# $Cu_{15}Si_4$ ($D8_6$) Structure: A15B4_cI76_220_ae_c-001

This structure previously used the label(s) `A15B4_cI76_220_ae_c`. Calls to these addresses will be redirected here.

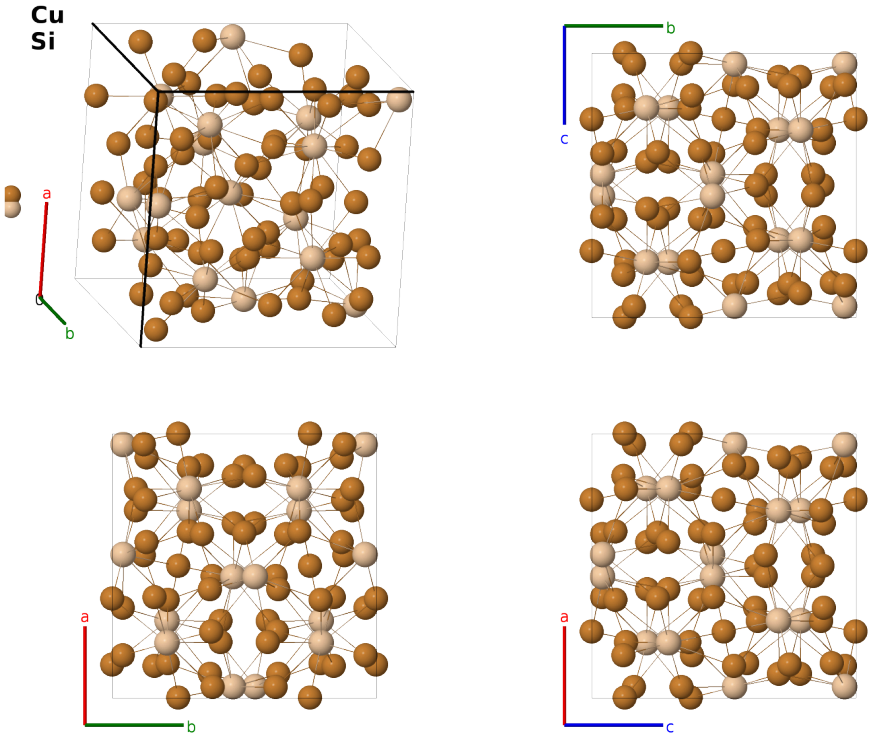
Cite this page as:


- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.


---

https://aflow.org/prototype-encyclopedia/MVX2

https://aflow.org/prototype-encyclopedia/A15B4_cI76_220_ae_c-001



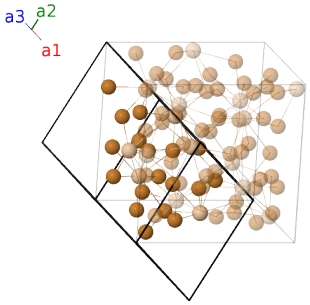

| | |
|---|---|
| **Prototype** | $Cu_{15}Si_4$ |
| **AFLOW prototype label** | A15B4_cI76_220_ae_c-001 |
| ***Strukturbericht* designation** | $D8_6$ |
| **ICSD** | 629165 |
| **CCDC** | 1753260 |
| **Pearson symbol** | cI76 |
| **Space group number** | 220 |
| **Space group symbol** | $I\bar{4}3d$ |
| **AFLOW prototype command** | `aflow --proto=A15B4_cI76_220_ae_c-001 --params=`$a, x_2, x_3, y_3, z_3$ |

**Other compounds with this structure**
$Cu_{15}As_4$, $Li_{15}Au_4$, $Li_{15}Ge_4$, $Li_{15}Si_4$, $Na_{15}Pb_4$

- (Mattern, 2007) take their data from (Mukherjee, 1969), and we use the ICSD information from that reference.

**Body-centered Cubic primitive vectors**

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}a\,\hat{\mathbf{z}}
\end{aligned}$$




**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$ | = | $\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$ | (12a) | Cu I |
| $\mathbf{B_2}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$ | = | $\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{z}}$ | (12a) | Cu I |
| $\mathbf{B_3}$ | = | $\frac{3}{8}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}}$ | (12a) | Cu I |
| $\mathbf{B_4}$ | = | $\frac{1}{8}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}}$ | (12a) | Cu I |
| $\mathbf{B_5}$ | = | $\frac{5}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$ | (12a) | Cu I |
| $\mathbf{B_6}$ | = | $\frac{7}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$ | (12a) | Cu I |
| $\mathbf{B_7}$ | = | $2x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$ | = | $ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$ | (16c) | Si I |
| $\mathbf{B_8}$ | = | $\frac{1}{2}\,\mathbf{a}_1 - \left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$ | (16c) | Si I |
| $\mathbf{B_9}$ | = | $-\left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$ | (16c) | Si I |
| $\mathbf{B_{10}}$ | = | $-\left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$ | = | $ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (16c) | Si I |
| $\mathbf{B_{11}}$ | = | $\left(2x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(2x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(2x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (16c) | Si I |
| $\mathbf{B_{12}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 - 2x_2\,\mathbf{a}_3$ | = | $-a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (16c) | Si I |
| $\mathbf{B_{13}}$ | = | $-2x_2\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$ | = | $a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (16c) | Si I |
| $\mathbf{B_{14}}$ | = | $-2x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (16c) | Si I |
| $\mathbf{B_{15}}$ | = | $(y_3 + z_3)\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3)\,\mathbf{a}_3$ | = | $ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{16}}$ | = | $\left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - \left(x_3 + y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ax_3\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{17}}$ | = | $(y_3 - z_3)\,\mathbf{a}_1 - \left(x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{18}}$ | = | $-\left(y_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$ | = | $ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} - a\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (48e) | Cu II |

| | | | | | | |
|---|---|---|---|---|---|---|
| $\mathbf{B_{19}}$ | = | $(x_3+y_3)\,\mathbf{a}_1+(y_3+z_3)\,\mathbf{a}_2+(x_3+z_3)\,\mathbf{a}_3$ | = | $az_3\,\hat{\mathbf{x}}+ax_3\,\hat{\mathbf{y}}+ay_3\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{20}}$ | = | $-\left(x_3+y_3-\frac{1}{2}\right)\,\mathbf{a}_1+\left(-y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2-(x_3-z_3)\,\mathbf{a}_3$ | = | $az_3\,\hat{\mathbf{x}}-ax_3\,\hat{\mathbf{y}}-a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{21}}$ | = | $\left(-x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_1+(y_3-z_3)\,\mathbf{a}_2-\left(x_3+z_3-\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-az_3\,\hat{\mathbf{x}}-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{y}}+ay_3\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{22}}$ | = | $(x_3-y_3)\,\mathbf{a}_1-\left(y_3+z_3-\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_3-z_3+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_3\,\hat{\mathbf{y}}-ay_3\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{23}}$ | = | $(x_3+z_3)\,\mathbf{a}_1+(x_3+y_3)\,\mathbf{a}_2+(y_3+z_3)\,\mathbf{a}_3$ | = | $ay_3\,\hat{\mathbf{x}}+az_3\,\hat{\mathbf{y}}+ax_3\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{24}}$ | = | $-(x_3-z_3)\,\mathbf{a}_1-\left(x_3+y_3-\frac{1}{2}\right)\,\mathbf{a}_2+\left(-y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}+az_3\,\hat{\mathbf{y}}-ax_3\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{25}}$ | = | $-\left(x_3+z_3-\frac{1}{2}\right)\,\mathbf{a}_1+\left(-x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_2+(y_3-z_3)\,\mathbf{a}_3$ | = | $ay_3\,\hat{\mathbf{x}}-az_3\,\hat{\mathbf{y}}-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{26}}$ | = | $\left(x_3-z_3+\frac{1}{2}\right)\,\mathbf{a}_1+(x_3-y_3)\,\mathbf{a}_2-\left(y_3+z_3-\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ay_3\,\hat{\mathbf{x}}-a\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{y}}+ax_3\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{27}}$ | = | $\left(x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{28}}$ | = | $\left(-x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_1-(y_3-z_3)\,\mathbf{a}_2-(x_3+y_3)\,\mathbf{a}_3$ | = | $-a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_3-\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{29}}$ | = | $-(x_3+z_3)\,\mathbf{a}_1+\left(y_3-z_3+\frac{1}{2}\right)\,\mathbf{a}_2-(x_3-y_3)\,\mathbf{a}_3$ | = | $a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(z_3-\frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{30}}$ | = | $(x_3-z_3)\,\mathbf{a}_1-(y_3+z_3)\,\mathbf{a}_2+\left(x_3-y_3+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(y_3-\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{31}}$ | = | $\left(y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{32}}$ | = | $-(y_3-z_3)\,\mathbf{a}_1-(x_3+y_3)\,\mathbf{a}_2+\left(-x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(x_3-\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{33}}$ | = | $\left(y_3-z_3+\frac{1}{2}\right)\,\mathbf{a}_1-(x_3-y_3)\,\mathbf{a}_2-(x_3+z_3)\,\mathbf{a}_3$ | = | $-a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(z_3-\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{34}}$ | = | $-(y_3+z_3)\,\mathbf{a}_1+\left(x_3-y_3+\frac{1}{2}\right)\,\mathbf{a}_2+(x_3-z_3)\,\mathbf{a}_3$ | = | $a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(y_3-\frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{35}}$ | = | $\left(x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{36}}$ | = | $-(x_3+y_3)\,\mathbf{a}_1+\left(-x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2-(y_3-z_3)\,\mathbf{a}_3$ | = | $a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(x_3-\frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{37}}$ | = | $-(x_3-y_3)\,\mathbf{a}_1-(x_3+z_3)\,\mathbf{a}_2+\left(y_3-z_3+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(z_3-\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (48e) | Cu II |
| $\mathbf{B_{38}}$ | = | $\left(x_3-y_3+\frac{1}{2}\right)\,\mathbf{a}_1+(x_3-z_3)\,\mathbf{a}_2-(y_3+z_3)\,\mathbf{a}_3$ | = | $-a\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(y_3-\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (48e) | Cu II |

## References


[1] M. Mattern, R. Seyrich, L. Wilde, C. Baehtz, M. Knapp, and J. Acker, *Phase formation of rapidly quenched Cu-Si alloys*, J. Alloys Compd. **429**, 211–215 (2007), doi:10.1016/j.jallcom.2006.04.046.

[2] K. P. Mukherjee, J. Bandyopadhyaya, and K. P. Gupta, *Phase relationship and crystal structure of intermediate phases in the Cu-Si system in the composition range of 17 to 25 at. pct Si*, Trans. Metal. Soc. AIME **245**, 2335–2338 (1969).


## Found in


[1] K. Sufryd, N. Ponweiser, P. Riani, K. W. Richter, and G. Cacciamani, *Experimental investigation of the Cu-Si phase diagram at x(Cu)*0.72, Intermetallics **19**, 1479–1488 (2011), doi:10.1016/j.intermet.2011.05.017.


## First cited in


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