Spinel (Al_2MgO_4, $H1_1$) Structure: A2BC4_cF56_227_c_b_e-001

This structure previously used the label(s) `A2BC4_cF56_227_d_a_e`. Calls to these addresses will be redirected here.

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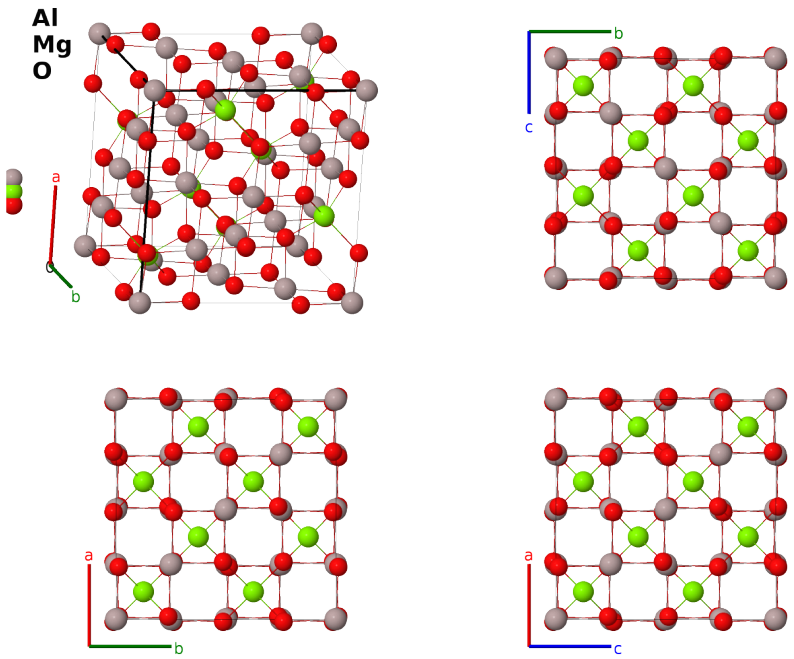
https://aflow.org/prototype-encyclopedia/MZYE

https://aflow.org/prototype-encyclopedia/A2BC4_cF56_227_c_b_e-001



Prototype	Al_2MgO_4
AFLOW prototype label	A2BC4_cF56_227_c_b_e-001
***Strukturbericht* designation**	$H1_1$
Mineral name	spinel
ICSD	26845
CCDC	1602224
Pearson symbol	cF56
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=A2BC4_cF56_227_c_b_e-001 --params=`a, x_3

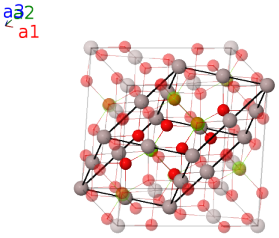
Other compounds with this structure

Al_2CdS_4, Al_2CrS_4, Al_2ZnSe_4, Cd_2VS_4, Co_2NiS_4, Co_3Se_4, Cr_2CdTe_4, Cr_2CoS_4, Cr_2CuS_4, Cr_2CuSe_4, Cr_2CoO_4, Cr_2FeO_4, Cr_2FeS_4, Cr_2HgS_4, Cr_2MnS_4, Cr_2SeZn_4, Cr_2ZrCd_4, Cr_2ZrSe_4, Ga_2CoS_4, Fe_2NiO_4, In_2CaS_4, In_2CdSe_4, In_2CrS_4, In_2FeS_4, In_2HgS_4, In_2MgS_4, In_2MnS_4, In_2NiS_4, In_2ZrCd_4, Ir_2CuS_4, Lu_2FeS_4, Lu_2MgS_4, Lu_2MnS_4, Mg_2GeO_4, Mn_2ZnTe_4, Na_2WO_4, Ni_2FeS_4, Sc_2FeS_4, Sc_2MnS_4, Sc_2MnSe_4, Ti_2CuS_4, V_2LiO_4, V_2CuS_4, V_2ZnO_4, Yb_2FeS_4, Yb_2MnS_4, Co_3O_4, Co_3S_4, Fe_3O_4, Fe_3S_4 (greigite), Ni_3S_4

- An *inverse spinel* has four Al atoms on the (8a) sites and (Al,Mg) alloyed on the (16d) sites.
- The binary $D7_2$ and ternary $H1_1$ spinel structures are for all intents and purposes identical. We could use $D7_2$ for the binary spinels and $H1_1$ for the ternaries, but historically this has not been the case. We dual-list this structure only to keep the historical record intact.
- (Hahn, 1955) has an extensive list of ternary spinels and inverse spinels.

Face-centered Cubic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(8b)	Mg I
$\mathbf{B_2}$	=	$\frac{5}{8}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$	=	$\frac{5}{8}a\,\hat{\mathbf{x}} + \frac{5}{8}a\,\hat{\mathbf{y}} + \frac{5}{8}a\,\hat{\mathbf{z}}$	(8b)	Mg I
$\mathbf{B_3}$	=	0	=	0	(16c)	Al I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(16c)	Al I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(3x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 - \left(3x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B_{10}}$	=	$-\left(3x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(3x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B_{13}}$	=	$-x_3\,\mathbf{a}_1 + \left(3x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B_{14}}$	=	$\left(3x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	O I

References

[1] P. Fischer, *Neutronenbeugungsuntersuchung der Strukturen von $MgAl_2O_4$-und $ZnAl_2O_4$-Spinellen, in Abhängigkeit von der Vorgeschichte*, Z. Krystallogr. **124**, 275–302 (1967), doi:10.1524/zkri.1967.124.16.275.

[2] H. Hahn, G. Frank, W. Klingler, A. D. Störger, and G. Störger, *Chalkogenide. VI. Über Ternäre Chalkogenide des Aluminiums, Galliums und Indiums mit Zink, Cadmium und Quecksilber*, Z. Anorganische und Allgemeine Chemie **279**, 241–270 (1955), doi:10.1002/zaac.19552790502.

Found in

[1] R. J. Hill, J. R. Craig, and G. V. Gibbs, *Systematics of the Spinel Structure Type*, Phys. Chem. Miner. **4**, 317–339 (1979).

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