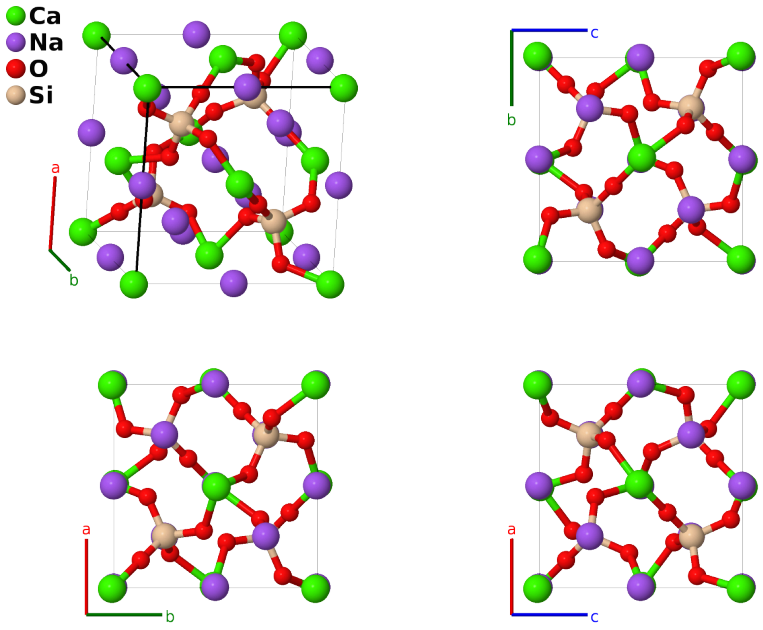
Na_2CaSiO_4 ($S6_6$) Structure: AB2C4D_cP32_198_a_2a_ab_a-001

This structure originally had the label `AB2C4D_cP32_198_a_2a_ab_a`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

https://aflow.org/p/MFVM

https://aflow.org/p/AB2C4D_cP32_198_a_2a_ab_a-001



Prototype	$CaNa_2O_4Si$
AFLOW prototype label	AB2C4D_cP32_198_a_2a_ab_a-001
***Strukturbericht* designation**	$S6_6$
ICSD	24235
Pearson symbol	cP32
Space group number	198
Space group symbol	$P2_13$
AFLOW prototype command	`aflow --proto=AB2C4D_cP32_198_a_2a_ab_a-001 --params=`$a, x_1, x_2, x_3, x_4, x_5, x_6, y_6, z_6$

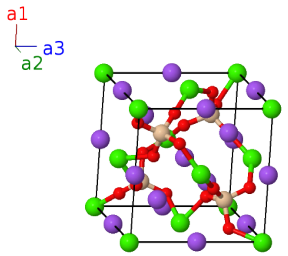
Other compounds with this structure
K_3CrO_4, Li_2SrSi_4

- Substitution of small fractions of rare earth elements onto the Ca site can produce photoluminescence.
- This is the crystal structure found by (Barth, 1932). The coordinates on p. 159 of (Hermann, 1937) are incorrect, as they do not properly transform Barth and Posnjak's coordinates in degrees to fractional coordinates. See (Hermann, 1937) pp. 557-8 for the correct coordinates.

- (Dollase, 1991) found that the SiO_4 tetrahedra were orientationally disordered, and that the resulting $Na_2Ca(SiO_4)$ structure took on the Heusler ($L1_2$) structure.

Simple Cubic primitive vectors

$$\begin{aligned}\mathbf{a_1} &= a\,\hat{\mathbf{x}}\\ \mathbf{a_2} &= a\,\hat{\mathbf{y}}\\ \mathbf{a_3} &= a\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B_2}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(x_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \left(x_1+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B_4}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1-\frac{1}{2}\right)\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_6}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_8}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2-\frac{1}{2}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(4a)	Na II
$\mathbf{B_{10}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Na II
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Na II
$\mathbf{B_{12}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3-\frac{1}{2}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(4a)	Na II
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{14}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(x_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 + \left(x_4+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{16}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4-\frac{1}{2}\right)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_{18}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \left(x_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a}_1 + \left(x_5+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Si I

$\mathbf{B_{20}}$	$=$	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2-x_5\,\mathbf{a}_3$	$=$	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_{21}}$	$=$	$x_6\,\mathbf{a}_1+y_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	$=$	$ax_6\,\hat{\mathbf{x}}+ay_6\,\hat{\mathbf{y}}+az_6\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{22}}$	$=$	$-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_1-y_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}-ay_6\,\hat{\mathbf{y}}+a\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{23}}$	$=$	$-x_6\,\mathbf{a}_1+\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_6-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_6\,\hat{\mathbf{x}}+a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(z_6-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{24}}$	$=$	$\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_2-z_6\,\mathbf{a}_3$	$=$	$a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}-az_6\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{25}}$	$=$	$z_6\,\mathbf{a}_1+x_6\,\mathbf{a}_2+y_6\,\mathbf{a}_3$	$=$	$az_6\,\hat{\mathbf{x}}+ax_6\,\hat{\mathbf{y}}+ay_6\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{26}}$	$=$	$\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_2-y_6\,\mathbf{a}_3$	$=$	$a\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}-ay_6\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{27}}$	$=$	$-\left(z_6-\frac{1}{2}\right)\,\mathbf{a}_1-x_6\,\mathbf{a}_2+\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(z_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}+a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{28}}$	$=$	$-z_6\,\mathbf{a}_1+\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_2-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-az_6\,\hat{\mathbf{x}}+a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{29}}$	$=$	$y_6\,\mathbf{a}_1+z_6\,\mathbf{a}_2+x_6\,\mathbf{a}_3$	$=$	$ay_6\,\hat{\mathbf{x}}+az_6\,\hat{\mathbf{y}}+ax_6\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{30}}$	$=$	$-y_6\,\mathbf{a}_1+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ay_6\,\hat{\mathbf{x}}+a\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{31}}$	$=$	$\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_1-\left(z_6-\frac{1}{2}\right)\,\mathbf{a}_2-x_6\,\mathbf{a}_3$	$=$	$a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(z_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}-ax_6\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{32}}$	$=$	$-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_1-z_6\,\mathbf{a}_2+\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}-az_6\,\hat{\mathbf{y}}+a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O II

References

[1] T. F. W. Barth and E. Posnjak, *Silicate structures of the cristobalite type: II. The crystal structure of Na_2CaSiO_4*, Z. Krystallogr. **81**, 370–375 (1932), doi:10.1524/zkri.1932.81.1.370.

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

[3] W. A. Dollase and C. R. Ross, *Crystal structure of orientationally disordered $Na_2(Ca,Sr)SiO_4$*, Z. Krystallogr. **197**, 13–26 (1991), doi:10.1524/zkri.1991.197.14.13.