

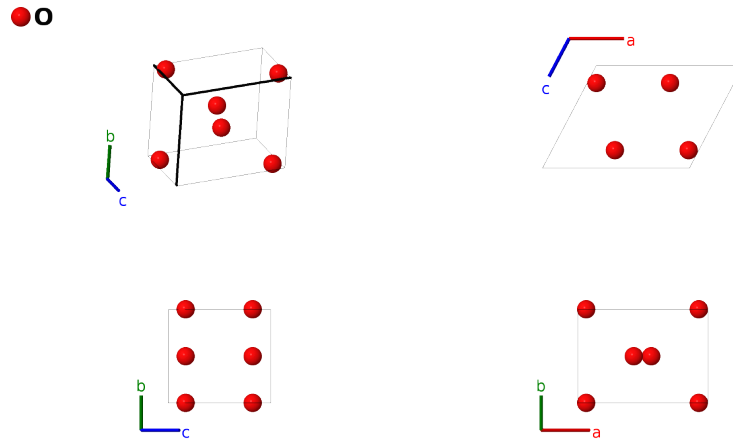
α -O₂ Structure: A_mC4_12_i-001

This structure originally had the label A_mC4_12_i. Calls to that address will be redirected here.

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<https://aflow.org/p/M3W6>

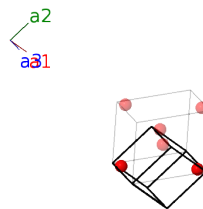
https://aflow.org/p/A_mC4_12_i-001



Prototype	O
AFLOW prototype label	A_mC4_12_i-001
ICSD	173933
Pearson symbol	mC4
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<code>aflow --proto=A_mC4_12_i-001 --params=a, b/a, c/a, β, x_1, z_1</code>

Base-centered Monoclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a\hat{x} - \frac{1}{2}b\hat{y} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{x} + \frac{1}{2}b\hat{y} \\ \mathbf{a}_3 &= c\cos\beta\hat{x} + c\sin\beta\hat{z} \end{aligned}$$



Basis vectors

	Lattice coordinates	=	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$=$	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4i) O I
\mathbf{B}_2	$=$	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(4i) O I

References

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