

# AFLOW V 3.1.137

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*          aflow - STEFANO CURTAROLO Duke University 2003-2017
*          High-Throughput ab-initio Computing Project
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AFLOW/ANRL Prototypes
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AFLOW implementation: Stefano Curtarolo and David Hicks

Citation Information: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, The AFLOW Library of Crystallographic Prototypes, *Comp. Mat. Sci.* (2016). (under review)

The AFLOW/ANRL Library consists of 288 crystallographic prototypes from the above paper. These prototypes have been programmed into AFLOW. The list of prototypes and how to call them can be found in `aflow_anrl.cpp`. The prototypes are generally listed in the order they appear in the paper (low space group number to high space group number).

Note: This implementation of the geometric prototypes allows for the creation of different structure prototypes depending on the parameters chosen. Therefore, these prototypes are quite general and powerful.

The general format for the command is as follows:

```
aflow --proto=label --params=a,b/a,c/a,alpha,beta,gamma,x1,y1,z1,x2,y2,z2,... [--hex]
```

Example:

```
aflow --proto=ABC4_oP12_16_ag_cd_2u --params=5.61,1.01069518717,1.61319073084,0.2,0.26,0.125,0.74,0.8,0.63
```

A description of each input is described below:

label: The label is a string that provides a great deal of information regarding the geometric prototype. The information is separated by underscores into different fields.

- Field 1: Stoichiometry
- Field 2: Pearson symbol
- Field 3: Space group number
- Field 4: Wyckoff letters (in alphabetic order) associated with species A
- Field 5: Wyckoff letters (in alphabetic order) associated with species B
- Field 6: Wyckoff letters (in alphabetic order) associated with species C
- ...
- ...
- ...

parameters: The parameters are necessary to create the structure prototype. The parameter information is separated by commas. The parameters are type double, which specify the degrees of freedom in the prototype.

- a,b/a,c/a : Magnitudes of lattice vectors. Note, there may not be a need to specify all magnitudes, since higher symmetry prototypes have lattice vector restrictions:
  - TRI/MCL/MCLC/ORC/ORCC/ORCF/ORCI: a,b/a,c/a
  - TET/BCT/HEX/RHL: a,c/a
  - CUB/FCC/BCC: a
- alpha,beta,gamma : Angles between lattice vectors. Note, there may not be a need to specify all angles, since higher symmetry prototypes have lattice vector restrictions:
  - TRI: alpha,beta,gamma
  - MCL/MCLC: beta

Rest: None

- $x_1, y_1, z_1, x_2, \dots$  : Coordinates of Wyckoff positions, which have a degree of variability. Caution: Order these parameters with care. The order of the Wyckoff positions is found in the paper.

[--hex]: For rhombohedral systems, there are two choices for representing the prototypes: rhombohedral (RHL) or hexagonal (HEX).

- RHL cell:  $a=b=c$  and  $\alpha=\beta=\gamma$  (better for ab-initio, smaller than HEX)
- HEX cell:  $a=b$  and  $\gamma=120$  (this cell is 3 times larger than the RHL)

The default representation is RHL. To show the prototype in the HEX representation, we add the --hex flag.

NOTE: Only applicable for rhombohedral systems.

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AFLOW/ANRL Prototypes

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