# NaO Structure: AB_hP12_189_fg_eh-001

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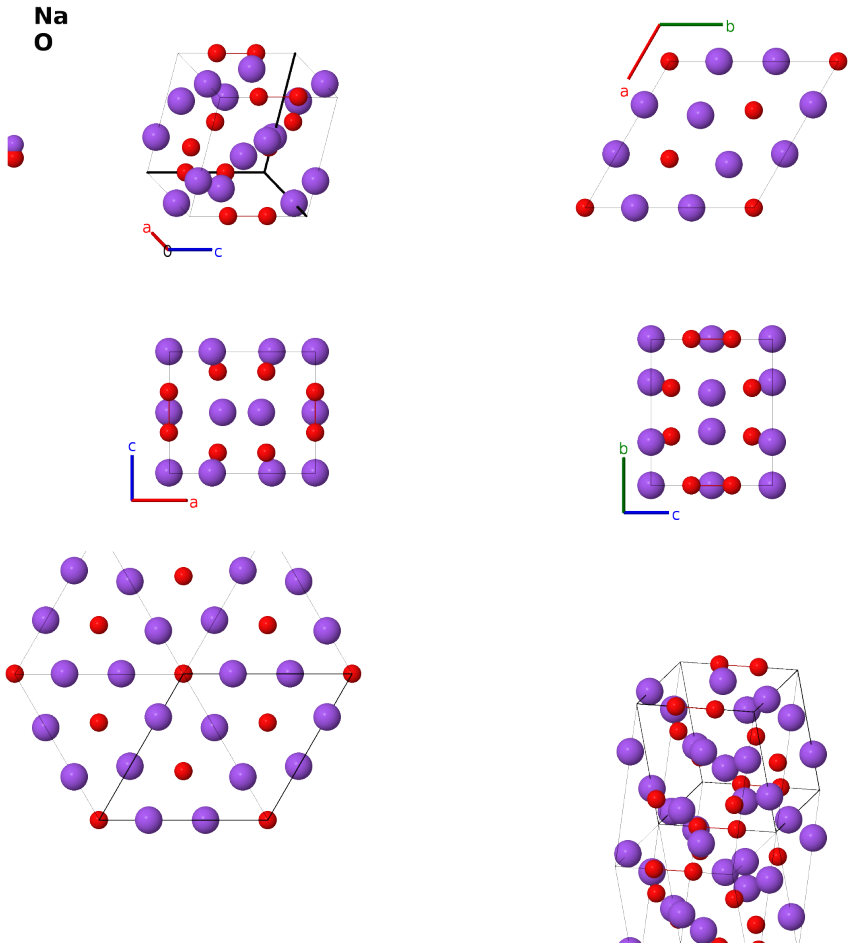
https://aflow.org/prototype-encyclopedia/PQWK

https://aflow.org/prototype-encyclopedia/AB_hP12_189_fg_eh-001




| | |
|---|---|
| **Prototype** | NaO |
| **AFLOW prototype label** | AB_hP12_189_fg_eh-001 |
| **ICSD** | 25526 |
| **CCDC** | 1601180 |
| **Pearson symbol** | hP12 |
| **Space group number** | 189 |
| **Space group symbol** | $P\bar{6}2m$ |

**AFLOW prototype command** `aflow --proto=AB_hP12_189_fg_eh-001 --params=`$a, c/a, z_1, x_2, x_3, z_4$

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**Other compounds with this structure**

CaAs, CaP, EuAs, KS, KSe, $\alpha$-KTe, $\alpha$-NaS, $\beta$-RbS, RbSe, RbTc, SrAs, SrP

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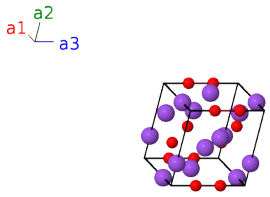
**Hexagonal primitive vectors**

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $z_1\,\mathbf{a}_3$ | = | $cz_1\,\hat{\mathbf{z}}$ | (2e) | O I |
| $\mathbf{B_2}$ | = | $-z_1\,\mathbf{a}_3$ | = | $-cz_1\,\hat{\mathbf{z}}$ | (2e) | O I |
| $\mathbf{B_3}$ | = | $x_2\,\mathbf{a}_1$ | = | $\frac{1}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$ | (3f) | Na I |
| $\mathbf{B_4}$ | = | $x_2\,\mathbf{a}_2$ | = | $\frac{1}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$ | (3f) | Na I |
| $\mathbf{B_5}$ | = | $-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$ | = | $-ax_2\,\hat{\mathbf{x}}$ | (3f) | Na I |
| $\mathbf{B_6}$ | = | $x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (3g) | Na II |
| $\mathbf{B_7}$ | = | $x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (3g) | Na II |
| $\mathbf{B_8}$ | = | $-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (3g) | Na II |
| $\mathbf{B_9}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (4h) | O II |
| $\mathbf{B_{10}}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (4h) | O II |
| $\mathbf{B_{11}}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (4h) | O II |
| $\mathbf{B_{12}}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (4h) | O II |

**References**


[1] H. Föppl, *Die Kristallstrukturen der Alkaliperoxyde*, Z. Anorganische und Allgemeine Chemie **291**, 12–50 (1957), doi:10.1002/zaac.19572910104.


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