α-ReO_3 ($D0_9$) Structure: A3B_cP4_221_c_b-001

This structure originally had the label `A3B_cP4_221_d_a`. Calls to that address will be redirected here.

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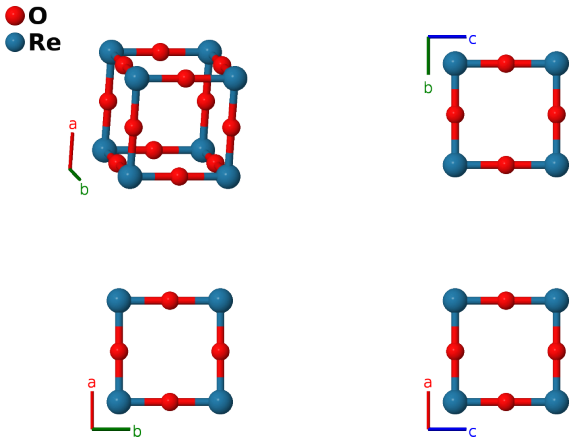
https://aflow.org/p/3DRV

https://aflow.org/p/A3B_cP4_221_c_b-001



Prototype	O_3Re
AFLOW prototype label	A3B_cP4_221_c_b-001
***Strukturbericht* designation**	$D0_9$
ICSD	16810
Pearson symbol	cP4
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	`aflow --proto=A3B_cP4_221_c_b-001 --params=`a

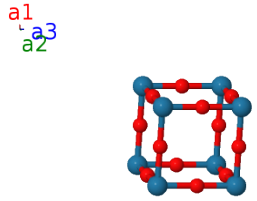
Other compounds with this structure

AlF_3, HfF_3, MoF_3, NCu_3, NNa_3, NbF_3, PbI_3, ScF_3, TaF_3, UO_3, WO_3

- Placing an atom on the origin, or (1a) Wyckoff position, transforms this into the cubic perovskite ($E2_1$) structure.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(1b)	Re I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(3c)	O I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(3c)	O I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(3c)	O I

References

[1] K. Meisel, *Rheniumtrioxyd. III. Mitteilung. Über die Kristallstruktur des Rheniumtrioxyds*, Z. Anorganische und Allgemeine Chemie **207**, 121–128 (1932), doi:10.1002/zaac.19322070113.

Found in

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