Phenakite (Be_2SiO_4, $S1_3$) Structure: A2B4C_hR42_148_2f_4f_f-001

This structure originally had the label `A2B4C_hR42_148_2f_4f_f`. Calls to that address will be redirected here.

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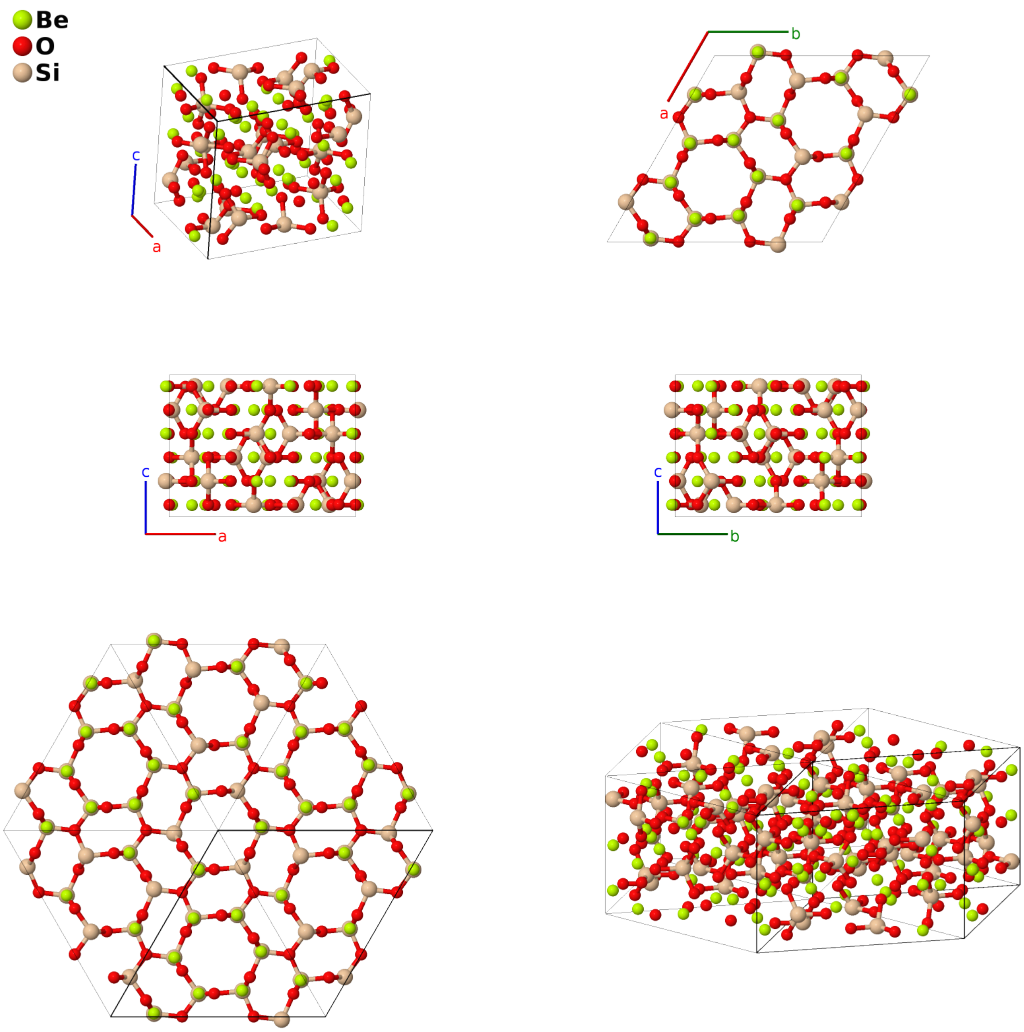
https://aflow.org/p/BQNX

https://aflow.org/p/A2B4C_hR42_148_2f_4f_f-001



Prototype	Be_2O_4Si
AFLOW prototype label	A2B4C_hR42_148_2f_4f_f-001
***Strukturbericht* designation**	$S1_3$
Mineral name	phenakite
ICSD	202275
Pearson symbol	hR42

Space group number 148

Space group symbol $R\overline{3}$

AFLOW prototype command `aflow --proto=A2B4C_hR42_148_2f_4f_f-001`
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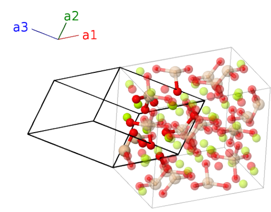
Other compounds with this structure

$LiZnPO_4$, Zn_2SiO4 (willemite), $(Zn, Mn)_2SiO_4$ (troostite)

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 - z_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_1 - 2y_1 + z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	Be I
$\mathbf{B_2}$	=	$z_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + y_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_1 - z_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_1 - y_1 - z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	Be I
$\mathbf{B_3}$	=	$y_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_1 - y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_1 + y_1 - 2z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	Be I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_1 - z_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_1 - 2y_1 + z_1)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	Be I
$\mathbf{B_5}$	=	$-z_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - y_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_1 - z_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_1 - y_1 - z_1)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	Be I
$\mathbf{B_6}$	=	$-y_1\,\mathbf{a}_1 - z_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 - y_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_1 + y_1 - 2z_1)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(6f)	Be I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 - 2y_2 + z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	Be II
$\mathbf{B_8}$	=	$z_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_2 - y_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	Be II
$\mathbf{B_9}$	=	$y_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 + y_2 - 2z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	Be II
$\mathbf{B_{10}}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 - 2y_2 + z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	Be II
$\mathbf{B_{11}}$	=	$-z_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_2 - z_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_2 - y_2 - z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	Be II
$\mathbf{B_{12}}$	=	$-y_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 + y_2 - 2z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	Be II
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{14}}$	=	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	O I

$\mathbf{B_{15}}$	=	$y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{16}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{17}}$	=	$-z_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{18}}$	=	$-y_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{19}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B_{20}}$	=	$z_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B_{21}}$	=	$y_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B_{22}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B_{23}}$	=	$-z_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_4 - z_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B_{24}}$	=	$-y_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B_{25}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_5 - 2y_5 + z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B_{26}}$	=	$z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_5 - z_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_5 - y_5 - z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B_{27}}$	=	$y_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B_{28}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_5 - 2y_5 + z_5)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B_{29}}$	=	$-z_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - y_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_5 - z_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_5 - y_5 - z_5)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B_{30}}$	=	$-y_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B_{31}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O IV
$\mathbf{B_{32}}$	=	$z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O IV
$\mathbf{B_{33}}$	=	$y_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O IV
$\mathbf{B_{34}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O IV
$\mathbf{B_{35}}$	=	$-z_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - y_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O IV
$\mathbf{B_{36}}$	=	$-y_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O IV
$\mathbf{B_{37}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 - 2y_7 + z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(6f)	Si I
$\mathbf{B_{38}}$	=	$z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + y_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_7 - y_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(6f)	Si I

$$\mathbf{B_{39}} = y_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3 = -\frac{1}{2}a\,(x_7 - y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 + y_7 - 2z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}} \quad (6f) \quad \text{Si I}$$

$$\mathbf{B_{40}} = -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 - 2y_7 + z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}} \quad (6f) \quad \text{Si I}$$

$$\mathbf{B_{41}} = -z_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - y_7\,\mathbf{a}_3 = \frac{1}{2}a\,(y_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_7 - y_7 - z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}} \quad (6f) \quad \text{Si I}$$

$$\mathbf{B_{42}} = -y_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3 = \frac{1}{2}a\,(x_7 - y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 + y_7 - 2z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}} \quad (6f) \quad \text{Si I}$$

References

[1] J. W. Downs and G. V. Gibbs, *An exploratory examination of the electron density and electrostatic potential of phenakite*, Am. Mineral. **72**, 769–777 (1987).

[2] R. M. Hazen and L. W. Finger, *High-Temperature Crystal Chemistry of Phenakite (Be_2SiO_4) and Chrysoberyl ($BeAl_2O_4$)*, Phys. Chem. Min. **14**, 426–434 (1987), doi:10.1007/BF00628819.