

# NH<sub>4</sub>Br (*B25*) Structure: AB4C\_tP12\_129\_c.i.a-001

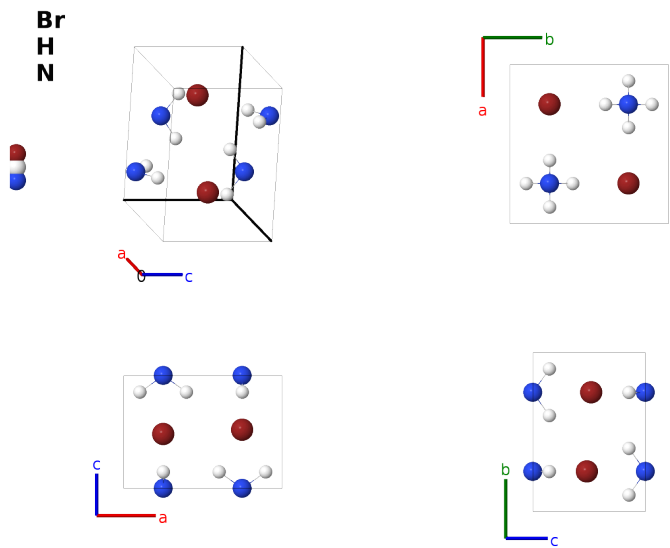
This structure previously used the label(s) **AB4C\_tP12\_129\_c.i.a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/G1GD>

[https://aflow.org/prototype-encyclopedia/AB4C\\_tP12\\_129\\_c.i.a-001](https://aflow.org/prototype-encyclopedia/AB4C_tP12_129_c.i.a-001)



|                                    |                                                                                                                     |
|------------------------------------|---------------------------------------------------------------------------------------------------------------------|
| Prototype                          | BrH <sub>4</sub> N                                                                                                  |
| AFLOW prototype label              | AB4C_tP12_129_c.i.a-001                                                                                             |
| <i>Strukturbericht</i> designation | <i>B25</i>                                                                                                          |
| ICSD                               | 26579                                                                                                               |
| CCDC                               | 1601970                                                                                                             |
| Pearson symbol                     | tP12                                                                                                                |
| Space group number                 | 129                                                                                                                 |
| Space group symbol                 | <i>P4/nmm</i>                                                                                                       |
| AFLOW prototype command            | <code>aflow --proto=AB4C_tP12_129_c.i.a-001<br/>--params=a, c/a, z<sub>2</sub>, y<sub>3</sub>, z<sub>3</sub></code> |

## Other compounds with this structure

NH<sub>4</sub>I

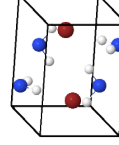
- Data was taken at -100°C using deuterium.

- The atomic positions were given for setting 1 of space group #129. We have shifted this to setting 2, placing the origin at the inversion site of the structure.

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### Simple Tetragonal primitive vectors

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




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### Basis vectors

|                   | Lattice<br>coordinates                                                              |     | Cartesian<br>coordinates                                                                          | Wyckoff<br>position | Atom<br>type |
|-------------------|-------------------------------------------------------------------------------------|-----|---------------------------------------------------------------------------------------------------|---------------------|--------------|
| $\mathbf{B}_1$    | $= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$                             | $=$ | $\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$                                 | (2a)                | N I          |
| $\mathbf{B}_2$    | $= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$                             | $=$ | $\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$                                 | (2a)                | N I          |
| $\mathbf{B}_3$    | $= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$          | $=$ | $\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$         | (2c)                | Br I         |
| $\mathbf{B}_4$    | $= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$          | $=$ | $\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$         | (2c)                | Br I         |
| $\mathbf{B}_5$    | $= \frac{1}{4} \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$                  | $=$ | $\frac{1}{4} a \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$                  | (8i)                | H I          |
| $\mathbf{B}_6$    | $= \frac{1}{4} \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$  | $=$ | $\frac{1}{4} a \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$  | (8i)                | H I          |
| $\mathbf{B}_7$    | $= -(y_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $-a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$ | (8i)                | H I          |
| $\mathbf{B}_8$    | $= y_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$                  | $=$ | $ay_3 \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$                  | (8i)                | H I          |
| $\mathbf{B}_9$    | $= \frac{3}{4} \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$  | $=$ | $\frac{3}{4} a \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$  | (8i)                | H I          |
| $\mathbf{B}_{10}$ | $= \frac{3}{4} \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$                  | $=$ | $\frac{3}{4} a \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$                  | (8i)                | H I          |
| $\mathbf{B}_{11}$ | $= (y_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$  | $=$ | $a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$  | (8i)                | H I          |
| $\mathbf{B}_{12}$ | $= -y_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$                 | $=$ | $-ay_3 \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$                 | (8i)                | H I          |

### References

- [1] H. A. Levy and S. W. Peterson, *Neutron Diffraction Determination of the Crystal Structure of Ammonium Bromide in Four Phases*, J. Am. Chem. Soc. **75**, 1536–1542 (1953), doi:10.1021/ja01103a006.

### First cited in

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