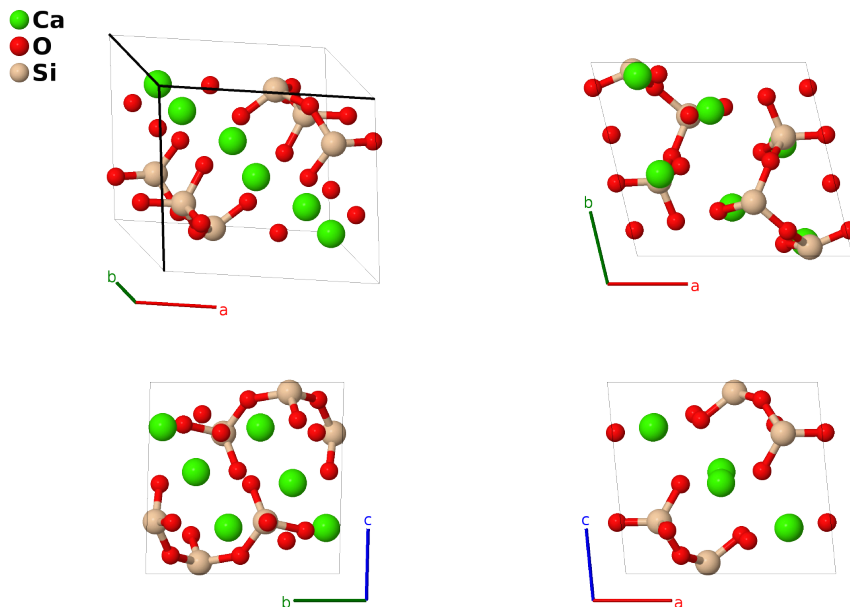# Wollastonite (CaSiO$_3$) Structure: AB3C_aP30_2_3i_9i_3i-001

This structure originally had the label `AB3C_aP30_2_3i_9i_3i`. Calls to that address will be redirected here.

https://aflow.org/p/89U5

https://aflow.org/p/AB3C_aP30_2_3i_9i_3i-001

|	
Prototype	CaO$_3$Si
AFLOW prototype label	AB3C_aP30_2_3i_9i_3i-001
Mineral name	wollastonite
ICSD	33702
Pearson symbol	aP30
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	aflow --proto=AB3C_aP30_2_3i_9i_3i-001 --params=$a, b/a, c/a, \alpha, \beta, \gamma, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}$

Other compounds with this structure

Ca$_2$NaHSi$_2$O$_9$ (pectolite)

- (Barnick, 1936) found a monoclinic structure for wollastonite, but that structure is now referred to as parawollastonite, with the current triclinic structure receiving the original name.

Triclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = b\cos\gamma\,\hat{\mathbf{x}} + b\sin\gamma\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c_x\,\hat{\mathbf{x}} + c_y\,\hat{\mathbf{y}} + c_z\,\hat{\mathbf{z}}$$

$$c_x = c\cos\beta$$

$$c_y = c(\cos\alpha - \cos\beta\cos\gamma)/\sin\gamma$$

$$c_z = \sqrt{c^2 - c_x^2 - c_y^2}$$
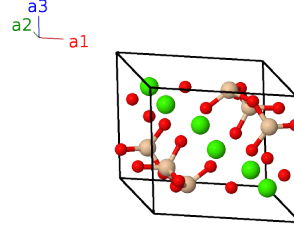
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a_1} + y_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	$=$	$(ax_1 + by_1\cos\gamma + c_x z_1)\,\hat{\mathbf{x}} + (by_1\sin\gamma + c_y z_1)\,\hat{\mathbf{y}} + c_z z_1\,\hat{\mathbf{z}}$	(2i)	Ca I
$\mathbf{B_2}$	$=$	$-x_1\,\mathbf{a_1} - y_1\,\mathbf{a_2} - z_1\,\mathbf{a_3}$	$=$	$-(ax_1 + by_1\cos\gamma + c_x z_1)\,\hat{\mathbf{x}} - (by_1\sin\gamma + c_y z_1)\,\hat{\mathbf{y}} - c_z z_1\,\hat{\mathbf{z}}$	(2i)	Ca I
$\mathbf{B_3}$	$=$	$x_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$(ax_2 + by_2\cos\gamma + c_x z_2)\,\hat{\mathbf{x}} + (by_2\sin\gamma + c_y z_2)\,\hat{\mathbf{y}} + c_z z_2\,\hat{\mathbf{z}}$	(2i)	Ca II
$\mathbf{B_4}$	$=$	$-x_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	$=$	$-(ax_2 + by_2\cos\gamma + c_x z_2)\,\hat{\mathbf{x}} - (by_2\sin\gamma + c_y z_2)\,\hat{\mathbf{y}} - c_z z_2\,\hat{\mathbf{z}}$	(2i)	Ca II
$\mathbf{B_5}$	$=$	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$(ax_3 + by_3\cos\gamma + c_x z_3)\,\hat{\mathbf{x}} + (by_3\sin\gamma + c_y z_3)\,\hat{\mathbf{y}} + c_z z_3\,\hat{\mathbf{z}}$	(2i)	Ca III
$\mathbf{B_6}$	$=$	$-x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$-(ax_3 + by_3\cos\gamma + c_x z_3)\,\hat{\mathbf{x}} - (by_3\sin\gamma + c_y z_3)\,\hat{\mathbf{y}} - c_z z_3\,\hat{\mathbf{z}}$	(2i)	Ca III
$\mathbf{B_7}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$(ax_4 + by_4\cos\gamma + c_x z_4)\,\hat{\mathbf{x}} + (by_4\sin\gamma + c_y z_4)\,\hat{\mathbf{y}} + c_z z_4\,\hat{\mathbf{z}}$	(2i)	O I
$\mathbf{B_8}$	$=$	$-x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-(ax_4 + by_4\cos\gamma + c_x z_4)\,\hat{\mathbf{x}} - (by_4\sin\gamma + c_y z_4)\,\hat{\mathbf{y}} - c_z z_4\,\hat{\mathbf{z}}$	(2i)	O I
$\mathbf{B_9}$	$=$	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$(ax_5 + by_5\cos\gamma + c_x z_5)\,\hat{\mathbf{x}} + (by_5\sin\gamma + c_y z_5)\,\hat{\mathbf{y}} + c_z z_5\,\hat{\mathbf{z}}$	(2i)	O II
$\mathbf{B_{10}}$	$=$	$-x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	$=$	$-(ax_5 + by_5\cos\gamma + c_x z_5)\,\hat{\mathbf{x}} - (by_5\sin\gamma + c_y z_5)\,\hat{\mathbf{y}} - c_z z_5\,\hat{\mathbf{z}}$	(2i)	O II
$\mathbf{B_{11}}$	$=$	$x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$(ax_6 + by_6\cos\gamma + c_x z_6)\,\hat{\mathbf{x}} + (by_6\sin\gamma + c_y z_6)\,\hat{\mathbf{y}} + c_z z_6\,\hat{\mathbf{z}}$	(2i)	O III
$\mathbf{B_{12}}$	$=$	$-x_6\,\mathbf{a_1} - y_6\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	$=$	$-(ax_6 + by_6\cos\gamma + c_x z_6)\,\hat{\mathbf{x}} - (by_6\sin\gamma + c_y z_6)\,\hat{\mathbf{y}} - c_z z_6\,\hat{\mathbf{z}}$	(2i)	O III
$\mathbf{B_{13}}$	$=$	$x_7\,\mathbf{a_1} + y_7\,\mathbf{a_2} + z_7\,\mathbf{a_3}$	$=$	$(ax_7 + by_7\cos\gamma + c_x z_7)\,\hat{\mathbf{x}} + (by_7\sin\gamma + c_y z_7)\,\hat{\mathbf{y}} + c_z z_7\,\hat{\mathbf{z}}$	(2i)	O IV
$\mathbf{B_{14}}$	$=$	$-x_7\,\mathbf{a_1} - y_7\,\mathbf{a_2} - z_7\,\mathbf{a_3}$	$=$	$-(ax_7 + by_7\cos\gamma + c_x z_7)\,\hat{\mathbf{x}} - (by_7\sin\gamma + c_y z_7)\,\hat{\mathbf{y}} - c_z z_7\,\hat{\mathbf{z}}$	(2i)	O IV
$\mathbf{B_{15}}$	$=$	$x_8\,\mathbf{a_1} + y_8\,\mathbf{a_2} + z_8\,\mathbf{a_3}$	$=$	$(ax_8 + by_8\cos\gamma + c_x z_8)\,\hat{\mathbf{x}} + (by_8\sin\gamma + c_y z_8)\,\hat{\mathbf{y}} + c_z z_8\,\hat{\mathbf{z}}$	(2i)	O V
$\mathbf{B_{16}}$	$=$	$-x_8\,\mathbf{a_1} - y_8\,\mathbf{a_2} - z_8\,\mathbf{a_3}$	$=$	$-(ax_8 + by_8\cos\gamma + c_x z_8)\,\hat{\mathbf{x}} - (by_8\sin\gamma + c_y z_8)\,\hat{\mathbf{y}} - c_z z_8\,\hat{\mathbf{z}}$	(2i)	O V
$\mathbf{B_{17}}$	$=$	$x_9\,\mathbf{a_1} + y_9\,\mathbf{a_2} + z_9\,\mathbf{a_3}$	$=$	$(ax_9 + by_9\cos\gamma + c_x z_9)\,\hat{\mathbf{x}} + (by_9\sin\gamma + c_y z_9)\,\hat{\mathbf{y}} + c_z z_9\,\hat{\mathbf{z}}$	(2i)	O VI

$$\mathbf{B_{18}} = -x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 = -\left(ax_9 + by_9\cos\gamma + c_x z_9\right)\hat{\mathbf{x}} - \left(by_9\sin\gamma + c_y z_9\right)\hat{\mathbf{y}} - c_z z_9\,\hat{\mathbf{z}} \qquad (2i) \qquad \text{O VI}$$

$$\mathbf{B_{19}} = x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = \left(ax_{10} + by_{10}\cos\gamma + c_x z_{10}\right)\hat{\mathbf{x}} + \left(by_{10}\sin\gamma + c_y z_{10}\right)\hat{\mathbf{y}} + c_z z_{10}\,\hat{\mathbf{z}} \qquad (2i) \qquad \text{O VII}$$

$$\mathbf{B_{20}} = -x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = -\left(ax_{10} + by_{10}\cos\gamma + c_x z_{10}\right)\hat{\mathbf{x}} - \left(by_{10}\sin\gamma + c_y z_{10}\right)\hat{\mathbf{y}} - c_z z_{10}\,\hat{\mathbf{z}} \qquad (2i) \qquad \text{O VII}$$

$$\mathbf{B_{21}} = x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = \left(ax_{11} + by_{11}\cos\gamma + c_x z_{11}\right)\hat{\mathbf{x}} + \left(by_{11}\sin\gamma + c_y z_{11}\right)\hat{\mathbf{y}} + c_z z_{11}\,\hat{\mathbf{z}} \qquad (2i) \qquad \text{O VIII}$$

$$\mathbf{B_{22}} = -x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 = -\left(ax_{11} + by_{11}\cos\gamma + c_x z_{11}\right)\hat{\mathbf{x}} - \left(by_{11}\sin\gamma + c_y z_{11}\right)\hat{\mathbf{y}} - c_z z_{11}\,\hat{\mathbf{z}} \qquad (2i) \qquad \text{O VIII}$$

$$\mathbf{B_{23}} = x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = \left(ax_{12} + by_{12}\cos\gamma + c_x z_{12}\right)\hat{\mathbf{x}} + \left(by_{12}\sin\gamma + c_y z_{12}\right)\hat{\mathbf{y}} + c_z z_{12}\,\hat{\mathbf{z}} \qquad (2i) \qquad \text{O IX}$$

$$\mathbf{B_{24}} = -x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3 = -\left(ax_{12} + by_{12}\cos\gamma + c_x z_{12}\right)\hat{\mathbf{x}} - \left(by_{12}\sin\gamma + c_y z_{12}\right)\hat{\mathbf{y}} - c_z z_{12}\,\hat{\mathbf{z}} \qquad (2i) \qquad \text{O IX}$$

$$\mathbf{B_{25}} = x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 = \left(ax_{13} + by_{13}\cos\gamma + c_x z_{13}\right)\hat{\mathbf{x}} + \left(by_{13}\sin\gamma + c_y z_{13}\right)\hat{\mathbf{y}} + c_z z_{13}\,\hat{\mathbf{z}} \qquad (2i) \qquad \text{Si I}$$

$$\mathbf{B_{26}} = -x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3 = -\left(ax_{13} + by_{13}\cos\gamma + c_x z_{13}\right)\hat{\mathbf{x}} - \left(by_{13}\sin\gamma + c_y z_{13}\right)\hat{\mathbf{y}} - c_z z_{13}\,\hat{\mathbf{z}} \qquad (2i) \qquad \text{Si I}$$

$$\mathbf{B_{27}} = x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 = \left(ax_{14} + by_{14}\cos\gamma + c_x z_{14}\right)\hat{\mathbf{x}} + \left(by_{14}\sin\gamma + c_y z_{14}\right)\hat{\mathbf{y}} + c_z z_{14}\,\hat{\mathbf{z}} \qquad (2i) \qquad \text{Si II}$$

$$\mathbf{B_{28}} = -x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3 = -\left(ax_{14} + by_{14}\cos\gamma + c_x z_{14}\right)\hat{\mathbf{x}} - \left(by_{14}\sin\gamma + c_y z_{14}\right)\hat{\mathbf{y}} - c_z z_{14}\,\hat{\mathbf{z}} \qquad (2i) \qquad \text{Si II}$$

$$\mathbf{B_{29}} = x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 = \left(ax_{15} + by_{15}\cos\gamma + c_x z_{15}\right)\hat{\mathbf{x}} + \left(by_{15}\sin\gamma + c_y z_{15}\right)\hat{\mathbf{y}} + c_z z_{15}\,\hat{\mathbf{z}} \qquad (2i) \qquad \text{Si III}$$

$$\mathbf{B_{30}} = -x_{15}\,\mathbf{a}_1 - y_{15}\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3 = -\left(ax_{15} + by_{15}\cos\gamma + c_x z_{15}\right)\hat{\mathbf{x}} - \left(by_{15}\sin\gamma + c_y z_{15}\right)\hat{\mathbf{y}} - c_z z_{15}\,\hat{\mathbf{z}} \qquad (2i) \qquad \text{Si III}$$

References

[1] M. J. Buerger and C. T. Prewitt, *The Crystal Structures of Wollastonite and Pectolite*, Proc. Natl. Acad. Sci. **47**, 1884–1888 (1961), doi:10.1073/pnas.47.12.1884.

[2] M. Barnick, *Strukturuntersuchung des natürlichen Wollastonits* (1936). Dissertation.