cases visual inspection of the studied structure is enough in order to guess which one could be the nearest  $S_n$  group, a practical solution is just to calculate this particular  $S_G(Q)$  value, or in case of doubt, a few  $S_G(Q)$  values for different  $S_n$  and pick the smallest one. A more detailed description of continuous shape measures and some of their applications in chemistry may be found in the following references [CCM]:

## 1.4 CSMs for quantum chemical objects

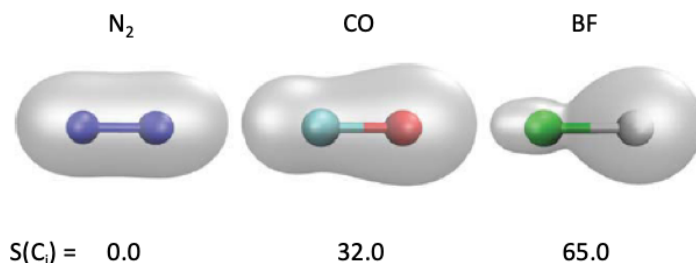
The use of the overlap  $\langle Q|P \rangle$  between two general objects  $Q$  and  $P$  allows the generalization of continuous symmetry and shape measures to more complex objects that cannot be simply described by a set of vertices, such as matrices or functions. In this case the definition of the continuous symmetry measure is:

$$S_G(Q) = \min \left[ 1 - \frac{\sum_{i=1}^h \langle Q | \hat{g}_i Q \rangle}{h \langle Q | Q \rangle} \right]$$

where  $Q$  is the given object and  $\hat{g}_i$  the  $h$  symmetry operations comprised in the finite point symmetry group  $G$ . The minimization in this case just refers to the orientation of the symmetry elements that define the symmetry operations in  $G$ . The key elements in this definition are the overlap terms  $\langle Q | \hat{g}_i Q \rangle$  between the original object  $Q$  and its image under all the  $h$  symmetry operations  $\hat{g}_i$  that form group  $G$ . The precise definition on how to obtain these overlaps depends, of course, on the nature of the object  $Q$ . For molecular orbitals as obtained in a quantum chemical calculation we have:

$$\langle \varphi | \hat{g}_i \varphi \rangle = \int \varphi(\mathbf{r}) \hat{g}_i \varphi(\mathbf{r}) d\tau$$

which is known as a SOEV (symmetry operation expectation value). For the electron density one can use an analogous expression for the corresponding SOEV by replacing the orbital (one electron wavefunction) by the whole electron density. Using this type of symmetry measures one is then able to compare the symmetry contents of the electronic structure of molecules, for instance by comparing the inversion symmetry measure for different diatomic molecules as in the example below:



The generalization of CSMs for functions, is of course, not limited to chemical applications and it permits extending the notion of continuous symmetry measures to geometrical objects beyond those defined by a set of vertices. A solid object of arbitrary shape, not restricted to a polyhedron, can be described by a function corresponding to a constant mass distribution, and its corresponding shape and symmetry measures can be easily computed by numerical integration to determine the SOEVs, avoiding the cumbersome minimization over vertex pairings that appear for objects that are defined by a set of vertices.

An interesting extension for functions which are not restricted to positive values, for instance, molecular orbitals, is the possibility of calculating continuous symmetry measures for each individual irreducible representation of a given point group. A more detailed description of the development and some applications of CSMs in quantum chemistry may be found in the following references [\[QCSMs\]](#):

**cosymlib** is available in both the GitHub and PyPI repositories (<https://pypi.org/project/cosymlib/>). Installation via PyPI is simpler and it is recommended for most users. Follow the instructions below to install **cosymlib** in your computer.

### 2.1 Installing cosymlib from PyPI (recommended)

This installation requires **pip** (<https://pip.pypa.io/en/stable/installing/>) to be installed in your system. We strongly recommend the use of python environments, for more details on this, refer to <https://docs.python.org/3/library/venv.html>. For most users the basic installation should proceed as follows:

1. Create a virtual environment at path <venv>

```
$ python3 -m venv <venv>
```

2. Activate this virtual environment

```
# on MAC / Linux
$ source <venv>/bin/activate

# on windows (powershell) [see note below]
C:\> <venv>\Scripts\Activate.ps1
```

3. Install **cosymlib**

```
$ pip install numpy
$ pip install cosymlib
```

4. Deactivate the virtual environment

```
$ deactivate
```

To use **cosymlib** you will need to activate the virtual environment every time that you open a new shell. On Linux/MAC all the scripts contained in **cosymlib** will be accessible in this environment:

```
$ source <venv>/bin/activate
$ <script_name> <script_options>
$ deactivate
```

On Windows, to execute the scripts you should type *python* followed by the full path of the script name:

```
C:\> python <venv>\Scripts\<script_name> <script_options>
```

---

**Note:** On Windows it may be necessary to add user execution permissions to activate the environment. To do this, open a powershell as administrator and type:

```
Set-ExecutionPolicy -ExecutionPolicy RemoteSigned -Scope CurrentUser
```

You should do this only once in order to gain execution permissions.

---

## 2.2 Installing cosymlib's source code

Alternatively, you can download the latest version of **cosymlib** from github using **git** (<https://git-scm.com>) and install it manually through the `setup.py` file using **setuptools** (<https://setuptools.readthedocs.io/>).

**cosymlib** contains libraries written in Fortran that require a compiler to build them. Before installing **cosymlib** make sure you have a working Fortran compiler installed in your system. For UNIX based systems you can install the GNU Fortran Compiler from package repositories by opening a terminal and typing the following commands:

- **Linux**

On YUM-based systems (Fedora/RedHat/CentOS)

```
sudo yum install yum-utils
```

On APT-based systems (Debian/Ubuntu)

```
sudo apt-get build-dep
```

- **Mac**

1. Install command-line tools:

```
xcode-select --install
```

2. Get Homebrew following the instructions at <https://brew.sh>, and install GCC formula by:

```
brew install gcc
```

- **Windows**

1. Install the Windows development environment **Visual Studio** (<https://developer.microsoft.com/en-us/windows/downloads/>)

2. Install C/Fortran compiler for Windows. We have tested and recommend **mingw** (<https://www.mingw-w64.org>)

To install **cosymlib**, download the source code using **git** in your computer by typing:

```
git clone https://github.com/GrupEstructuraElectronicaSimetria/cosymlib.git
```

This creates a copy of the repository in your computer. You can keep it updated by synchronizing it with the GitHub repository by using the command:

```
git pull
```

Once this is done, move to the repository root directory (where `setup.py` is found) and type the following command to install **cosymlib**:

```
python setup.py install --user
```

---

**Note:** The `requirements.txt` file located at the repository root directory contains a list of all dependency python modules needed for **cosymlib** to run. If any of them are missing in your system you will need to install them before running **cosymlib**.

---

In both cases (PyPI & Github installations) the code will be installed as a **python** module. To check that it is properly installed you can run the **python** interpreter and execute:

```
import cosymlib
```

If the execution does not show any errors, then **cosymlib** has been installed successfully.

---

**Note:** For users with Apple M1, the **scipy** library might not properly install when following the instructions above. To solve this, install it manually:

```
brew install openblas
brew install lapack
brew install python
pip install cython pybind11 pythran numpy
OPENBLAS=$(brew --prefix openblas) CFLAGS="-falign-functions=8 ${CFLAGS}" pip install_
↪--no-use-pep517 scipy==1.7.0
```

---

**Note:** When using an IDE, remember to select the python interpreter in the homebrew path. To find it:

```
which python3
>> /opt/homebrew/bin/python3
```



## CHAPTER 3

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### How to use cosymlib

---

**Cosymlib** is a python library for computing continuous symmetry & shape measures (CSMs & CShMs). Besides using the APIs contained in **cosymlib** to build your own custom-made python programs we have also written some general scripts to perform standard tasks such as calculating a continuous shape measure for a given structure without the need of writing a python script. All this general task scripts are called using a similar syntax which includes the name of the script, the name of the file containing the structural data, and optional arguments specifying the tasks we want to perform:

```
$ script filename -task1 -task2 ... -taskn
```

For instance, consider a `struct.xyz` file containing the following structural information for a  $H_4$  molecule in an approximately square geometry:

```
4
H4 Quadrangle
H   1.1   0.9   0.0
H  -1.0   1.1   0.0
H  -0.9  -1.2   0.0
H   1.1  -1.0   0.0
```

If we would like to compute the square shape measure  $S(SP-4)$  for this 4-vertex polygon we simply can call the shape script indicating the name of our `.xyz` file containing the coordinates and use the `-m` flag (m stands for measure) with the `SP-4` label to indicate that we want to compute a shape measure using a perfect square (`SP-4` stands for square planar structure with 4 vertices) as the reference shape:

```
$ shape struct.xyz -m SP-4
```

and the shape script will call the APIs in **cosymlib** to read first our input file, generate a molecule object, calculate the  $S(SP-4)$  continuous shape measure for it, and print the result of the calculation on the screen:

```
-----
COSYMLIB v0.10.5
Electronic Structure & Symmetry Group
Institut de Quimica Teorica i Computacional (IQTC)
```

(continues on next page)

(continued from previous page)

```
Universitat de Barcelona
```

```
-----  
Structure      SP-4  
H4,            0.520,  
-----
```

```
End of calculation  
-----
```

If, for instance, we also want the coordinates for the square with the optimal overlap with our problem structure, we just need to include the `-s` flag (where `s` stands for structure) in our call:

```
$ shape struct.xyz -m SP-4 -s
```

A longer, explicit version for some flags is also available using a double `-` sign. With these explicit flags the previous command becomes:

```
$ shape struct.xyz --measure SP-4 --structure
```

The general task scripts include also `gsym` and `cchir` for calculating continuous symmetry and chirality measures for polyhedral structures, `shape_map` for plotting shape maps, as well as the `esym` and `mosym` scripts for the continuous symmetry analysis of electron densities and the pseudosymmetry analysis of molecular orbitals, respectively.

Besides these six basic scripts, we have also developed `cosym`, a general script that allows to perform any of the basic calculations above. We could, for instance, use directly `cosym` to calculate the previous shape measure using the following command:

```
$ cosym struct.xyz -shp_m SP-4 -s
```

Note that when using `cosym` some of the optional flags in `shape` change to indicate which type of calculation we would like to perform. For instance, `-m` becomes `-shp_m` to distinguish it from a symmetry measure ( `-m` flag in `sym`) that becomes `-sym_m` when called from `cosym`. On the other hand, other arguments such as `-s`, which have the same meaning when calculating shape, symmetry or chirality measures, remain unchanged when used in combination with the general `cosym` script.

Taking into account the users of our previous programs, we have also written a stand-alone script `shape_classic` which is able to read an `old_shape.dat` input file containing both the structural information and the necessary keywords to run a full CShM calculation as it was done in our previous `SHAPE` program.

In the sections below you can find a detailed description of all stand-alone scripts as well as all APIs included in the present distribution of **cosymlib**.

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## 3.1 General task scripts

The **cosymlib** library includes several scripts to perform basic tasks that can be run in a terminal as command line instructions, without the need of writing a full python script. The following subsections describe the general usage of all of them.

---



### 3.1.1 shape

`shape` can be used for computing continuous shape measures (CShMs) for geometrical structures defined by the cartesian coordinates for a set of vertices, for instance, a molecular structure defined by the positions of the atomic nuclei.

The minimal information needed to run `shape` is an input file containing the coordinates of a set of vertices. Since `shape` is mainly intended to be used in the context of structural chemistry, the main source of structural information will be a `fname.xyz` file containing a molecular geometry in xyz format ([http://en.wikipedia.org/wiki/XYZ\\_file\\_format](http://en.wikipedia.org/wiki/XYZ_file_format)).

An example of a `cocl6.xyz` file with the structure for a perfect octahedral  $\text{CoCl}_6$  fragment with 2.4Å Co-Cl inter-atomic distances is:

```
7
CoCl6
Co    0.0    0.0    0.0
Cl   -2.4    0.0    0.0
Cl    2.4    0.0    0.0
Cl    0.0    2.4    0.0
Cl    0.0   -2.4    0.0
Cl    0.0    0.0    2.4
Cl    0.0    0.0   -2.4
```

The first line in the file indicates the number of atoms (vertices in the geometric structure), the second line contains a free-format descriptive title, and the following lines (as many as indicated in the first line) contain a label (usually the atomic symbol) and the cartesian coordinates x, y, z for each atom (vertex) in the structure.

`fname.xyz` files read by `shape` may contain a single structure as in the previous example or multiple structures (all with the same number N of atoms). In this case you must append a

```
N
Structure_name
label_1  x1  y1  z1
...
label_N  xN  yN  zN
```

block for each structure, without leaving any blank lines between them. Note that even if the number of vertices N must be the same for all structures, it is mandatory to include it explicitly for each block.

Shape is also able to read input structures from files in other formats used in structural chemistry. A detailed description of the structural files read by `shape` can be found in the information on input formats section.

The basic call to the `shape` script must provide the the file containing the input structure and the reference shape with respect to which the shape measure is calculated.

```
$ shape input_file -m SH
```

where `input_file` is a file containing the structural information in a valid format, for instance a `.xyz` file, `-m` requests a shape measure calculation, and is `SH` a label indicating a given reference structure, for instance `SP-4` for a square or `OC-6` for an octahedron. Note that the reference shape must be compatible with the problem structure, i. e., they must both contain the same number of atoms (vertices). To obtain a list of the labels for the reference structures compatible with a given input structure you may use:

```
$ shape input_file -l
```

If `input_file` contains, for instance, a structure with 6 atoms (vertices) you will get the following output on screen:

Available reference structures with 6 Vertices:

Label	Sym	Info
HP-6	D6h	Hexagon
PPY-6	C5v	Pentagonal pyramid
OC-6	Oh	Octahedron
TPR-6	D3h	Trigonal prism
JPPY-6	C5v	Johnson pentagonal pyramid J2

We can then use this information to compute the desired continuous shape measure

```
$ shape input_file -m OC-6
```

if we want to compute the octahedral shape measure. For a file containing a perfect octahedron of carbon atoms:

```
6
C6_octa
  C  -1.0   0.0   0.0
  C   1.0   0.0   0.0
  C   0.0   1.0   0.0
  C   0.0  -1.0   0.0
  C   0.0   0.0   1.0
  C   0.0   0.0  -1.0
```

the program will return:

```
Starting...
-----
COSYM v0.7.4
Electronic Structure Group,  Universitat de Barcelona
-----

Structure      OC-6

C6_octa,       0.000

End of cosym calculation
```

Indicating that it is indeed a perfect octahedron,  $S(\text{OC-6}) = 0.000$ . If we want to know how far this octahedron is from the reference triangular prism we may use:

```
$ shape input_file -m TPR-6
```

which returns a value of  $S(\text{TPR-6}) = 16.737$ . Note that since shape measures are independent from size, position, or orientation of the problem structure, we would obtain exactly the same values for any perfect octahedron in `input_file`.

When studying the shape of the coordination sphere around a given atom, let us say a transition metal atom  $M$  surrounded by  $n$  atoms  $L$  coming from the surrounding ligands, it is possible to consider just the  $L_n$  polyhedron or a centered  $ML_n$  “polyhedron”. We will obtain different information from each calculation. While considering the  $L_n$  polyhedron, we will know how different it is from the ideal references, but if we are interested in distortions due to displacements of the central atom from the geometric center we will need to compare the centered  $ML_n$  “polyhedron” with the ideal references where the central atom is located at the geometric center of the object. Since the central  $M$  atom and the  $n$  surrounding ligands are not equivalent (no  $M \leftrightarrow L$  permutations are allowed when computing the shape measure) it is necessary to indicate that the structure in `input_file` corresponds to a centered  $ML_n$  polyhedron and not to a simple  $L_{n+1}$  polyhedron. This is achieved by including the `-c N` flag in the shape command,

where N is an integer number indicating the position of the central atom in `input_file` (for a file with multiple structures the central atom should be in the same position for all of them). If one uses the `cocl6.xyz` file above as `input_file` indicating that the first atom in the structure (the Co atom) is in the center (`-c 1`)

```
$ shape cocl6.xyz -l -c 1
```

we get the following valid labels:

```
Available reference structures with 6 Vertices:
```

Label	Sym	Info
HP-6	D6h	Hexagon
PPY-6	C5v	Pentagonal pyramid
OC-6	Oh	Octahedron
TPR-6	D3h	Trigonal prism
JPPY-6	C5v	Johnson pentagonal pyramid J2

note that, although these labels the same as those for a structure with 6 atoms where we do not include a central atom, a calculation including the `-c N` flag is not equivalent to a calculation where the central atom is ignored, that is just for the  $L_n$  polyhedron. If one wants to calculate the shape measure just for the “empty”  $L_n$  shell one needs to prepare a different input file deleting the line corresponding to the central atom and reducing the number of atoms by 1.

If we try omitting the `-c N` flag for the `cocl6.xyz` file we get a different result. Using

```
$ shape cocl6.xyz -l
```

we find:

```
Available reference structures with 7 Vertices:
```

Label	Sym	Info
HP-7	D7h	Heptagon
HPY-7	C6v	Hexagonal pyramid
PBPY-7	D5h	Pentagonal bipyramid
COC-7	C3v	Capped octahedron
CTPR-7	C2v	Capped trigonal prism
JBPY-7	D5h	Johnson pentagonal bipyramid J13
JETPY-7	C3v	Johnson elongated triangular pyramid J7

which are the possible reference structures for empty  $L_7$  polyhedra, since now the Co atom is being considered on equal foot to all other six Cl atoms, even if this might make no sense from a chemical point of view. The list of currently available reference structures in the cosymlib program is at [the page end](#).

To calculate the octahedral shape measure for the  $\text{CoCl}_6$  structure contained in the `cocl6.xyz` file we will use:

```
$ shape cocl6.xyz -c 1 -m OC-6
```

which will return a  $S(\text{OC-6}) = 0.000$  value since the six Cl atoms in the structure form a perfect octahedron with the Co atom sitting exactly in its geometric center. Note also that, as shown in this example, the position of the `-c N` and `-m OC-6` flags, or the `input_file` in the call to the shape script is totally irrelevant and any combination such as:

```
$ shape cocl6.xyz -c 1 -m OC-6
$ shape -c 1 -m OC-6 cocl6.xyz
$ shape -m OC-6 cocl6.xyz -c 1
```

will result in exactly the same CShM calculation.

Sometimes we are not just interested in the shape measure, that is, how far our problem shape is from the ideal reference, but also we would like to have the coordinates of the ideal reference shape with the size, position, and orientation that is closest to our problem shape. To achieve this we just need to include the `-s` flag in our call.

Let us consider a `struct.xyz` file containing the geometry for an approximately square  $H_4$  molecule.

```
4
H4 Quadrangle
H    1.1    0.9    0.0
H   -1.0    1.1    0.0
H   -0.9   -1.2    0.0
H    1.1   -1.0    0.0
```

If we want to know how far it is from having a perfectly square geometry and which is the closest square to its actual distorted structure we may use:

```
$ shape struct.xyz -m SP-4 -s
```

which will yield:

**Starting...**

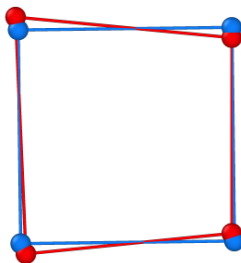
```
-----
COSYM v0.7.4
Electronic Structure Group, Universitat de Barcelona
-----
```

```
Structure      SP-4
```

```
H4,            0.520
```

```
4
H4
H    1.100000    0.900000    0.000000
H   -1.000000    1.100000    0.000000
H   -0.900000   -1.200000    0.000000
H    1.100000   -1.000000    0.000000
4
H4_SP-4
H    1.100000    1.000000    0.000000
H   -0.975000    0.975000    0.000000
H   -0.950000   -1.100000    0.000000
H    1.125000   -1.075000    0.000000
```

from which we find that the problem structure has an approximate square planar geometry with a small departure from the ideal shape,  $S(SP-4) = 0.520$ , together with the coordinates of the problem structure and its closest ideal (square) structure, which we can use to plot the superposition of problem structure (in red) and the ideal reference (in blue):



Other optional flags to control the execution of shape are:

`shape -h` (no input file needed) returns a list of all available flags and their use

Running `shape` with the `-o file_name` flag prints all output into the `file_name` file

Running `shape` with the `-r` flag prints the coordinates of the reference shape in a file named `Ln.xyz` or `M Ln.xyz` where `n` is the number of vertices of the polyhedron.

The `-info` flag may be used to print the coordinates of the input structure

You may use `-fixp` to disable the minimization over the permutation of vertices while searching for the shape measure. If you include the `-fixp` in your call, the minimization will be carried out considering only the distance between the *i*-th vertex in the problem structure with the *i*-th vertex in the reference shape. Although this option allows a drastic reduction of the computational cost, it should be used with care since the actual shape measure is defined for the permutation that gives the lowest value of *S*. For large structures the `-fixp` option will probably be the only way of obtaining a shape measure, but this procedure is only justified for structures with small distortions from the reference structure. Before doing the actual calculation it will be necessary to run `shape` with the `-r` flag to print the coordinates of the reference shape and order the vertices in the problem structure accordingly.

A quite useful flag is `-cref filename` that allows the user to specify a custom reference structure in the filename file. Use this option if you want to use a reference structure different from any of those provided by `shape`. To use this feature you will need to include the `-m custom` flag in your call:

```
$ shape input_file -m custom -cref filename
```

Besides the shorthand version of the flags described above, it is also possible to use an explicit version by writing them preceded by a double `--` sign. The explicit versions of the flags are:

Short Flag	Explicit flag
<code>-h</code>	<code>--help</code>
<code>-m</code>	<code>--measure</code>
<code>-l</code>	<code>--labels</code>
<code>-s</code>	<code>--structure</code>
<code>-o</code>	<code>--output_name</code>
<code>-c</code>	<code>--central_atom</code>
<code>-r</code>	<code>--references</code>
<code>-cref</code>	<code>--custom_ref</code>
<code>-fixp</code>	<code>--fix_permutation</code>

Sometimes, to avoid a cumbersome repetition of several flags in the call of the `shape` module we may write all flags in an input file and just call `shape` indicating the file with the structural input and the file with the options of the

calculation. For example, if the original call is:

```
$ shape struct.xyz -c 1 -m OC-6 -s -o struct.out
```

You can create a new file called `struct.yml` (the name for the file can be freely chosen and does not need to be the same as for the structure) containing the options in YAML format (<http://en.wikipedia.org/wiki/YAML>):

```
central_atom : 1
measure      : OC-6
structure    : True
output       : struct.out
```

and then call `shape` just using:

```
$ shape struct.xyz struct.yml
```

Note that you must use the explicit version of the flags in the `.yml` file. If a flag such as `-s` does not need any additional argument, you must include `True` in the `.yml` file.

---

### 3.1.2 shape\_classic

To run `shape_classic` you only need an `old_shape.dat` input file containing both the structural information and the necessary keywords to run a full CShM calculation as in the old SHAPE program:

```
$ shape_classic old_shape.dat
```

The script will perform all tasks indicated in the input file, creating the necessary output files, normally `old_shape.out` and `old_shape.tab` with the same information as when using our previous SHAPE program. Follow the link below for a pdf version of the user guide for SHAPE ver. 2.1 where you will find all information to perform a continuous shape analysis using this option.

SHAPE ver. 2.1 User's guide

---

### 3.1.3 gsym

In the case of running a continuous symmetry measure (CSM), the `gsym` script is required plus an input file containing a geometric structure as the one used in the `shape` script. Since the main difference with the continuous shape measures is that the reference structure now must contain one or more symmetry elements, the user will need to specify which symmetry operation wants to analyse for the input geometry. The  $Th_8$  molecule can be a good example to show the  $S_4$  symmetry that the molecule contains. The `Th8.xyz` file is shown below:

```
8
Th8
Th -16.80062 -0.55052 -13.74098
Th -12.80008 -0.09601 -14.54017
Th -15.57778 1.38797 -17.17300
Th -20.18823 -1.83274 -15.67222
Th -16.79762 -4.14442 -15.76983
Th -12.79709 -3.68990 -16.56902
Th -18.96539 0.10576 -19.10423
Th -15.57478 -2.20592 -19.20184
```

The simplest way to compute the  $S_4$ CSM measure for Th<sub>8</sub> is to run the following command:

```
$ gsym Th8.xyz -m S4
```

which is equivalent to:

```
$ gsym -m S4 Th8.xyz
```

and will return the CSM result in the cosymplib format:

```
-----
COSYMLIB v0.9.5
Electronic Structure & Symmetry Group
Institut de Quimica Teorica i Computacional (IQTC)
Universitat de Barcelona
-----
```

```
Evaluating symmetry operation : S4
```

```
th8          0.000
```

```
-----
                        End of calculation
-----
```

If the user wants to save this information in a file, the `-o` (or `--output`) flag should be added as well as the output file name. For example, the following call will execute the previous CSM calculation and will store the information in the Th8.txt file:

```
$ gsym Th8.xyz -m S4 -o Th8.txt
```

Additional commands (or flags) can be added to the command line to control the type of calculation that will be run. For example, the `-c N` command, where *N* is the position of an atom of the input file, explicitly tells the program which atom acts as a central atom of the molecule and that only could permut by himself. Alternatively, the `--center x y z`, where *x*, *y* and *z* are the 3D coordinates of a point in space, will set the origin of a structure. Similarly, the `-s` and `-l` commands work as in the shape case. The first returns the coordinates of the ideal reference geometry with the size, position, and orientation that is closest to our problem shape and belongs to a symmetry group. The second gives information of the available symmetry groups in cosymplib

```
Available symmetry groups
```

```
E      Identity Symmetry
Ci     Inversion Symmetry Group
Cs     Reflection Symmetry Group
Cn     Rotational Symmetry Group (n: rotation order)
Sn     Rotation-Reflection Symmetry Group (n: rotation-reflection order)
```

The `--info` flag may be used to print the coordinates of the input structure. Supplementary, other flags are available to the user to control if the calculation should take into account the connectivity `--ignore_connectivity`, the atom nature `--ignore_atoms_labels`, the connectivity threshold that controls if two atoms are connected `--connectivity_thresh` or the file that contains a custom connectivity `--connectivity_file`. In the last case, the format of the connectivity file should be as follow,

```
1      2      3      4      5
2      1
3      1
```

(continues on next page)

(continued from previous page)

```
4    1
5    1
```

where each number is related to the position of the each atom on the input file. For example, in the first line, the connectivity file tells the program that the atom in position one of the the input file is connected to the second, third, fourth and fifth atoms, while the second line tells that the second atom is only connected to the first atom. For a methane molecule where the input file is written as follow,

```
5
Methane
  C      0.0000      0.0000      0.0000
  H      0.5288      0.1610      0.9359
  H      0.2051      0.8240     -0.6786
  H      0.3345     -0.9314     -0.4496
  H     -1.0685     -0.0537      0.1921
```

the connectivity file force the carbon atom to be connected to all hydrogen atoms and viceversa. Finally, a list of available flags and their uncontracted form is listed below.

Short Flag	Explicit flag
-h	--help
-m	--measure
-s	--structure
-c	--central_atom
-o	--output
-l	--labels
-v	--version

Note: the actual program only runs for  $C_n$ ,  $C_s$ ,  $C_i$  and  $S_n$  symmetry groups as well as their symmetry operations.

---

### 3.1.4 cchir

The `cchir` script allows the user to calculate the chirality of a structure by calculating the continuous symmetry measure of the  $S_n$  improper rotation group. By default the `-m` flag will measure the  $S_1$  symmetry which is equivalent ot the  $C_s$  symmetry group. However, the user can control the order of the impropert rotation by the `-order n` flag where  $n=1,2,4,6,\dots$ . Other additional flags derived from the `gsym` script that have the same interaction with the chirality measure are available and list below. For more information of these commands go to `gsym` subsection of this page.

Common cchir and gsym commands
-o or --ouput
-c or --central_atom
-v or --version
--info
--center

---



### 3.1.5 esym

We are currently working on this feature of the program regarding the electronic structure symmetry of molecules, therefore the actual script is under construction.

---

### 3.1.6 cosym

This script is a general script that cover all the previous scripts.

---

## 3.2 Specific task scripts

In this section the specific task scripts are described.

---

### 3.2.1 shape\_map

The `shape_map` script calculate the continuous shape measures of a single or multiple structures with two reference structures in the same way the `shape` script does. However, it computes additional information like the minimum distortion pathway between the two reference structures, plus the deviation and the generalized coordinate of each user's structure. The most common commands available in the script are similar to the commands found in the `shape` script. The required commands are the `-m_1 SH1`` (or `--measure_1`) and the `-m_2 SH2` flags, where SH1 and SH2 are the reference structure labels available in the program. Additionally, these flags can be substituted by the `-m_custom_1 SH1` or the `-m_custom_2 SH2` to indicate the program that SH1 and/or SH2 are the files containing a custom reference structure. Moreover, a set of flags are available to control the different plot options on the `shape_map`. The `--min_dev MIN_DEV` and `--max_dev MAX_DEV` will only show the structures that are between the minimum and maximum deviation values (MIN\_DEV and MAX\_DEV), while the `--min_gco MIN_GCO` and `--max_gco MAX_GCO` show the structure that are at the MIN\_GCO to MAX-GCO range of the generalized coordinate. In addition, the user can plot more resolution minimal distortion pathways by setting the number of structures needed to compute the curve with the `--n_points N_POINTS` flag.

Finally, a set of mutual flags found in all scripts is available and listed below:

Short Flag	Explicit flag
-h	--help
-l	--labels
-o	--output_name
-c	--central_atom
-v	--version

---

## 3.3 Using cosymlib's APIs

The current API's are under construction and a set of tutorials will be provide in a near future.

## 3.4 Shape references

Here are the available shape reference's labels and their symmetry that can be used by the shape program.

Vertices	Label	Shape	Symmetry
2	L-2	Linear	$D_{\infty h}$
	vT-2	Divacant tetrahedron (V-shape, 109.47°)	$C_{2v}$
	vOC-2	Tetravacant octahedron (L-shape, 90.00°)	$C_{2v}$
3	TP-3	Trigonal planar	$D_{3h}$
	vT-3	Pyramid <sup>b</sup> (vacant tetrahedron)	$C_{3v}$
	fac-vOC-3	fac-Trivacant octahedron	$C_{3v}$
	mer-vOC-3	mer-Trivacant octahedron (T-shape)	$C_{2v}$
4	SP-4	Square	$D_{4h}$
	T-4	Tetrahedron	$T_d$
	SS-4	Seesaw or sawhorse <sup>b</sup> (cis-divacant octahedron)	$C_{2v}$
	vTBPY-4	Axially vacant trigonal bipyramid	$C_{3v}$
5	PP-5	Pentagon	$D_{5h}$
	vOC-5	Vacant octahedron <sup>b</sup> (Johnson square pyramid, J1)	$C_{4v}$
	TBPY-5	Trigonal bipyramid	$D_{3h}$
	SPY-5	Square pyramid <sup>c</sup>	$C_{4v}$
	JTBPY-5	Johnson trigonal bipyramid (J12)	$D_{3h}$
6	HP-6	Hexagon	$D_{6h}$
	PPY-6	Pentagonal pyramid	$C_{5v}$
	OC-6	Octahedron	$O_h$
	TPR-6	Trigonal prism	$D_{3h}$
	JPPY-6	Johnson pentagonal pyramid (J2)	$C_{5v}$
7	HP-7	Heptagon	$D_{7h}$
	HPY-7	Hexagonal pyramid	$C_{6v}$
	PBPY-7	Pentagonal bipyramid	$D_{5h}$
	COC-7	Capped octahedron <sup>a</sup>	$C_{3v}$
	CTPR-7	Capped trigonal prism <sup>a</sup>	$C_{2v}$
	JPBPY-7	Johnson pentagonal bipyramid (J13)	$D_{5h}$
	JETPY-7	Elongated triangular pyramid (J7)	$C_{3v}$
8	OP-8	Octagon	$D_{8h}$
	HPY-8	Heptagonal pyramid	$C_{7v}$
	HBPY-8	Hexagonal bipyramid	$D_{6h}$
	CU-8	Cube	$O_h$
	SAPR-8	Square antiprism	$D_{4d}$
	TDD-8	Triangular dodecahedron	$D_{2d}$
	JGBF-8	Johnson - Gyrobifastigium (J26)	$D_{2d}$
	JETBPY-8	Johnson - Elongated triangular bipyramid (J14)	$D_{3h}$
	JBTP-8	Johnson - Biaugmented trigonal prism (J50)	$C_{2v}$
	BTPR-8	Biaugmented trigonal prism	$C_{2v}$
	JSD-8	Snub disphenoid (J84)	$D_{2d}$
	TT-8	Triakis tetrahedron	$T_d$
	ETBPY-8	Elongated trigonal bipyramid (see 8)	$D_{3h}$
9	EP-9	Enneagon	$D_{9h}$
	OPY-9	Octagonal pyramid	$C_{8v}$
	HBPY-9	Heptagonal bipyramid	$D_{7h}$
	JTC-9	Triangular cupola (J3) = trivacant cuboctahedron	$C_{3v}$
	JCCU-9	Capped cube (Elongated square pyramid, J8)	$C_{4v}$
	CCU-9	Capped cube	$C_{4v}$

Continued on next page

Table 1 – continued from previous page

Vertices	Label	Shape	Symmetry
	JCSAPR-9	Capped sq. antiprism (Gyroelongated square pyramid J10)	$C_{4v}$
	CSAPR-9	Capped square antiprism	$C_{4v}$
	JTCTPR-9	Tricapped trigonal prism (J51)	$D_{3h}$
	TCTPR-9	Tricapped trigonal prism	$D_{3h}$
	JTDIC-9	Tridiminished icosahedron (J63)	$C_{3v}$
	HH-9	Hula-hoop	$C_{2v}$
	MFF-9	Muffin	$C_s$
10	DP-10	Decagon	$D_{10h}$
	EPY-10	Enneagonal pyramid	$C_{9v}$
	OBPY-10	Octagonal bipyramid	$D_{8h}$
	PPR-10	Pentagonal prism	$D_{5h}$
	PAPR-10	Pentagonal antiprism	$D_{5d}$
	JBCCU-10	Bicapped cube (Elongated square bipyramid J15)	$D_{4h}$
	JBCSAPR-10	Bicapped square antiprism (Gyroelongated square bipyramid J17)	$D_{4d}$
	JMBIC-10	Metabidiminshed icosahedron (J62)	$C_{2v}$
	JATDI-10	Augmented tridiminshed icosahedron (J64)	$C_{3v}$
	JSPC-10	Sphenocorona (J87)	$C_{2v}$
	SDD-10	Staggered dodecahedron (2:6:2) <sup>c</sup>	$D_2$
	TD-10	Tetradecahedron (2:6:2)	$C_{2v}$
	HD-10	Hexadecahedron (2:6:2, or 1:4:4:1)	$D_{4h}$
11	HP-11	Hendecagon	$D_{11h}$
	DPY-11	Decagonal pyramid	$C_{10v}$
	EBPY-11	Enneagonal bipyramid	$D_{9h}$
	JCPPR-11	Capped pent. Prism (Elongated pentagonal pyramid J9)	$C_{5v}$
	JCPAPR-11	Capped pent. antiprism (Gyroelongated pentagonal pyramid J11)	$C_{5v}$
	JaPPR-11	Augmented pentagonal prism (J52)	$C_{2v}$
	JASPC-11	Augmented sphenocorona (J87)	$C_s$
12	DP-12	Dodecagon	$D_{12h}$
	HPY-12	Hendecagonal pyramid	$C_{11v}$
	DBPY-12	Decagonal bipyramid	$D_{10h}$
	HPR-12	Hexagonal prism	$D_{6h}$
	HAPR-12	Hexagonal antiprism	$D_{6d}$
	TT-12	Truncated tetrahedron	$T_d$
	COC-12	Cuboctahedron	$O_h$
	ACOC-12	Anticuboctahedron (Triangular orthobicupola J27)	$D_{3h}$
	IC-12	Icosahedron	$I_h$
	JSC-12	Square cupola (J4)	$C_{4v}$
	JEPBPY-12	Elongated pentagonal bipyramid (J16)	$D_{6h}$
	JBAPPR-12	Biaugmented pentagonal prism (J53)	$C_{2v}$
	JSPMC-12	Sphenomegacorona (J88)	$C_s$
20	DD-20	Dodecahedron <sup>d</sup>	$I_h$
24	TCU-24	Truncated cube	$O_h$
	TOC-24	Truncated octahedron	$O_h$
48	TCOC-48	Truncated cuboctahedron	$O_h$
60	TRIC-60	Truncated icosahedron (fullerene)	$I_h$

a Non regular polyhedron.

b A regular polyhedron with one or two vertices removed.

c Spherical distribution of vertices with mass center at the origin (apical-basal bond angles of 104.45°).

d For polyhedra with more than 12 vertices the calculation times may be unpractical, for now avoid this calculations

an upgrade is coming soon.

e This is a chiral polyhedron. It must be noticed that the algorithm used by Shape does not distinguish the two enantiomers of a chiral shape. Therefore, whenever a chiral reference polyhedron is used, the resulting shape measures may not refer to that specific polyhedron but to its enantiomer.

Slides and notebooks used in the course “Symmetry & Shape in Structural Chemistry” given by P. Alemany at the Universidad de Santiago de Chile (USACH) from 5-9 June 2023.

The notebooks and the associated data files give an overview of the main uses of the *cosymlib*. They can be run directly on *Google colab* without the need of installing locally the *cosymlib* in the user’s computer. If the *cosymlib* is installed in the user’s computer, the notebooks can be also run locally or, alternatively, the commands included in them may be directly executed, without the need of the notebook. For a routine calculation of CSMs & CShMs we recommend to download and install the *cosymlib* in your computer and run the scripts directly, without the need of using notebooks.

## 4.1 Slides

Introduction

Molecular Shapes

Molecular Symmetry

Polyhedra in Chemistry

Continuous Symmetry Measures

Group Theory

Representation Theory

Irreducible Representations

## 4.2 Notebooks & data files

You can execute directly the notebooks in Google Colab just by clicking at the links below or you may download the notebooks to your computer and run them there. To do this you will need to install the *cosymlib* in your computer and download also the data files associated to each notebook. If you run the notebooks in your computer you don’t need to

execute the first cells loading the *cosymlib* and loading the data files, just make sure that the data files are in the same folder where you have the .ipynb files.

### 4.3 Point Group Determinaton:

[Download notebook](#) [Download datafile 1](#) [Download datafile 2](#) [Download datafile 3](#)

### 4.4 Continuous Symmetry Measures:

[Download notebook](#) [Download datafile 1](#) [Download datafile 2](#) [Download datafile 3](#)

### 4.5 Shape Measures:

[Download notebook](#) [Download datafile 1](#) [Download datafile 2](#) [Download datafile 3](#)  
[Download datafile 4](#) [Download datafile 5](#)

### 4.6 Symmetry Measures for the Electronic Structure:

### 4.7 Data files with additional molecular structures:

adamantane allene ammonia benzenetriol c5\_cp C60 C70 Co\_complex 18-crown-6 cubane  
cyclobutane cyclohex\_chair diborane difluoroethene dodecaborate dodecahedrane  
ethane ethylene ferrocene\_ec ferrocene\_st Ge9 H2O H2O2 methane Os2Cl8 SF6  
snub\_dodecahedron trisen\_co twistane vanadate h2o2\_path CrN6 Eu\_coord\_9







## CHAPTER 5

---

Useful links

---



Electronic  
Structure  
Group



Institut de Química Teòrica  
i Computacional  
UNIVERSITAT DE BARCELONA



Donostia International Physics Center

Prof. David Avnir Homepage

Dr. Inbal Tuvi-Arad Homepage

# Kimika Teorikoa

Euskal Herriko Unibertsitatea

## 6.1 Cosymlib

**class** `cosymlib.Cosymlib` (*structures*, *ignore\_atoms\_labels=False*, *ignore\_connectivity=False*, *connectivity=None*, *connectivity\_thresh=None*, *charge\_eh=0*, *mode=0*, *precision=3*)

This class contains all the high level methods used in the command line interface scripts. The methods return formatted results of multiple molecules calculations

### Parameters

- **structures** (*list*, *Geometry*, *Molecule*) – List of *Geometry* or *Molecule*
- **ignore\_atoms\_labels** (*bool*) – Ignore atomic element labels in symmetry calculations
- **ignore\_connectivity** (*bool*) – Ignore connectivity in symmetry calculations
- **connectivity** (*list*) – List of pairs of atom indices that are considered connected
- **connectivity\_thresh** (*bool*) – Connectivity threshold (Ionic radius is used as reference)

**get\_geometries** ()

Get the geometries

**Returns** List of *Geometry* objects

**Return type** list

**get\_molecule\_path\_deviation** (*shape\_label1*, *shape\_label2*, *central\_atom=0*)

Get molecule path deviation

### Parameters

- **shape\_label1** (*str*) – First shape reference label
- **shape\_label2** (*str*) – Second shape reference label

- **central\_atom** (*int*) – Position of the central atom

**get\_n\_atoms** ()

Get the number of atoms if all structures contains the same number of atoms, else raise exception.

**Returns** Number of atoms

**Return type** int

**get\_point\_group** (*tol=0.01*)

Get the point group of all structures

**Parameters** **tol** (*float*) – Tolerance

**Returns** a list of point group labels

**Return type** list

**get\_shape\_measure** (*label, kind, central\_atom=0, fix\_permutation=False*)

Get shape measure

**Parameters**

- **label** (*str*) – Reference shape label
- **kind** (*str*) – function name suffix
- **central\_atom** (*int*) – Position of the central atom
- **fix\_permutation** (*bool*) – Do not permute atoms during shape calculations

**Returns** Shape measures

**Return type** list

**molecules**

Get the molecules

**Returns** List of *Molecule* objects

**Return type** list

**print\_chirality\_measure** (*order=1, central\_atom=0, center=None, permutation=None, output=<\_io.TextIOWrapper name='<stdout>' mode='w' encoding='UTF-8'>*)

Prints the chirality measure

**Parameters**

- **order** (*int*) – Order of the chirality measure (1: Cs, 2: Ci, n: S<sub>n</sub>)
- **central\_atom** (*int*) – Position of the central atom
- **center** (*int*) – Center of symmetry in Cartesian coordinates. If None center is optimized
- **permutation** (*list, tuple*) – Define permutation
- **output** (*hook*) – Display hook

**print\_esym\_orientation** (*group, axis=None, axis2=None, center=None, out-put=<\_io.TextIOWrapper name='<stdout>' mode='w' encoding='UTF-8'>*)

Prints down an xyz file of the molecule with the orientation\_axis

**Parameters**

- **group** (*string*) – Symmetry group

- **axis** (*list*) – Main symmetry axis of group
- **axis2** (*list*) – Secondary symmetry axis of group
- **center** (*list, tuple*) – Center
- **output** (*hook*) – Display hook

```
print_geometric_measure_info(label, multi=1, central_atom=0, center=None, out-
                             put=<_io.TextIOWrapper    name='<stdout>'    mode='w'
                             encoding='UTF-8'>)
```

Prints geometric symmetry measure verbose

#### Parameters

- **label** (*str*) – Symmetry point group label
- **multi** (*int*) – Number of symmetry axis to find
- **central\_atom** (*int*) – Position of the central atom
- **center** (*list*) – Center of symmetry in Cartesian coordinates. If None center is optimized
- **output** – Display hook

Type hook

```
print_geometric_symmetry_measure(label, central_atom=0, center=None, per-
                                mutation=None, output=<_io.TextIOWrapper
                                name='<stdout>' mode='w' encoding='UTF-8'>)
```

Prints geometric symmetry measure in format

#### Parameters

- **label** (*str*) – Symmetry point group label
- **central\_atom** (*int*) – Position of the central atom
- **center** (*list, tuple*) – Center of symmetry in Cartesian coordinates. If None center is optimized
- **permutation** (*list, tuple*) – Define permutation
- **output** (*hook*) – Display hook

```
print_info()
```

Prints general information about the structures

```
print_minimum_distortion_path_shape(shape_label1, shape_label2, central_atom=0,
                                     min_dev=None, max_dev=None, min_gco=None,
                                     max_gco=None, num_points=20, output=None)
```

Print the minimum distortion path

#### Parameters

- **shape\_label1** (*str*) – First reference shape label
- **shape\_label2** (*str*) – Second reference shape label
- **central\_atom** (*int*) – Position of the central atom
- **min\_dev** (*float*) –
- **max\_dev** (*float*) –
- **min\_gco** (*float*) –

- **max\_gco** (*float*) –
- **num\_points** (*int*) – Number of points
- **output1** (*hook*) – Display hook

```
print_point_group (tol=0.01, output=<_io.TextIOWrapper name='<stdout>' mode='w' encoding='UTF-8'>)
```

Print point group of all structures

**Parameters** *tol* (*float*) – Tolerance

```
print_shape_measure (shape_reference, central_atom=0, fix_permutation=False, output=<_io.TextIOWrapper name='<stdout>' mode='w' encoding='UTF-8'>)
```

Prints the shape measure of all structures in format

**Parameters**

- **shape\_reference** (*list*) – List of references and/or geometries
- **central\_atom** (*int*) – Position of the central atom
- **fix\_permutation** (*bool*) – Do not permute atoms during shape calculations
- **output** (*hook*) – Display hook

```
print_shape_structure (shape_reference, central_atom=0, fix_permutation=False, output=<_io.TextIOWrapper name='<stdout>' mode='w' encoding='UTF-8'>)
```

Prints the nearest shape structure in format

**Parameters**

- **shape\_reference** (*list*) – List of references and/or geometries
- **central\_atom** (*int*) – Position of the central atom
- **fix\_permutation** (*bool*) – Do not permute atoms during shape calculations
- **output** (*hook*) – Display hook

```
print_symmetry_nearest_structure (label, central_atom=0, center=None, permutation=None, output=<_io.TextIOWrapper name='<stdout>' mode='w' encoding='UTF-8'>)
```

Prints the nearest structure to ideal symmetric structure

**Parameters**

- **label** (*str*) – Symmetry point group label
- **central\_atom** (*int*) – Position of the central atom
- **center** (*int*) – Center of symmetry in Cartesian coordinates. If None center is optimized
- **permutation** (*list*, *tuple*) – Define permutation
- **output** (*hook*) – Display hook

## 6.2 Molecule

```
class cosymlib.molecule.Molecule (geometry, electronic_structure=None, name=None)
```

This is the main class that contains all the information and calculations methods that can apply to a single molecule. The functionality is divided in two objects: Geometry and Electronic Structure. In the base class

(Molecule) implements the methods that require both the electronic structure and molecular geometry information such as the symmetry of the wave function.

#### Parameters

- **geometry** (*Geometry*, *Molecule*) – The geometry
- **electronic\_structure** (*ElectronicStructure*, *str*) – The electronic structure
- **name** (*str*) – Molecule name

#### **electronic\_structure**

Get the electronic structure

**Returns** The electronic structure

**Return type** *ElectronicStructure*

#### **geometry**

Get the geometry

**Returns** The geometry

**Return type** *Geometry*

#### **get\_charge()**

Get the charge of the molecule

#### **get\_connectivity()**

Get the atoms connectivity

**Returns** the atoms connectivity

**Return type** list

#### **get\_n\_atoms()**

Get the number of atoms

**Returns** number of atoms

**Return type** int

#### **get\_pointgroup(tol=0.01)**

Get the symmetry point group

**Parameters** **tol** (*float*) – The tolerance

**Returns** The point group label

**Return type** str

#### **get\_positions()**

Get the positions in Cartesian coordinates

**Returns** the coordinates

**Return type** list

#### **get\_symbols()**

Get the atomic elements symbols

**Returns** the symbols

**Return type** list

## 6.3 Geometry

**class** `cosymlib.molecule.geometry.Geometry` (*positions*, *symbols=()*, *name=""*, *connectivity=None*, *connectivity\_thresh=1.2*)

This class contains the methods related to shape and geometric symmetry calculations

### Parameters

- **positions** (*list*) – Cartesian coordinates
- **symbols** (*list*) – Atomic elements symbols
- **name** (*str*) – Geometry name
- **connectivity** (*list*) – Connectivity list
- **connectivity\_thresh** (*float*) – Connectivity threshold

### Example

```
water = Geometry(positions=[[0.0, 0.0, 0.0],
                           [0.0, 1.0, 0.0],
                           [0.0, 0.0, 1.0],
                           symbols=['O', 'H', 'H'],
                           name='water molecule',
                           connectivity=[[1, 2], [1, 3]])
```

**get\_connectivity** ()

Get connectivity as a list of pairs of connected atoms

**Returns** The connectivity

**Return type** list

**get\_n\_atoms** ()

Get the number of atoms

**Returns** number of atoms

**Return type** int

**get\_pointgroup** (*tol=0.01*)

Get the symmetry point group

**Parameters** *tol* (*float*) – The tolerance

**Returns** The point group

**Return type** str

**get\_positions** ()

Get the positions in Cartesian coordinates

**Returns** the coordinates

**Return type** list

**get\_shape\_measure** (*shape\_label*, *central\_atom=0*, *fix\_permutation=False*)

Get the Shape measure

### Parameters

- **shape\_label** (*str*) – Reference shape label
- **central\_atom** (*int*) – the central atom position



- **fix\_permutation** (*bool*) – Do not permute atoms

**Returns** The measure

**Return type** float

**get\_symbols** ()

Get the atomic elements symbols

**Returns** the symbols

**Return type** list

**get\_symmetry\_measure** (*label, central\_atom=0, center=None, multi=1, permutation=None*)

Get the symmetry measure

**Parameters**

- **label** (*str*) – Symmetry point group
- **central\_atom** (*int*) – central atom position (0 if no central atom)
- **center** (*list*) – center of the measure in Cartesian coordinates
- **permutation** (*list, tuple*) – define permutation

**Returns** The symmetry measure

**Return type** float

**get\_symmetry\_nearest\_structure** (*label, central\_atom=0, center=None, multi=1, permutation=None*)

Returns the nearest ideal structure

**Parameters**

- **label** (*str*) – symmetry point group
- **central\_atom** (*int*) – central atom position (0 if no central atom)
- **center** (*list*) – center of the measure in Cartesian coordinates
- **permutation** (*list, tuple*) – Define permutation

**Returns** The structure

**Return type** *Geometry*

**get\_symmetry\_permutation** (*label, central\_atom=0, center=None, multi=1, permutation=None*)

Get the optimum atoms permutation for geometrical symmetry measures

**Parameters**

- **label** (*str*) – Symmetry point group
- **central\_atom** (*int*) – central atom position (0 if no central atom)
- **center** (*list*) – center of the measure in Cartesian coordinates
- **permutation** (*list, tuple*) – define permutation

**Returns** The symmetry measure

**Return type** float

## 6.4 Electronic structure

```
class cosymlib.molecule.electronic_structure.ElectronicStructure (basis, orbital_coefficients,  
                                                                multiplicity=None, alpha_energies=None,  
                                                                beta_energies=None, alpha_occupancy=None,  
                                                                beta_occupancy=None)
```

This class contains basically the access to electronic structure data

### Parameters

- **basis** (*dict*) – The basis set
- **orbital\_coefficients** (*list*) – Molecular orbital coefficients
- **multiplicity** (*int*) – The multiplicity
- **alpha\_energies** (*list*) – Alpha molecular orbital energies in Hartree
- **beta\_energies** (*list*) – Beta molecular orbital energies in Hartree
- **alpha\_occupancy** (*list*) – Occupancy of alpha orbitals
- **beta\_occupancy** (*list*) – Occupancy of beta orbitals

### **alpha\_electrons**

get the number of alpha electrons

**Returns** alpha electrons

### **alpha\_energies**

get the energies of the alpha molecular orbitals

**Returns** the energies

### **basis**

get the basis set name

**Returns** basis set

### **beta\_electrons**

get the number of beta electrons

**Returns** beta electrons

### **beta\_energies**

get the energies of the beta molecular orbitals

**Returns** the energies

### **coefficients\_a**

get the alpha molecular orbitals coefficients

**Returns** the alpha molecular orbitals

### **coefficients\_b**

get the beta molecular orbitals coefficients

**Returns** the beta molecular orbitals

**multiplicity**

get the multiplicity

**Returns** the multiplicity**s2**get the expected value of spin square operator  $S^2 = (s * (s + 1))$ **Returns**  $S^2$ 

**Cosymlib** is being developed by the **Electronic Structure & Symmetry (ESS)** group at the Department de Ciència de Materials i Química Física and the Institut de Química Teòrica i Computacional (IQTUB). University of Barcelona.

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