# $NH_4Br$ ($B25$) Structure: AB4C_tP12_129_c_i_a-001

This structure originally had the label `AB4C_tP12_129_c_i_a`. Calls to that address will be redirected here.

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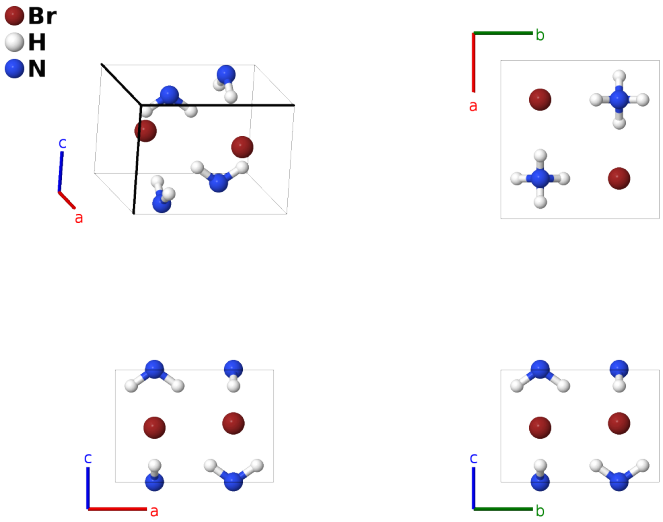
https://aflow.org/p/G1GD

https://aflow.org/p/AB4C_tP12_129_c_i_a-001



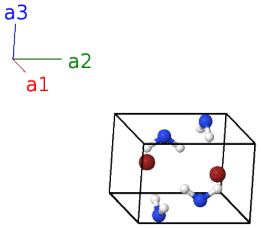

| | |
|---|---|
| **Prototype** | $BrH_4N$ |
| **AFLOW prototype label** | AB4C_tP12_129_c_i_a-001 |
| ***Strukturbericht* designation** | $B25$ |
| **ICSD** | 26579 |
| **Pearson symbol** | tP12 |
| **Space group number** | 129 |
| **Space group symbol** | $P4/nmm$ |
| **AFLOW prototype command** | `aflow --proto=AB4C_tP12_129_c_i_a-001 --params=`$a, c/a, z_2, y_3, z_3$ |

**Other compounds with this structure**
$NH_4I$

- 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.

### Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$




### Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom 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 |
| $\mathbf{B_6}$ | = | $\frac{1}{4}\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (8i) | H I |
| $\mathbf{B_7}$ | = | $-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (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 |
| $\mathbf{B_9}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (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 |
| $\mathbf{B_{11}}$ | = | $\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (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.