

# NH<sub>4</sub>I<sub>3</sub> (D<sub>016</sub>) Structure: A3B\_oP16\_62\_3c\_c-002

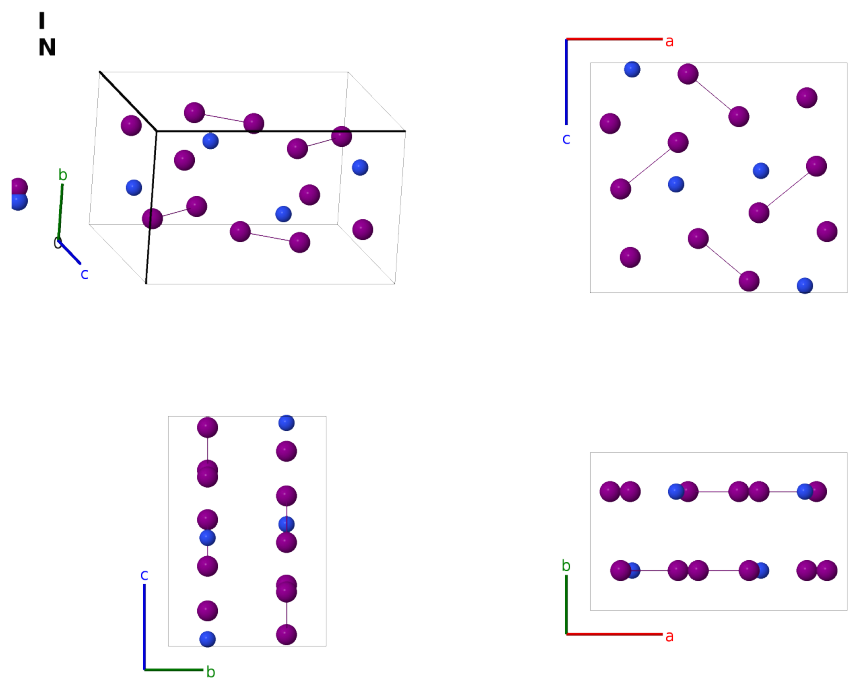
This structure previously used the label(s) **A3B\_oP16\_62\_3c\_c**. Calls to these addresses will be redirected here.

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/DE18>

[https://aflow.org/prototype-encyclopedia/A3B\\_oP16\\_62\\_3c\\_c-002](https://aflow.org/prototype-encyclopedia/A3B_oP16_62_3c_c-002)



|                                    |                                                                                                                                                                                                              |
|------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype                          | I <sub>3</sub> (NH <sub>4</sub> )                                                                                                                                                                            |
| AFLOW prototype label              | A3B_oP16_62_3c_c-002                                                                                                                                                                                         |
| <i>Strukturbericht</i> designation | D <sub>016</sub>                                                                                                                                                                                             |
| ICSD                               | 22128                                                                                                                                                                                                        |
| CCDC                               | 1598912                                                                                                                                                                                                      |
| Pearson symbol                     | oP16                                                                                                                                                                                                         |
| Space group number                 | 62                                                                                                                                                                                                           |
| Space group symbol                 | <i>Pnma</i>                                                                                                                                                                                                  |
| AFLOW prototype command            | <code>aflow --proto=A3B_oP16_62_3c_c-002</code><br><code>--params=a, b/a, c/a, x<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub></code> |

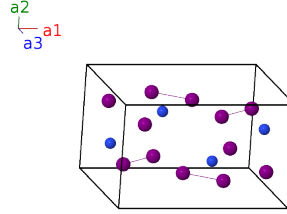
## Other compounds with this structure

CsI<sub>3</sub>, CsBr<sub>3</sub>

- (Cheesman, 1970) gives the positions of the atoms in Cartesian coordinates, which we have translated into the standard Wyckoff notation.
- The hydrogen positions are not given, so the NH<sub>4</sub> molecules are centered on the (4c) Wyckoff position.
- With the NH<sub>4</sub> molecules treated as a single entity, NH<sub>4</sub>I<sub>3</sub> has the same AFLOW label, A3B\_oP16\_62\_3c\_c, as Bi<sub>3</sub>Ni. The structures are generated by the same symmetry operations with different sets of parameters (**--params**) specified in their corresponding CIF files.

## Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



## Basis vectors

|                   | Lattice<br>coordinates                                                                                                    |     | Cartesian<br>coordinates                                                                                                               | Wyckoff<br>position | Atom<br>type |
|-------------------|---------------------------------------------------------------------------------------------------------------------------|-----|----------------------------------------------------------------------------------------------------------------------------------------|---------------------|--------------|
| $\mathbf{B}_1$    | $= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$                                                        | $=$ | $ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$                                                        | (4c)                | I I          |
| $\mathbf{B}_2$    | $= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (4c)                | I I          |
| $\mathbf{B}_3$    | $= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$                                                       | $=$ | $-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$                                                       | (4c)                | I I          |
| $\mathbf{B}_4$    | $= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$  | $=$ | $a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$  | (4c)                | I I          |
| $\mathbf{B}_5$    | $= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$                                                        | $=$ | $ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$                                                        | (4c)                | I II         |
| $\mathbf{B}_6$    | $= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (4c)                | I II         |
| $\mathbf{B}_7$    | $= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$                                                       | $=$ | $-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$                                                       | (4c)                | I II         |
| $\mathbf{B}_8$    | $= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$  | $=$ | $a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$  | (4c)                | I II         |
| $\mathbf{B}_9$    | $= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$                                                        | $=$ | $ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$                                                        | (4c)                | I III        |
| $\mathbf{B}_{10}$ | $= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (4c)                | I III        |
| $\mathbf{B}_{11}$ | $= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$                                                       | $=$ | $-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$                                                       | (4c)                | I III        |
| $\mathbf{B}_{12}$ | $= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$  | $=$ | $a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$  | (4c)                | I III        |
| $\mathbf{B}_{13}$ | $= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$                                                        | $=$ | $ax_4 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$                                                        | (4c)                | NH I         |
| $\mathbf{B}_{14}$ | $= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (4c)                | NH I         |
| $\mathbf{B}_{15}$ | $= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$                                                       | $=$ | $-ax_4 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$                                                       | (4c)                | NH I         |
| $\mathbf{B}_{16}$ | $= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$  | $=$ | $a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$  | (4c)                | NH I         |

## References

- [1] G. H. Cheesman and A. J. T. Finney, *Refinement of the structure of ammonium triiodide,  $NH_4I_3$* , Acta Crystallogr. Sect. B **26**, 906–908 (1970), doi:10.1107/S0567740870003357.

## Found in

- [1] A. J. T. Finney, *The Structure and Stability of Simple Tri-Iodides* (1973). Ph.D. Thesis, University of Tasmania.

## First cited in

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.