

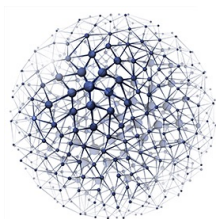
# AFLOW Prototype Encyclopedia: Generating crystallographic structures

David Hicks

AFLOW – CMSAS Online

*Session 4 (2:00PM-3:30PM)*

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**AFLOW**  
Automatic - FLOW for Materials Discovery



# The search for prototypes

catalogs of structure prototypes



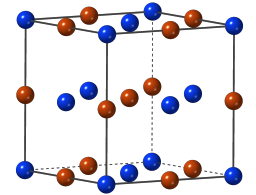
computational hurdles

arbitrary designations

Ex:

compound name: NaCl or MgO

*Strukturbericht*: B1



knowledge of crystallography

Ex:

space group #216

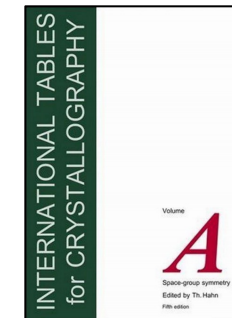
Wyckoff position:

Ag 4 a 0, 0, 0

↑  
multiplicity

↑  
letter designation

↑  
representative coordinate



coordinates

Ag 0, 0, 0

Ag 0, 1/2, 1/2

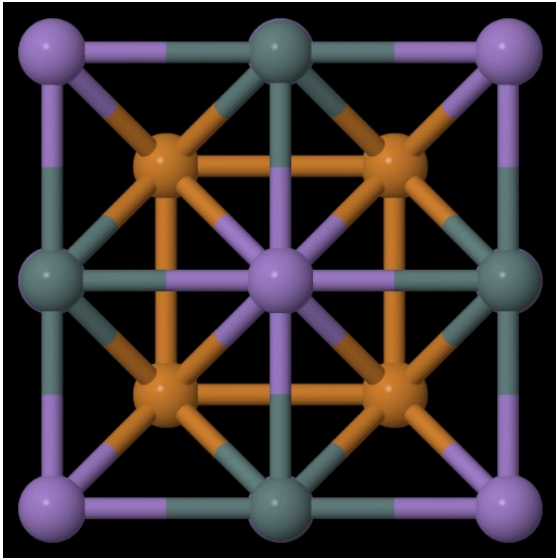
Ag 1/2, 0, 1/2

Ag 1/2, 1/2, 0

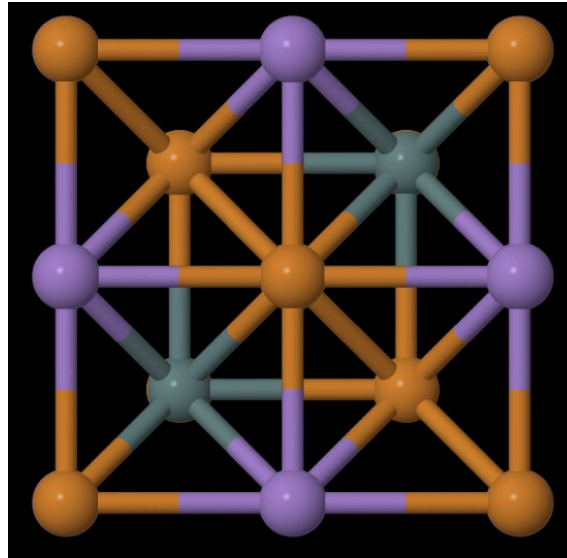
lack methods for materials generation

# AFLOW: Crystallographic prototypes

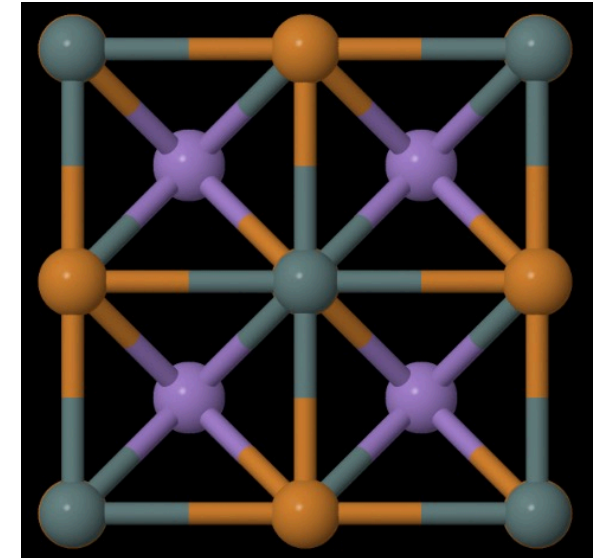
- AFLOW contains built-in structural prototypes:



Prototype T0001:  
Heusler structure



Prototype T0002:  
Anti-Heusler structure



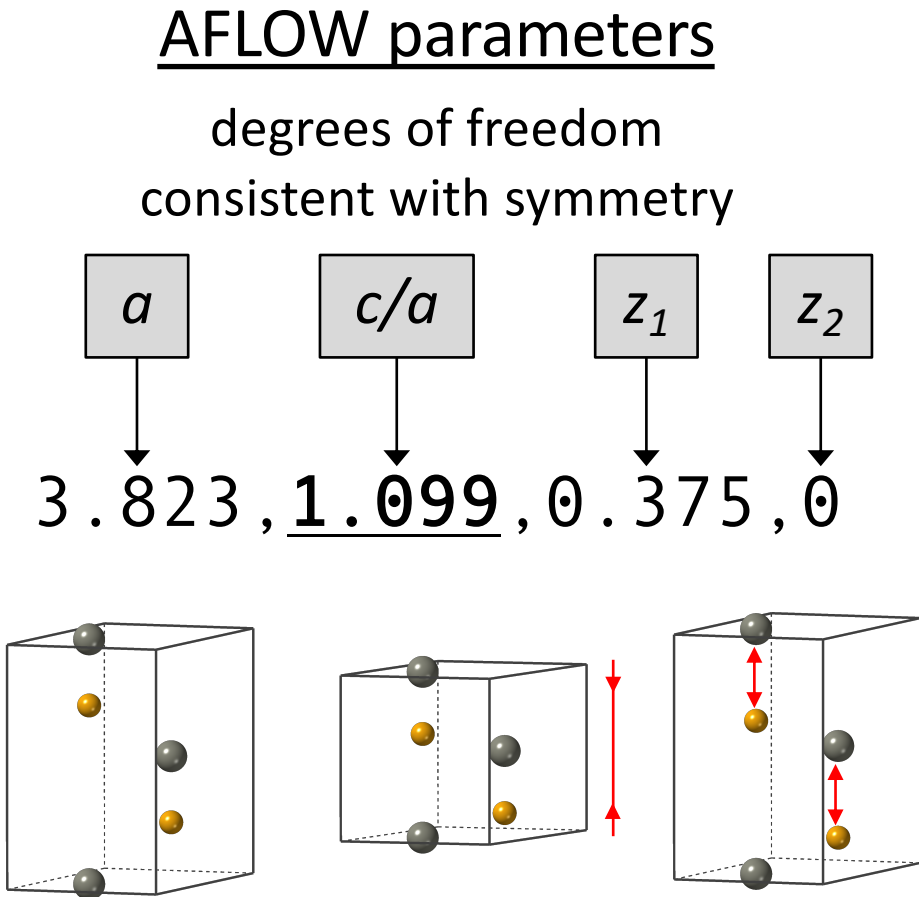
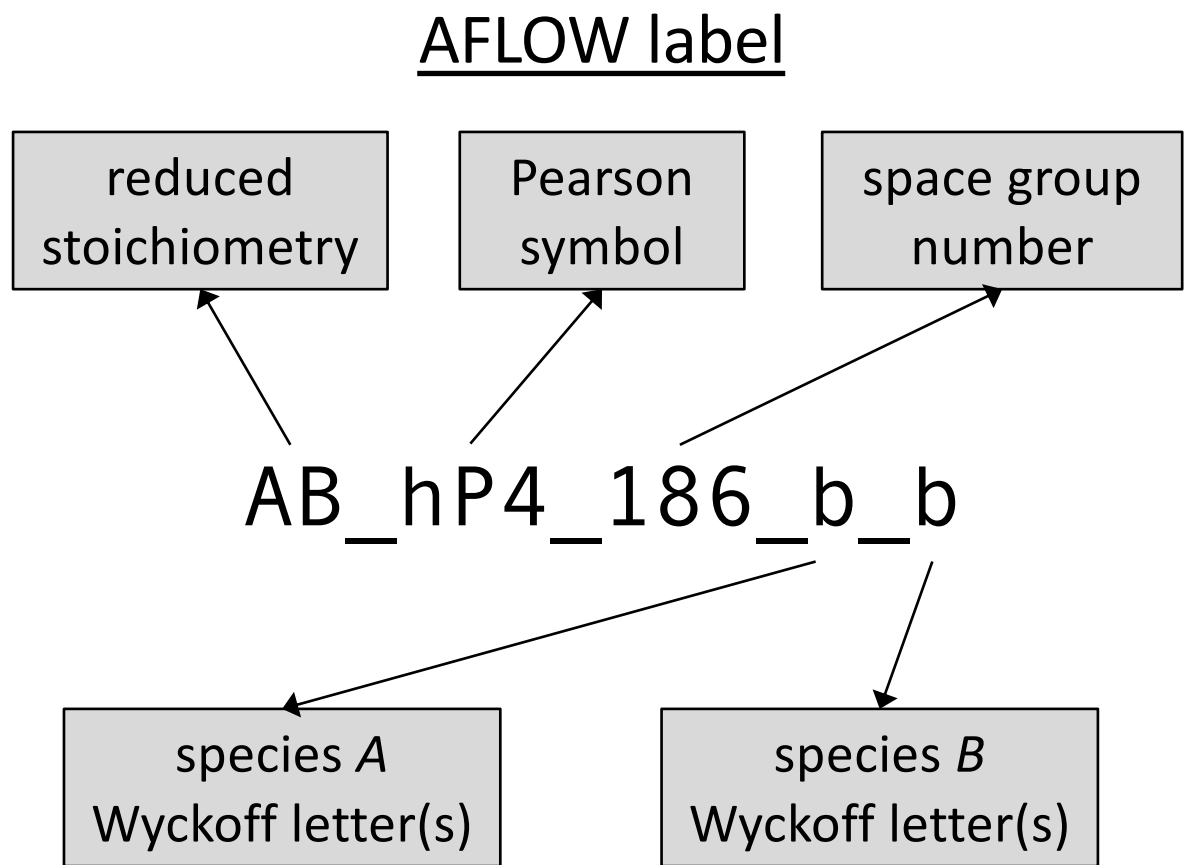
Prototype T0003:  
Half-Heusler structure

- Decorating prototypes with different elements allows for automated creation of new hypothetical materials
- ~1,100 prototypes available at [aflow.org/prototype-encyclopedia](http://aflow.org/prototype-encyclopedia)



# Standard designation and generation

Descriptive label and method for generation (*e.g.*, wurtzite)



# Online application

www.aflow.org/prototype-encyclopedia

Space Group Pearson Symbol Strukturbericht Chemical Symbols Prototype Index Crystal Info Search prototypes... search

AFLOW

## ENCYCLOPEDIA OF CRYSTALLOGRAPHIC PROTOTYPES

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: Part 1, *Comput. Mater. Sci.* **136**, S1-S828 (2017). (doi=10.1016/j.commatsci.2017.01.017)

D. Hicks, M. J. Mehl, E. G. Goett, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, The AFLOW Library of Crystallographic Prototypes: Part 2, *Comput. Mater. Sci.* **161**, S1-S1011 (2019). (doi=10.1016/j.commatsci.2018.10.043)

search by structure descriptors

Number of prototypes in the encyclopedia: **1100**

Search by common name or composition...

search

Search prototypes via space group, Pearson symbol, Strukturbericht designation, and chemical symbols.

Space Group	Pearson Symbol	Strukturbericht
Chemical Symbols	Prototype Index	AFLOW-XtalFinder

### Corundum ( $\text{Al}_2\text{O}_3$ , $D_{5h}$ ) Structure: A2B3\_hr10\_167\_c\_e

load supercell load block

primitive conventional both

Wigner-Seitz : {0 0 0} atom # toggle

axis a axis b axis c

unitcell on unitcell off

balls balls & sticks

save PNG+Jmol

console JS\_CONSOLE

Prototype	: $\text{Al}_2\text{O}_3$
AFLOW prototype label	: A2B3_hr10_167_c_e
Strukturbericht designation	: $D_{5h}$
Pearson symbol	: hR10
Space group number	: 167
Space group symbol	: $R\bar{3}c$
AFLOW prototype command	: aflow --proto=A2B3_hr10_167_c_e [--hex] --params=a,c/a,x1,x2

View the structure from several different perspectives  
View the primitive and conventional unit cells

general prototype info



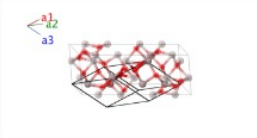
# Online application

www.aflow.org/prototype-encyclopedia

View the structure from several different perspectives  
View the primitive and conventional cell

• Hexagonal settings of this structure can be obtained with the option --hex.

**Rhombohedral primitive vectors:**

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2} a \hat{x} - \frac{1}{2\sqrt{3}} a \hat{y} + \frac{1}{3} c \hat{z} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}} a \hat{y} + \frac{1}{3} c \hat{z} \\ \mathbf{a}_3 &= -\frac{1}{2} a \hat{x} - \frac{1}{2\sqrt{3}} a \hat{y} + \frac{1}{3} c \hat{z} \end{aligned}$$


**Basis vectors:**

	Lattice Coordinates	Cartesian Coordinates	Wyckoff Position	Atom 1
B <sub>1</sub>	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$x_1 c \hat{z}$	(4c)	Al
B <sub>2</sub>	$(\frac{1}{2} - x_1) \mathbf{a}_1 + (\frac{1}{2} - x_1) \mathbf{a}_2 + (\frac{1}{2} - x_1) \mathbf{a}_3$	$(\frac{1}{2} - x_1) c \hat{z}$	(4c)	Al
B <sub>3</sub>	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$-x_1 c \hat{z}$	(4c)	Al
B <sub>4</sub>	$(\frac{1}{2} + x_1) \mathbf{a}_1 + (\frac{1}{2} + x_1) \mathbf{a}_2 + (\frac{1}{2} + x_1) \mathbf{a}_3$	$(\frac{1}{2} + x_1) c \hat{z}$	(4c)	Al
B <sub>5</sub>	$x_2 \mathbf{a}_1 + (\frac{1}{2} - x_2) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$\frac{1}{8}(4x_2 - 1) a \hat{x} + \frac{\sqrt{3}}{8}(1 - 4x_2) a \hat{y} + \frac{1}{4} c \hat{z}$	(6e)	O
B <sub>6</sub>	$\frac{1}{4} \mathbf{a}_1 + x_2 \mathbf{a}_2 + (\frac{1}{2} - x_2) \mathbf{a}_3$	$\frac{1}{8}(4x_2 - 1) a \hat{x} - \frac{\sqrt{3}}{8}(1 - 4x_2) a \hat{y} + \frac{1}{4} c \hat{z}$	(6e)	O
B <sub>7</sub>	$(\frac{1}{2} - x_2) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + x_2 \mathbf{a}_3$	$-\frac{1}{4}(4x_2 - 1) a \hat{x} + \frac{1}{4} c \hat{z}$	(6e)	O
B <sub>8</sub>	$-x_2 \mathbf{a}_1 + (\frac{1}{2} + x_2) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-\frac{1}{8}(4x_2 + 3) a \hat{x} + \frac{1}{8\sqrt{3}}(1 + 12x_2) a \hat{y} + \frac{5}{12} c \hat{z}$	(6e)	O
B <sub>9</sub>	$\frac{3}{4} \mathbf{a}_1 - x_2 \mathbf{a}_2 + (\frac{1}{2} + x_2) \mathbf{a}_3$	$-\frac{1}{8}(4x_2 - 1) a \hat{x} - \frac{1}{8\sqrt{3}}(5 + 12x_2) a \hat{y} + \frac{5}{12} c \hat{z}$	(6e)	O
B <sub>10</sub>	$(\frac{1}{2} + x_2) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - x_2 \mathbf{a}_3$	$\frac{1}{4}(4x_2 + 1) a \hat{x} + \frac{1}{2\sqrt{3}} a \hat{y} + \frac{5}{12} c \hat{z}$	(6e)	O

**References**

- L. W. Finger and R. M. Hazen, *Crystal structure and compression of rubite to 46 kbar*, J. Appl. Phys. **49**, 5823–5826 (1978), doi:10.1063/1.324598.

**Geometry files**

- CIF
- POSCAR

lattice and atom information  
(symbolic notation)

prototype generator

• CIF  
• POSCAR

**Prototype Generator**

aflow --proto=A2B3\_hR10\_167\_c\_e --params=

a  c/a  x<sub>1</sub>

x<sub>2</sub>

**Species:**

A  B

VASP Output QE Output FHI-AIMS Output ABINIT Output WYCKAR Output CIF Output Refresh Jmol

**Running:**

```
aflow --proto=A2B3_hR10_167_c_e:Al:O --params=4.7607,2.72957758313,0.35216,0.5561
```

**Output:**

```
AlO/A2B3_hR10_167_c_e params=4.7607,2.72957758313,0.35216,0.5561 SG#=167 [ANRL doi: 10.1016/j.commat.2017.01.017 (part 1), doi: 10.1016/j.commat.2018.10.043 (part 2)]
1.000000
2.3803500000000000 -1.37429571326553 4.331566666666900
0.0000000000000000 2.74859142653105 4.331566666666900
-2.3803500000000000 -1.37429571326553 4.331566666666900
4 6
Direct[10] [A4B6]
0.3521600000000000 0.3521600000000000 0.3521600000000000 Al
0.1478400000000000 0.1478400000000000 0.1478400000000000 Al
-0.3521600000000000 -0.3521600000000000 -0.3521600000000000 Al
0.8521600000000000 0.8521600000000000 0.8521600000000000 Al
0.5561000000000000 -0.0561000000000000 0.2500000000000000 O
0.2500000000000000 0.5561000000000000 -0.0561000000000000 O
-0.0561000000000000 0.2500000000000000 0.5561000000000000 O
-0.5561000000000000 1.0561000000000000 0.7500000000000000 O
0.7500000000000000 -0.5561000000000000 1.0561000000000000 O
1.0561000000000000 0.7500000000000000 -0.5561000000000000 O
```

# Prototype commands

- AFLOW Crystallographic Prototype Encyclopedia (approx. 1,100)

```
aflow --proto=AB_hP4_186_b_b --params=3.823,1.638,0.375,0.0
```

label

parameters

- AFLOW Standard Prototypes (approx. 700)

```
aflow --proto=T0001.A2BC
```

- generally numbered labels
- hard-coded prototypes; no degrees of freedom



# Create geometry files

- Decorate rock-salt prototype AB\_cF8\_225\_a\_b with MgO:

```
aflow --proto=AB_cF8_225_a_b:Mg:O --params=3.5
```

```
MgO/AB_cF8_225_a_b params=3.5 SG#=225
```

```
1.000000
```

```
0.0000000000000000 1.7500000000000000 1.7500000000000000
```

```
1.7500000000000000 0.0000000000000000 1.7500000000000000
```

```
1.7500000000000000 1.7500000000000000 0.0000000000000000
```

```
1 1
```

```
Direct(2) [A1B1]
```

```
0.0000000000000000 0.0000000000000000 0.0000000000000000
```

```
0.5000000000000000 0.5000000000000000 0.5000000000000000
```

```
Mg  
O
```

- Variety of possible geometry file formats by adding options:

VASP

```
--vasp
```

CIF

```
--cif
```

FHI-AIMS

```
--aims
```

Quantum Espresso

```
--qe
```

ABINIT

```
--abinit
```

ELK

```
--elk
```

# Create geometry files

- Control atomic site decoration:

```
aflow --proto=AB_cF8_225_a_b.BA:Mg:0 --params=3.5
```

```
Mg0/AB_cF8_225_a_b.BA params=3.5 SG=225
```

```
1.000000
```

```
0.0000000000000000 1.7500000000000000 1.7500000000000000
```

```
1.7500000000000000 0.0000000000000000 1.7500000000000000
```

```
1.7500000000000000 1.7500000000000000 0.0000000000000000
```

```
1 1
```

```
Direct(2) [A1B1]
```

```
0.5000000000000000 0.5000000000000000 0.5000000000000000 Mg
```

```
0.0000000000000000 0.0000000000000000 0.0000000000000000 0
```

- Automatic volume scaling based on atomic elements:

```
aflow --proto=AB_cF8_225_a_b.AB:Mg:0 --params=-1
```

```
Mg0/AB_cF8_225_a_b.AB params=-1 SG=225
```

```
-30.600100
```

```
0.0000000000000000 0.5000000000000000 0.5000000000000000
```

```
0.5000000000000000 0.0000000000000000 0.5000000000000000
```

```
0.5000000000000000 0.5000000000000000 0.0000000000000000
```

# Create geometry files

- Enumerated parameter sets:

```
aflow --proto=AB2C_oP16_62_c_2c_c.ABC:Cu:S:Sb  
--params=-1,0.630741110003,2.4086075108,0.2522,0.8276,0.6221,0.095,0.8706,0.8244,0.226,0.06333
```

VS

```
aflow --proto=AB2C_oP16_62_c_2c_c-001 ABC:Cu:S:Sb
```

- Don't know what parameter sets are available?

```
aflow --proto=AB2_oP6_58_a_g
```

```
anrl::getANRLParameters(): ERROR - AB2_oP6_58_a_g has 3 preset parameter set(s):  
AB2_oP6_58_a_g-001 : -1,1.03044871795,0.673076923077,0.275,0.325  
AB2_oP6_58_a_g-002 : -1,0.917942176871,0.601615646259,0.66667,0.25  
AB2_oP6_58_a_g-003 : -1,1.22049228277,0.761913333033,0.2004,0.3787  
AB2_oP6_58_a_g-004 : -1,1.1965466,0.67115528,0.8682,0.5945  
AB2_oP6_58_a_g-005 : -1,1.2288051,0.58567724,0.414,0.068
```

# Generate aflow.in files

- Use Heusler prototype T0001.A2BC to create aflow.in file for Cu<sub>2</sub>TiZn:

```
aflow --aflow_proto=T0001.A2BC:Cu:Ti:Zn
```

- Comma separated prototypes:

```
aflow --aflow_proto=T0001.A2BC,TFCC001.ABC:Ag,Au,Cu,Fe:Mn,Ti:Zn
```

- Comma separated species:

```
aflow --aflow_proto=T0001.A2BC:Ag,Au,Cu,Fe:Mn,Ti:Zn
```

- Include degrees of freedom for relevant prototypes:

```
aflow --aflow_proto=AB_cF8_225_a_b.AB:Mg:0 --params=-1
```

# Available prototypes

- List of prototypes:

AFLOW Prototype Encyclopedia

```
aflow --protos
```

OR

```
http://aflow.org/prototype-encyclopedia
```

- Search for specific prototypes:

```
aflow --prototype_labels --nspecies=2 --stoichiometry=1,2 --sg=225
```

```
583,584,691.AB,691.BA,1027.AB,1027.BA,1218.AB,1218.BA,AB2_cF12_225_a_c
```

- Additional information is available in README:

```
aflow --readme=prototypes
```

# Exercises

1. [ONLINE EXERCISE] Generate POSCARs for the following structures via the AFLOW online generator: 1) diamond, 2) caswellsilverite, 3) spinel (ternary), 4) calaverite (Struk. C34), 5) brookite, 6) sulvanite. What are the AFLOW labels of these structures?
2. Generate structures for the prototype A\_hR1\_166\_a using an element and value of a of your choice, with c/a values of 0.5, 0.612, 1.0, 1.225, 1.5, 2.45, and 3.0. Calculate the space group (--aflowSG) of each of the structures.
3. Generate the Heusler structure (T0001.A2BC) and decorate with elements of your choice. Determine the space group, Wyckoff positions, and Pearson symbol of this prototype. What would the corresponding AFLOW prototype label be?



# More information

AFLOW Prototypes README:

```
aflow --readme=prototypes
```

AFLOW Prototype articles:

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: Part 1*, *Comp. Mat. Sci.* **136** Supplement, S1–S828 (2017).  
doi:[10.1016/j.commatsci.2017.01.017](https://doi.org/10.1016/j.commatsci.2017.01.017)

D. Hicks, M.J. Mehl, E. Gossett, C. Toher, O. Levy, R.M. Hanson, G.L.W. Hart, and S. Curtarolo,  
*The AFLOW Library of Crystallographic Prototypes: Part 2*, *Comp. Mat. Sci.* **161** Supplement, S1-S1011 (2019).  
doi: [10.1016/j.commatsci.2018.10.043](https://doi.org/10.1016/j.commatsci.2018.10.043)

D. Hicks, M.J. Mehl, M. Esters, C. Oses, O. Levy, G.L.W. Hart, C. Toher, and S. Curtarolo,  
*The AFLOW Library of Crystallographic Prototypes: Part 3*, in press, *Comp. Mat. Sci.* (2021).  
[arXiv:2012.05961](https://arxiv.org/abs/2012.05961)