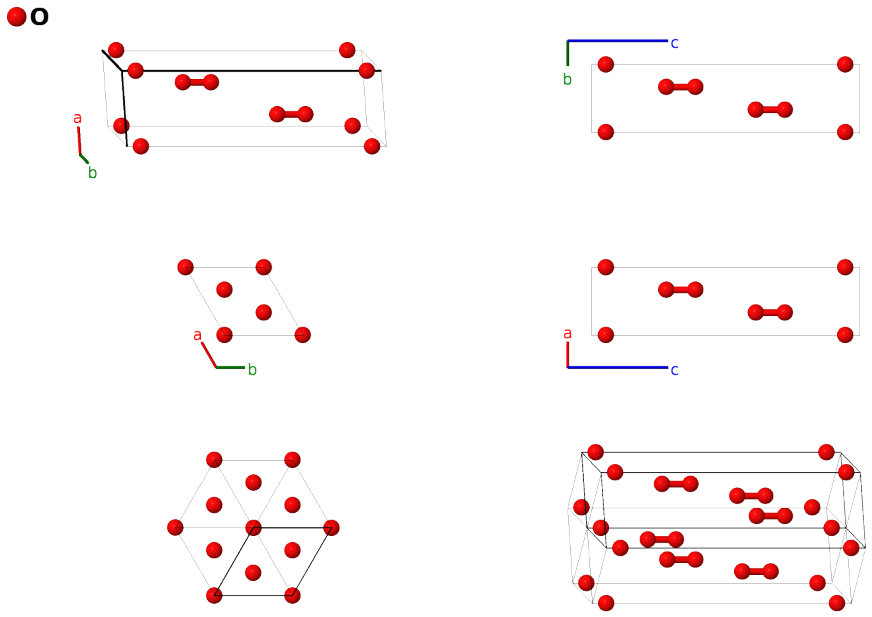
β-O_2 Structure: A_hR2_166_c-003

This structure originally had the label `A_hR2_166_c.beta-O`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/KTH0

https://aflow.org/p/A_hR2_166_c-003

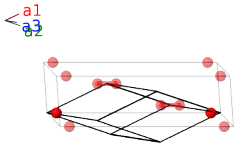


Prototype	O
AFLOW prototype label	A_hR2_166_c-003
ICSD	173934
Pearson symbol	hR2
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A_hR2_166_c-003 --params=`$a, c/a, x_1$

- α-As ($A7$), rhombohedral graphite, and β-O have the same AFLOW prototype label, A_hR2_166_c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files. Hexagonal settings of rhombohedral structures can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-cx_1\,\hat{\mathbf{z}}$	(2c)	O I

References

[1] R. J. Meier and R. B. Helmholdt, *Neutron-diffraction study of α- and β-oxygen*, Phys. Rev. B **29**, 1387–1393 (1984), doi:10.1103/PhysRevB.29.1387.