β-O_2 Structure: A_hR2_166_c-003

This structure previously used the label(s) `A_hR2_166_c.beta-O`. Calls to these addresses will be redirected here.

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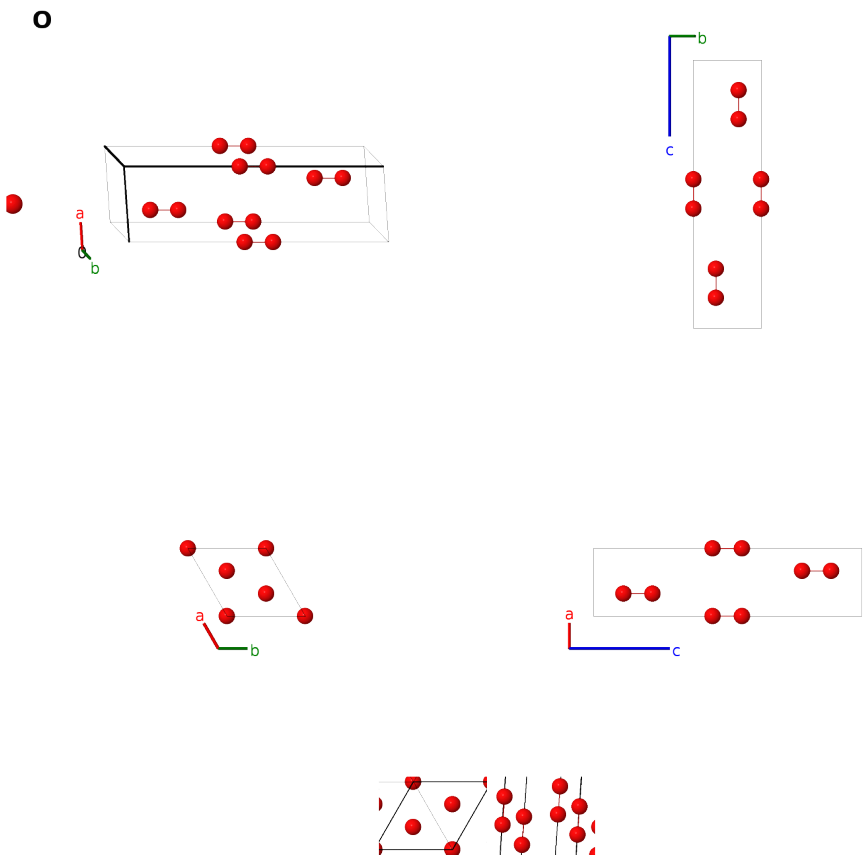
https://aflow.org/prototype-encyclopedia/KTH0

https://aflow.org/prototype-encyclopedia/A_hR2_166_c-003



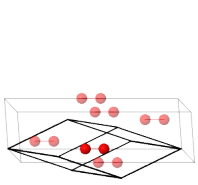
Prototype	O
AFLOW prototype label	A_hR2_166_c-003
ICSD	173934
CCDC	1688831
Pearson symbol	hR2
Space group number	166
Space group symbol	$R\bar{3}m$

AFLOW prototype command `aflow --proto=A_hR2_166_c-003 --params=`$a, c/a, x_1$

- Solid oxygen can be found in the α-O_2 phase below 24K and in the β-O_2 phase between 24 and 44K, with γ-O_2, stable between 44 and 54K, in the β-F_2 structure (Meier, 1984).
- Data for β-O_2 was taken at 30K.
- 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



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.

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