$MgSO_4$ Structure: ABC4_oC24_63_c_a_fg-001

This structure previously used the label(s) `AB4C_oC24_63_a_fg_c`. Calls to these addresses will be redirected here.

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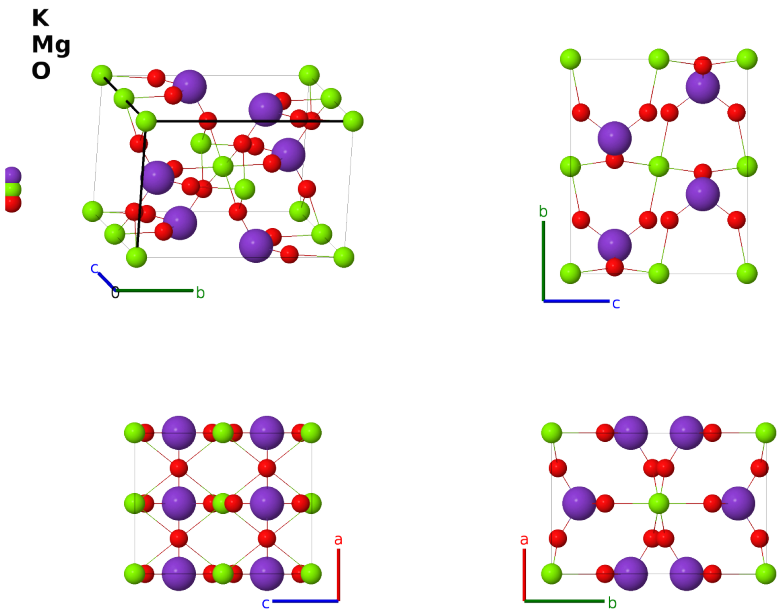
https://aflow.org/prototype-encyclopedia/FNXT

https://aflow.org/prototype-encyclopedia/ABC4_oC24_63_c_a_fg-001



Prototype	MgO_4S
AFLOW prototype label	ABC4_oC24_63_c_a_fg-001
ICSD	16759
CCDC	1597308
Pearson symbol	oC24
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=ABC4_oC24_63_c_a_fg-001 --params=`$a, b/a, c/a, y_2, y_3, z_3, x_4, y_4$

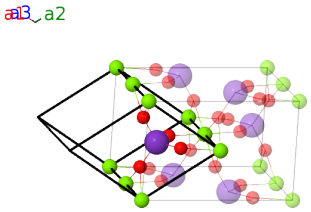
Other compounds with this structure

$CdCrO_4$, $CoCrO_4$, $CuCrO_4$, $MgCrO_4$, $MnCrO_4$, $NiCrO_4$, $ZnCrO_4$, $AlPO_4$, β-$CrPO_4$, $FePO_4$, $InPO_4$, $TlPO_4$, $TlPO_4$, VPO_4, $CdSO_4$, $CoSO_4$, $CuSO_4$, $FeSO_4$, $NiSO_4$, $ZnSO_4$, $CoSeO_4$, $CuSeO_4$, $MnSeO_4$, $ZnSeO_4$, $CrVO_4$, $FeVO_4$, $InVO_4$, $TlVO_4$

- (Baran, 1998) gives $CrVO_4$ or β-$CrPO_4$ as the prototype for this structure.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Mg I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Mg I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	K I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	K I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_7}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_8}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_9}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B_{10}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B_{11}}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B_{12}}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	O II

References

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[2] E. J. Baran, *Review: Materials belonging to the $CrVO_4$ structure type: preparation, crystal chemistry and physicochemical properties*, J. Mater. Sci. **33**, 2479–2497 (1998), doi:10.1023/A:1004380530309.

Found in

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

First cited in

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