

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

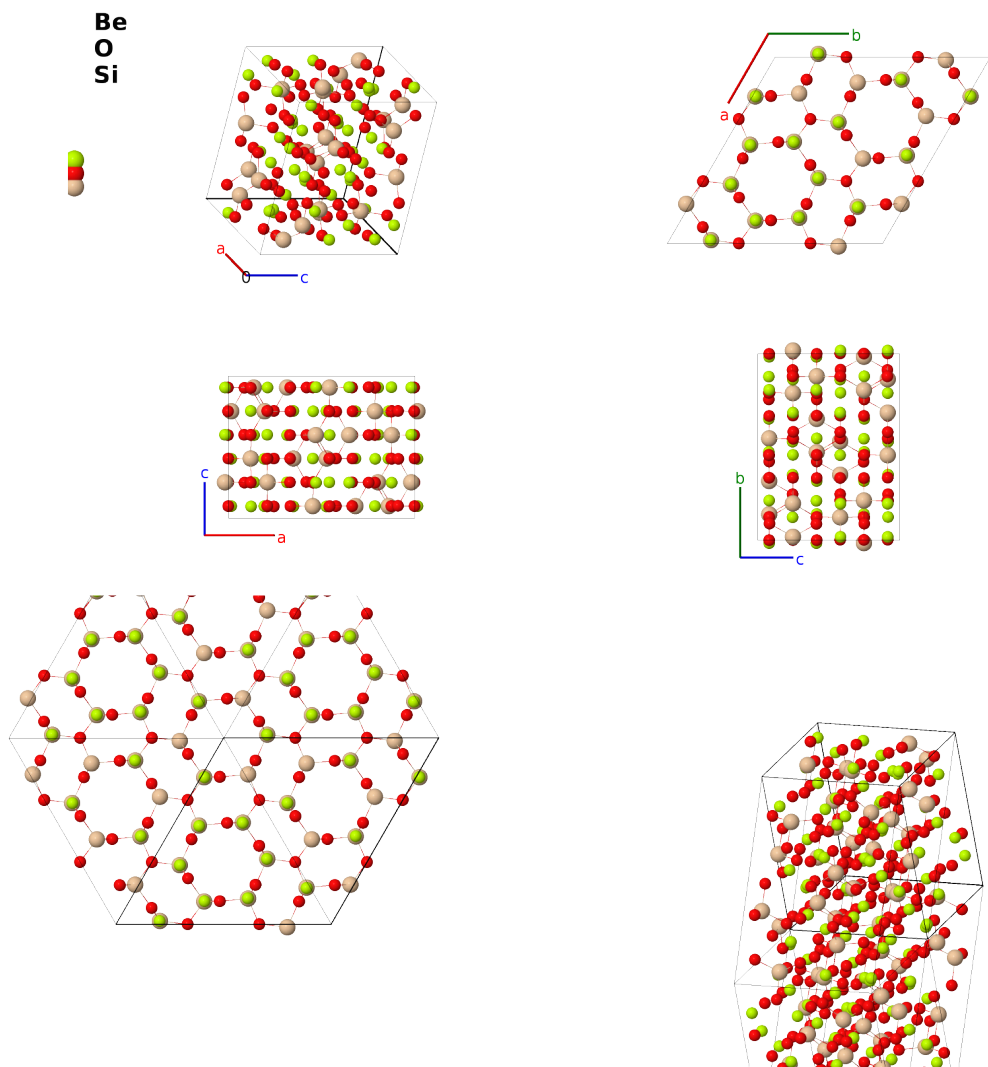
This structure previously used the label(s) **A2B4C_hR42_148_2f_4f_f**. Calls to these addresses will be redirected here.

Cite this page as:

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- 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/prototype-encyclopedia/BQNX>

https://aflow.org/prototype-encyclopedia/A2B4C_hR42_148_2f_4f_f-001



Prototype	$\text{Be}_2\text{O}_4\text{Si}$
AFLOW prototype label	A2B4C_hR42_148_2f_4f_f-001
<i>Strukturbericht</i> designation	$S1_3$
Mineral name	phenakite

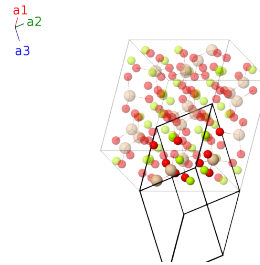
ICSD	202275
CCDC	1706859
Pearson symbol	hR42
Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	aflow --proto=A2B4C_hR42_148_2f_4f_f-001 --params= $a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

Other compounds with this structure

Li_2MoO_4 , Li_2WO_4 , LiZnPO_4 , Zn_2SiO_4 (willemite), $(\text{Zn}, \text{Mn})_2\text{SiO}_4$ (troostite)

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
\end{aligned}$$



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

$$\begin{aligned}
\mathbf{B}_{36} &= -y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3 &= \frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) &\text{O IV} \\
\mathbf{B}_{37} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= \frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6f) &\text{Si I} \\
\mathbf{B}_{38} &= z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + y_7 \mathbf{a}_3 &= -\frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6f) &\text{Si I} \\
\mathbf{B}_{39} &= y_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3 &= -\frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6f) &\text{Si I} \\
\mathbf{B}_{40} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6f) &\text{Si I} \\
\mathbf{B}_{41} &= -z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - y_7 \mathbf{a}_3 &= \frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6f) &\text{Si I} \\
\mathbf{B}_{42} &= -y_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3 &= \frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6f) &\text{Si I}
\end{aligned}$$

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.

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