$Ca_3Al_2O_6$ ($E9_1$) Structure: A2B3C6_cP33_221_cd_ag_fh-001

This structure originally had the label `A2B3C6_cP33_221_cd_ag_fh`. Calls to that address will be redirected here.

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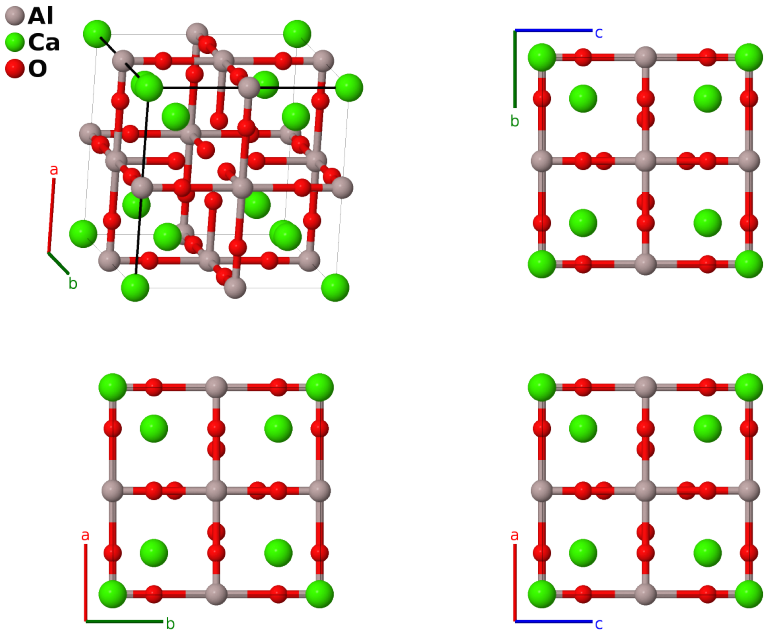
https://aflow.org/p/TZEN

https://aflow.org/p/A2B3C6_cP33_221_cd_ag_fh-001

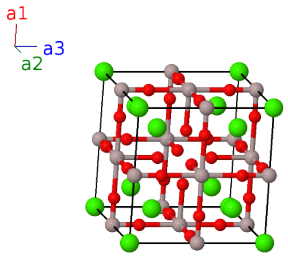


Prototype	$Al_2Ca_3O_6$
AFLOW prototype label	A2B3C6_cP33_221_cd_ag_fh-001
***Strukturbericht* designation**	$E9_1$
ICSD	151369
Pearson symbol	cP33
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	`aflow --proto=A2B3C6_cP33_221_cd_ag_fh-001 --params=`a, x_4, x_5, x_6

- (Steele, 1929) do not use the standard Wyckoff position notation to describe the atomic positions, so we use the parameters found in (Herman, 1937). An alternative description of the structure places the O-I atoms on the (6e) $(\pm x, 0, 0)\ldots$ site rather than the (6f) site.
- (Mondal, 1975) reanalyzed this structure and concluded that the true structure was one where the lattice constant was doubled and contained 264 atoms. See the $Ca_3Al_2O_6$ (A2B3C6_cP264_205_2d_ab2c2d_6d) structure page.

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
$\mathbf{B_1}$	=	0	=	0	(1a)	Ca 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)	Al 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)	Al 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)	Al I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(3d)	Al II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(3d)	Al II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{z}}$	(3d)	Al II
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_9}$	=	$-x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{14}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(8g)	Ca II
$\mathbf{B_{15}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(8g)	Ca II
$\mathbf{B_{16}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(8g)	Ca II
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(8g)	Ca II
$\mathbf{B_{18}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(8g)	Ca II
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(8g)	Ca II
$\mathbf{B_{20}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(8g)	Ca II
$\mathbf{B_{21}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(8g)	Ca II
$\mathbf{B_{22}}$	=	$x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_6\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(12h)	O II
$\mathbf{B_{23}}$	=	$-x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$-ax_6\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(12h)	O II
$\mathbf{B_{24}}$	=	$x_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12h)	O II
$\mathbf{B_{25}}$	=	$-x_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12h)	O II
$\mathbf{B_{26}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{z}}$	(12h)	O II
$\mathbf{B_{27}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{z}}$	(12h)	O II
$\mathbf{B_{28}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_6\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}}$	(12h)	O II
$\mathbf{B_{29}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_6\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}}$	(12h)	O II

$\mathbf{B_{30}}$	=	$x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12h)	O II
$\mathbf{B_{31}}$	=	$-x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12h)	O II
$\mathbf{B_{32}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(12h)	O II
$\mathbf{B_{33}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(12h)	O II

References

[1] F. A. Steele and W. P. Davey, *The Crystal Structure of Tricalcium Aluminate*, J. Am. Chem. Soc. **51**, 689–697 (1929), doi:10.1021/ja01383a001.

[2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturebericht Band II, 1928-1932* (Akademsiche Verlagsgesellschaft M. B. H, Leipzig, 1937).

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[1] P. Mondal and J. W. Jeffery, *The crystal structure of tricalcium aluminate, $Ca_3Al_2O_6$*, Acta Crystallogr. Sect. B **31**, 689–697 (1975), doi:10.1107/S0567740875003639.