# **Manual of m-CBAC charge assignment script**

## *List of scripts*

1. **m-CBAC\_Ver\_1.0.sh**: Main program for the charge assignment.
2. **secondlayr.f90** and s**ort\_colum.py**: Algorithms for determining the connectivity of atoms.
3. **Database\_0th.txt, Database\_1st.txt, and Database\_2nd.txt**: Developed databases for 0th, 1st, and 2nd layer connectivity patterns, respectively.

## *Input files*

The input MOF structure file has to be in **CIF** format with a *P1* symmetry. Further information (e.g., bond, angle, etc.) are not needed. A sample CIF input file is provided, and it is recommended to use the same format.

## *Run the program*

1. Place all CIF files for charge assignments in the same directory with the scripts mentioned above.
2. In Linux command line, type: “**bash m-CBAC\_Ver\_1.0.sh”**. The program will automatically scan all CIF files within the same folder and assign charges accordingly.

## *Output files*

1. A new CIF file named “**FINAL\_<structure cif name>**” will be created after running the main program.
2. Two log files will also be created:
   1. **float.list**: a list of MOFs if floating ions or solvents are detected.
   2. **unknowm\_element.list**: a list of MOFs having elements that are not included in the database.