CubeSym

Software to calculate the continuos measures of symmetry (CMS) of the electronic density from a gaussian cube formatted file.

Requisites

Python 2.7
numpy
matplotlib
scypy

Usage

This software has no configuration files. All the requested options should be input by command line flags. Options **-g** or **-c** selects the electronic density input source and are mandatory. Other flags are optional. Each parameter has a default value. Use **-h** to check the default values and get additional information.

Electronic density from analytic potential

CubeSym can generate a analytical density as a sum of tridimensional gaussian functions. This is specified by **-g** flag:

-g *potentialfile*

Reads the gaussian parameters from *potentialfile*. This file is a plain text file containing the following information:

-Definition of the grid

Limit_inf_X Limit_sup_X Number_of_points
Limit_inf_Y Limit_sup_Y Number_of_points
Limit_inf_Z Limit_sup_Z Number_of_points

-Definition of gaussian functions.

Each function is defined in one line. The firsts 3 values are the cartesian coordinates in which the function is centered. The next value is the total integration of the function and finally, the last one, is the function width.

X1 Y1 Z1 Integration1 Width 1
X2 Y2 Z2 Integration2 Width 2
.. … … …….. …..

Each function is calculated as:

$$g(x,y,z) = A\left(e^{-\frac{(x-x_0)^2}{2c^2}} + e^{-\frac{(y-y_0)^2}{2c^2}} + e^{-\frac{(z-z_0)^2}{2c^2}} \right)$$

were *c* is the width *(x_0 y_0 z_0)* define the center position and *A* is the normalization constant defined as:

$$A = \frac{Integration}{\left(c\sqrt{2\pi}\right)^3}$$

If a line starts with "#", the line is ignored. Use this for comments.

Cube file load

-c cubefile

Reads electronic density from a generic cube file. This option is incompatible with **-g**.

Set rotation order

-o value

Defines the rotational symmetry measure to be calculated.

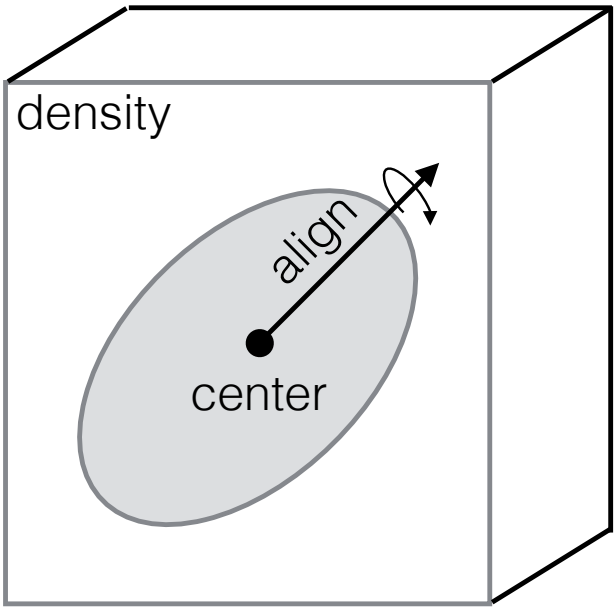
Set alignment of the density

—center X Y Z

Defines the position of the center of symmetry. By default is 0 0 0.

—align X Y Z

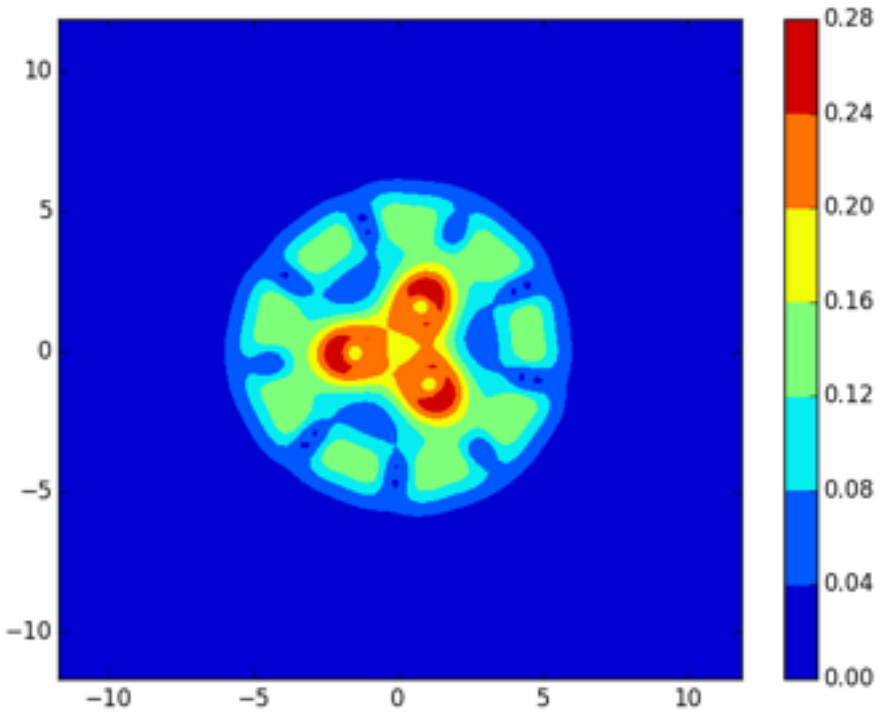
Defines the vector (from center coordinates) that indicate the direction of the rotation axis. The measure will be done respect to this axis.



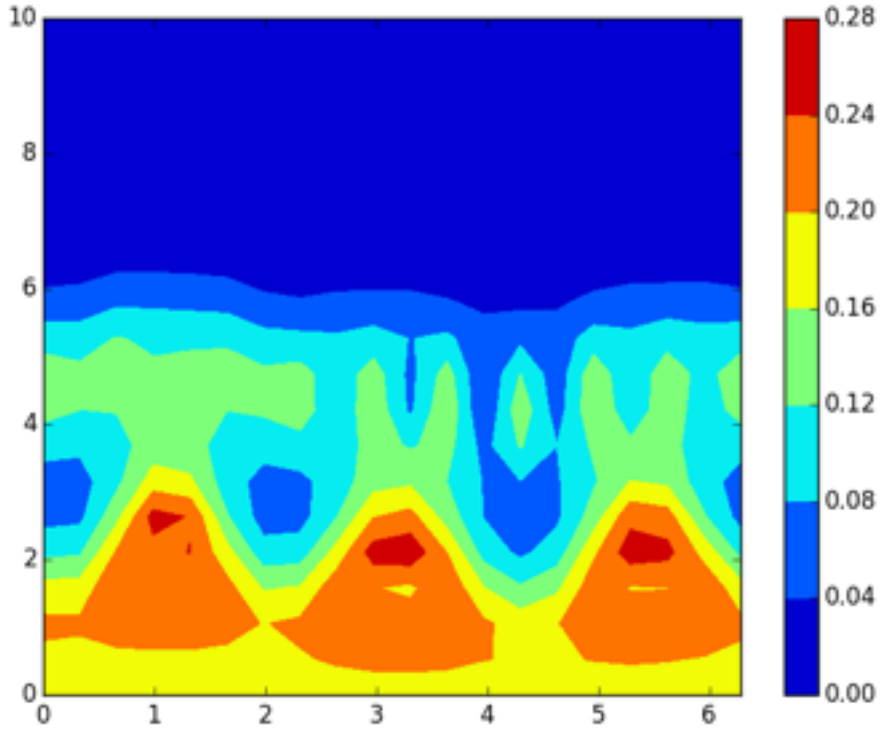
Check density

-ps coordinate

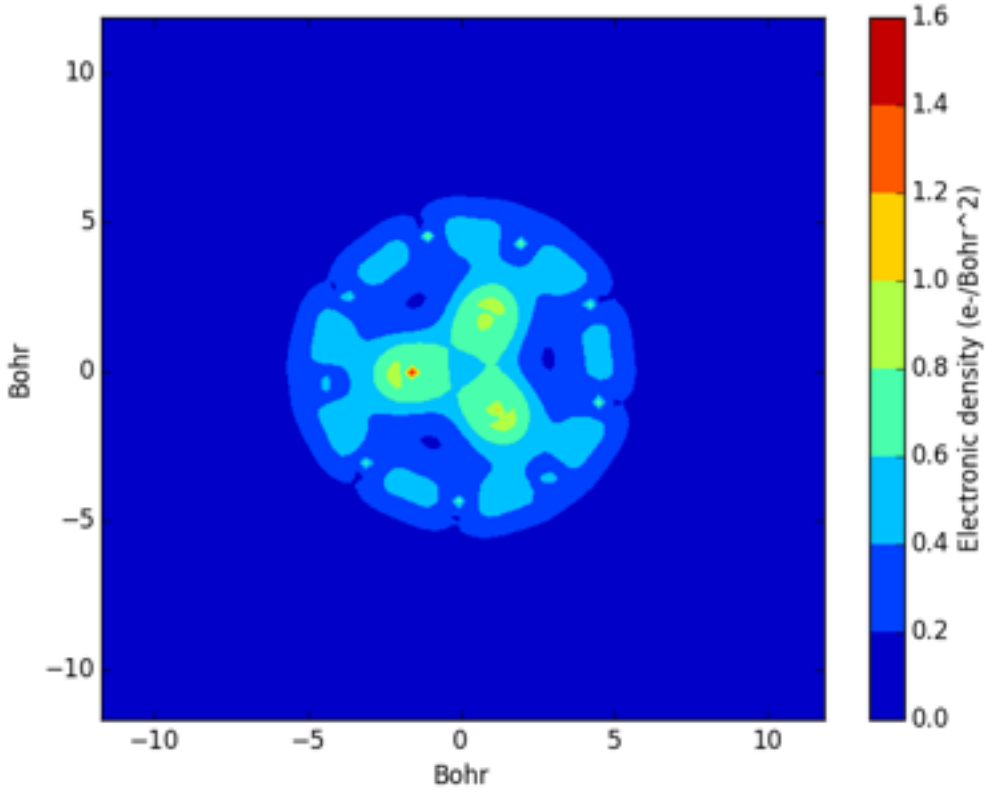
Plot a density slide along rotation axis in a contour plot. *coordinate* if a float number that defines the position of the slide.to be plotted



Plot a density slide in cylindrical coordinates. when **-r** option is also set.**-ps** coordinate



-pf precision
Plot the integration along z coordinate. This integration is calculated as the sum of slides perpendicular to z using the rectangle method. *precision* indicated the width of each rectangle.



Request measure

-m number_of_slides

Calculates the symmetry measure along the axis defined by **align** and **center**. Number_of_slides define the number of slides that will be calculated and printed. The range is calculated automatically from cube/gaussianfile density limits.

```
#     coordinate     measure(C5)       overlap        density2        density
     0.00000000      0.00000000      0.00000000      0.00000000      0.00000000
     0.34482759      0.12653913      0.14521883      0.14540282      1.00480419
     0.68965517      0.34634496      0.33466530      0.33582843      2.16332205
     1.03448276      0.62632812      0.57901804      0.58266745      3.51367389
```

coordinate: position along the align axis (or the radius in radial calculations)
measure: CMS measure

$$\frac{1}{N\rho^2}\sum_i^N \rho_i\rho$$

where ρ if the electronic density, ρ_i is the rotated density and N is the number of rotations.

overlap: integration of the average of the overlap of all rotations.

$$\frac{1}{N}\sum_i^N \rho_i\rho$$

density2: integration of the square electronic density

$$\rho^2$$

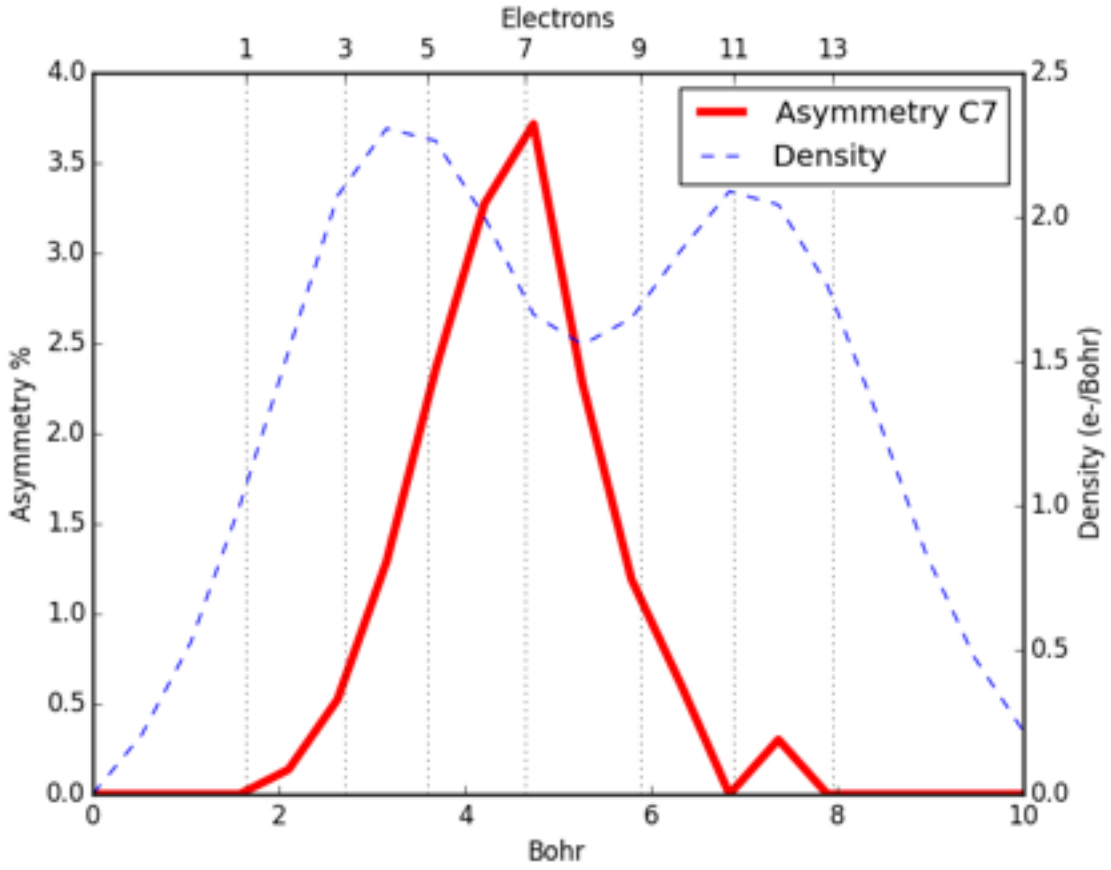
density: integration of the electronic density

$$\rho$$

Plot results

-p

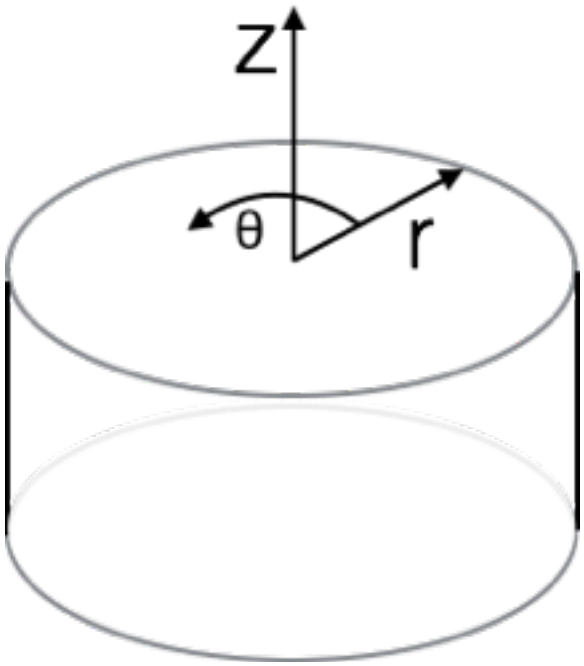
Plot the symmetry measure and electronic density. To use this feature, **-m** should also be set.



Set radial

-r

Set the measure of symmetry to be calculated along the radius instead of z axis. This direction is perpendicular to the rotation axis.



Set radial grid

—r_grid N_z N_θ N_r

Set the grid that will be used to build the cylindrical coordinates. This grid is used for the integration of the density and overlaps in cylindrical coordinates. Increasing the grid will make the calculation slower but will increase the accuracy.

—measure_error value

When overlap and density are very close the measure of symmetry could be very inaccurate, specially when this integrals are almost 0. When the difference between both integrals is bellow this number CMS is set as 0. By default is 1E-5 e^{-2}.

Examples

Example 1

Calculate the C9 CMS of the electronic density in a cube file (C3B9.cube). The molecule is oriented along the the axis 0 0 1. Integrate 30 sides of the density, show the results on screen and plot of the density and symmetry measure.

$ cubesym -c C3B9.cube --center 0.1 0.2 0.1 --align 0 0 1 -o 9 -m 30 -p

Example 2

Load cube file C3B9.cube and calculate the C3 CMS along the radius. Integrate 30 slides and show it on screen.

.$ cubesym -c C3B9.cube -r -o 3 -m 30

Example 3

Load analytical potential composed by gaussian functions from file1 and calculate the C5 symmetry measure along the radius. The density is aligned along the axis 1 0 0.

$ cubesym -g file1 -r --align 1 0 0 -o 5 -m 30

Example 4

Plot a slide of the density aligned in (0 1 0) direction. This slide correspond to the plane perpendicular to (0, 2.1, 0).

$ cubesym -g file1 -ps 2.1 --align 0 1 0