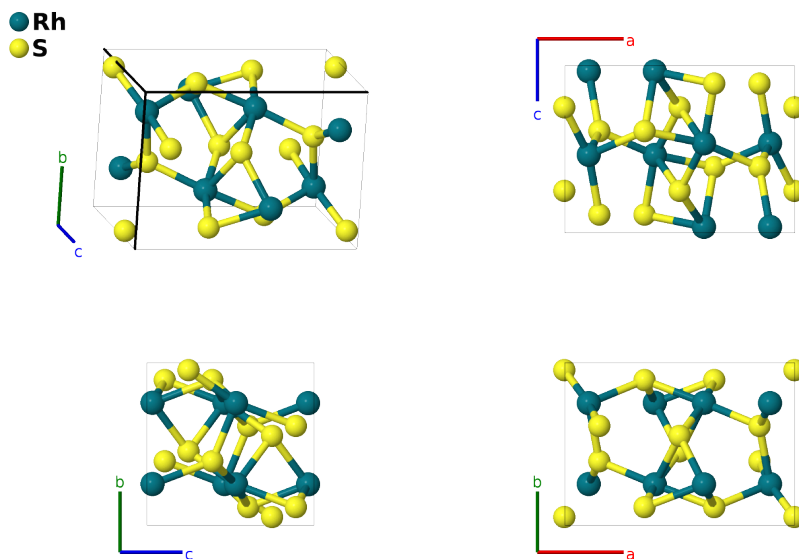# $Rh_2O_3$ Structure: A2B3_oP20_60_d_cd-001

This structure originally had the label `A2B3_oP20_60_d_cd`. Calls to that address will be redirected here.

https://aflow.org/p/WEMD

https://aflow.org/p/A2B3_oP20_60_d_cd-001



| | |
|---|---|
| **Prototype** | $Rh_2O_3$ |
| **AFLOW prototype label** | A2B3_oP20_60_d_cd-001 |
| **ICSD** | 15344 |
| **Pearson symbol** | oP20 |
| **Space group number** | 60 |
| **Space group symbol** | $Pbcn$ |
| **AFLOW prototype command** | aflow --proto=A2B3_oP20_60_d_cd-001 --params=$a, b/a, c/a, y_1, x_2, y_2, z_2, x_3, y_3, z_3$ |

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**Other compounds with this structure**

$Rh_2S_2Se$, $Rh_2SSe_2$, $Rh_2Se_3$, $Ir_2S_3$

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- (Villars, 2016) gives an incorrect link for the primary reference (Parthé, 1967). (Downs, 2003) has the correct reference.

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**Simple Orthorhombic primitive vectors**

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
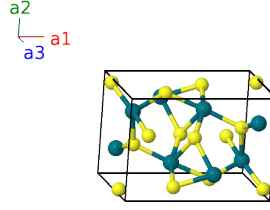


## Basis vectors

|  |  | Lattice coordinates |  | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | $=$ | $y_1\,\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$ | $=$ | $by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4c) | S I |
| $\mathbf{B_2}$ | $=$ | $\frac{1}{2}\,\mathbf{a_1} - \left(y_1 - \frac{1}{2}\right)\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$ | $=$ | $\frac{1}{2}a\,\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (4c) | S I |
| $\mathbf{B_3}$ | $=$ | $-y_1\,\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$ | $=$ | $-by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (4c) | S I |
| $\mathbf{B_4}$ | $=$ | $\frac{1}{2}\,\mathbf{a_1} + \left(y_1 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$ | $=$ | $\frac{1}{2}a\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4c) | S I |
| $\mathbf{B_5}$ | $=$ | $x_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$ | $=$ | $ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (8d) | Rh I |
| $\mathbf{B_6}$ | $=$ | $-\left(x_2 - \frac{1}{2}\right)\mathbf{a_1} - \left(y_2 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_2 + \frac{1}{2}\right)\mathbf{a_3}$ | $=$ | $-a\left(x_2 - \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\hat{\mathbf{z}}$ | (8d) | Rh I |
| $\mathbf{B_7}$ | $=$ | $-x_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} - \left(z_2 - \frac{1}{2}\right)\mathbf{a_3}$ | $=$ | $-ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\hat{\mathbf{z}}$ | (8d) | Rh I |
| $\mathbf{B_8}$ | $=$ | $\left(x_2 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_2 - \frac{1}{2}\right)\mathbf{a_2} - z_2\,\mathbf{a_3}$ | $=$ | $a\left(x_2 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$ | (8d) | Rh I |
| $\mathbf{B_9}$ | $=$ | $-x_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} - z_2\,\mathbf{a_3}$ | $=$ | $-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$ | (8d) | Rh I |
| $\mathbf{B_{10}}$ | $=$ | $\left(x_2 + \frac{1}{2}\right)\mathbf{a_1} + \left(y_2 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_2 - \frac{1}{2}\right)\mathbf{a_3}$ | $=$ | $a\left(x_2 + \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\hat{\mathbf{z}}$ | (8d) | Rh I |
| $\mathbf{B_{11}}$ | $=$ | $x_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} + \left(z_2 + \frac{1}{2}\right)\mathbf{a_3}$ | $=$ | $ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\hat{\mathbf{z}}$ | (8d) | Rh I |
| $\mathbf{B_{12}}$ | $=$ | $-\left(x_2 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_2 + \frac{1}{2}\right)\mathbf{a_2} + z_2\,\mathbf{a_3}$ | $=$ | $-a\left(x_2 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (8d) | Rh I |
| $\mathbf{B_{13}}$ | $=$ | $x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$ | $=$ | $ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (8d) | S II |
| $\mathbf{B_{14}}$ | $=$ | $-\left(x_3 - \frac{1}{2}\right)\mathbf{a_1} - \left(y_3 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$ | $=$ | $-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$ | (8d) | S II |
| $\mathbf{B_{15}}$ | $=$ | $-x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} - \left(z_3 - \frac{1}{2}\right)\mathbf{a_3}$ | $=$ | $-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\hat{\mathbf{z}}$ | (8d) | S II |
| $\mathbf{B_{16}}$ | $=$ | $\left(x_3 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_3 - \frac{1}{2}\right)\mathbf{a_2} - z_3\,\mathbf{a_3}$ | $=$ | $a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (8d) | S II |
| $\mathbf{B_{17}}$ | $=$ | $-x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$ | $=$ | $-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (8d) | S II |
| $\mathbf{B_{18}}$ | $=$ | $\left(x_3 + \frac{1}{2}\right)\mathbf{a_1} + \left(y_3 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_3 - \frac{1}{2}\right)\mathbf{a_3}$ | $=$ | $a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\hat{\mathbf{z}}$ | (8d) | S II |
| $\mathbf{B_{19}}$ | $=$ | $x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$ | $=$ | $ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$ | (8d) | S II |
| $\mathbf{B_{20}}$ | $=$ | $-\left(x_3 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_3 + \frac{1}{2}\right)\mathbf{a_2} + z_3\,\mathbf{a_3}$ | $=$ | $-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (8d) | S II |

## References

[1] E. Parthé, E. Hohnke, and F. Hulliger, *A new structure type with octahedron pairs for Rh$_2$S$_3$, Rh$_2$Se$_3$ and Ir$_2$S$_3$*, Acta Cryst. **23**, 832–840 (1967), doi:10.1107/S0365110X67003767.

**Found in**

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

[2] P. Villars, *Rh$_2$S$_3$ orth Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.