Akermanite ($Ca_2MgSi_2O_7$, $S5_3$) Structure: A2BC7D2_tP24_113_e_a_cef_e-001

This structure originally had the label `A2BC7D2_tP24_113_e_a_cef_e`. Calls to that address will be redirected here.

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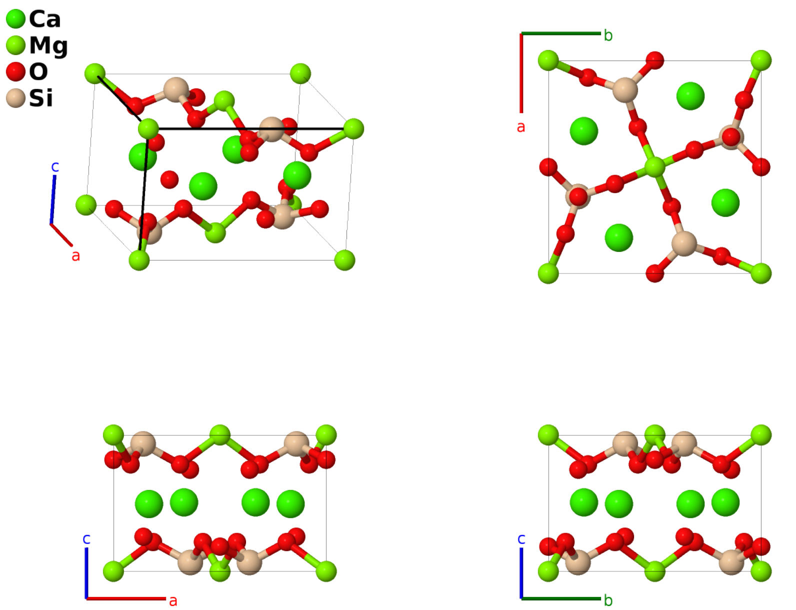
https://aflow.org/p/QV01

https://aflow.org/p/A2BC7D2_tP24_113_e_a_cef_e-001



Prototype	Ca_2MgO_7Si
AFLOW prototype label	A2BC7D2_tP24_113_e_a_cef_e-001
***Strukturbericht* designation**	$S5_3$
Mineral name	akermanite
ICSD	50065
Pearson symbol	tP24
Space group number	113
Space group symbol	$P\bar{4}2_1m$
AFLOW prototype command	`aflow --proto=A2BC7D2_tP24_113_e_a_cef_e-001` `--params=`$a, c/a, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, y_6, z_6$

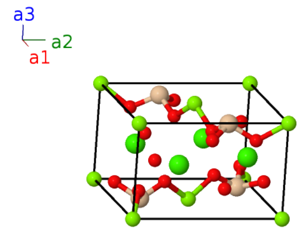
Other compounds with this structure

$Ba_2MnGe_2O_7$, $Ca_2B_2SiO_7$ (okayamalite), $Ca_2BeSi_2O_7$ (gugiaite), $Ca_2ZnSi_2O_7$ (hardystonite), $Sr_2MnGe_2O_7$, $Sr_2MnGe_2S_6O$, $Sr_2ZrSi_2O_7$, $Ca_2Al(AlSi)O_7$ (gehlenite), $(Ca, Na)_2(Al, Mg, Fe)(Si_2O_7)$ (alumoakermanite), $(Ca, Na)_2(Al, Mg, Fe)(Si, Al)_2O_7$ (melilite), $(Ca, Na)_2(Mg, Al, Si)_3O_7$

- Akermanite is an end point of the mineral melilite, which, like thortveitite (S2$_1$), is a sorosilicate, a mineral containing isolated Si_2O_7 or related groups. We have followed (Parthé, 1997) and use akermanite to represent the entire class of materials.
- We use the ambient pressure data from (Yang, 1997) to describe the structure.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Mg I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(2a)	Mg I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_2\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B_7}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B_8}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{11}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{12}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_{15}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_{16}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{18}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{19}}$	=	$y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{20}}$	=	$-y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{21}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{22}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{23}}$	=	$-\left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-a\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{24}}$	=	$\left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$a\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	O III

References

[1] H. Yang, R. M. Hazen, R. T. Downs, and L. W. Finger, *Structural change associated with the incommensurate-normal phase transition in akermanite, $Ca_2MgSi_2O_7$, at high pressure*, Phys. Chem. Minerals **24**, 510–519 (1997), doi:10.1007/s002690050066.

[2] E. Parthé, L. Gelato, B. Chabot, M. Penso, K. Cenzula, and R. Gladyshevskii, *Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types*, *Gmelin Handbook of Inorganic and Organometallic Chemistry*, vol. 2 (Springer-Verlag, Berlin, Heidelberg, 1993), 8 edn., doi:10.1007/978-3-662-02909-1_3.