# $Hg_2O_2NaI$ Structure: A2BCD2_hP18_180_f_c_b_i-001

This structure originally had the label `A2BCD2_hP18_180_f_c_b_i`. Calls to that address will be redirected here.

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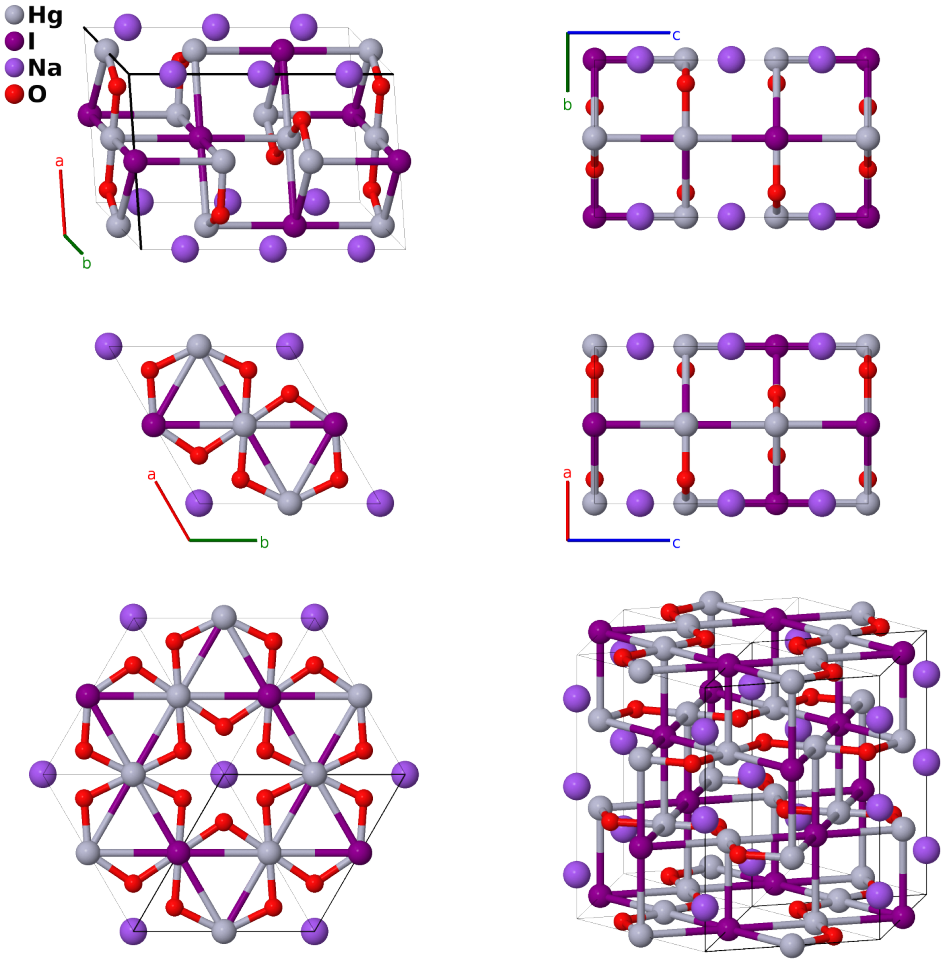
https://aflow.org/p/TQ0B

https://aflow.org/p/A2BCD2_hP18_180_f_c_b_i-001

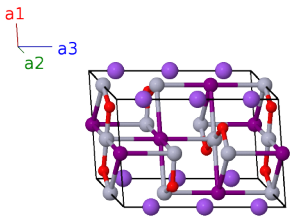



| | |
|---|---|
| **Prototype** | $Hg_2INaO_2$ |
| **AFLOW prototype label** | A2BCD2_hP18_180_f_c_b_i-001 |
| **ICSD** | 14125 |
| **Pearson symbol** | hP18 |
| **Space group number** | 180 |
| **Space group symbol** | $P6_222$ |
| **AFLOW prototype command** | `aflow --proto=A2BCD2_hP18_180_f_c_b_i-001 --params=`$a, c/a, z_3, x_4$ |

- This structure can also be found in the enantiomorphic space group $P6_422$ #181.

### Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$




### Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}c\,\hat{\mathbf{z}}$ | (3b) | Na I |
| $\mathbf{B_2}$ | = | $\frac{1}{6}\,\mathbf{a}_3$ | = | $\frac{1}{6}c\,\hat{\mathbf{z}}$ | (3b) | Na I |
| $\mathbf{B_3}$ | = | $\frac{5}{6}\,\mathbf{a}_3$ | = | $\frac{5}{6}c\,\hat{\mathbf{z}}$ | (3b) | Na I |
| $\mathbf{B_4}$ | = | $\frac{1}{2}\,\mathbf{a}_1$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$ | (3c) | I I |
| $\mathbf{B_5}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{2}{3}c\,\hat{\mathbf{z}}$ | (3c) | I I |
| $\mathbf{B_6}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{3}c\,\hat{\mathbf{z}}$ | (3c) | I I |
| $\mathbf{B_7}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (6f) | Hg I |
| $\mathbf{B_8}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + \left(z_3 + \frac{2}{3}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_3 + 2)\,\hat{\mathbf{z}}$ | (6f) | Hg I |
| $\mathbf{B_9}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{3}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + c\left(z_3 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$ | (6f) | Hg I |
| $\mathbf{B_{10}}$ | = | $\frac{1}{2}\,\mathbf{a}_2 - \left(z_3 - \frac{2}{3}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_3 - 2)\,\hat{\mathbf{z}}$ | (6f) | Hg I |
| $\mathbf{B_{11}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (6f) | Hg I |
| $\mathbf{B_{12}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{3}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - c\left(z_3 - \frac{1}{3}\right)\,\hat{\mathbf{z}}$ | (6f) | Hg I |
| $\mathbf{B_{13}}$ | = | $x_4\,\mathbf{a}_1 + 2x_4\,\mathbf{a}_2$ | = | $\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}$ | (6i) | O I |
| $\mathbf{B_{14}}$ | = | $-2x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$ | = | $-\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{2}{3}c\,\hat{\mathbf{z}}$ | (6i) | O I |
| $\mathbf{B_{15}}$ | = | $x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$ | = | $-\sqrt{3}ax_4\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$ | (6i) | O I |
| $\mathbf{B_{16}}$ | = | $-x_4\,\mathbf{a}_1 - 2x_4\,\mathbf{a}_2$ | = | $-\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}$ | (6i) | O I |
| $\mathbf{B_{17}}$ | = | $2x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$ | = | $\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{2}{3}c\,\hat{\mathbf{z}}$ | (6i) | O I |
| $\mathbf{B_{18}}$ | = | $-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$ | = | $\sqrt{3}ax_4\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$ | (6i) | O I |

### References


[1] K. Aurivillius, *Least-Squares Refinement of the Crystal Structures of Orthorhombic HgO and of $Hg_2O_2NaI$*, Acta Chemica Scand. **18**, 1305–1306 (1964), doi:10.3891/acta.chem.scand.18-1305.