Dioptase [$Cu_6(Si_6O_{18})\cdot 6H_2O$] Structure: AB2C4D_hR48_148_f_2f_4f_f-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

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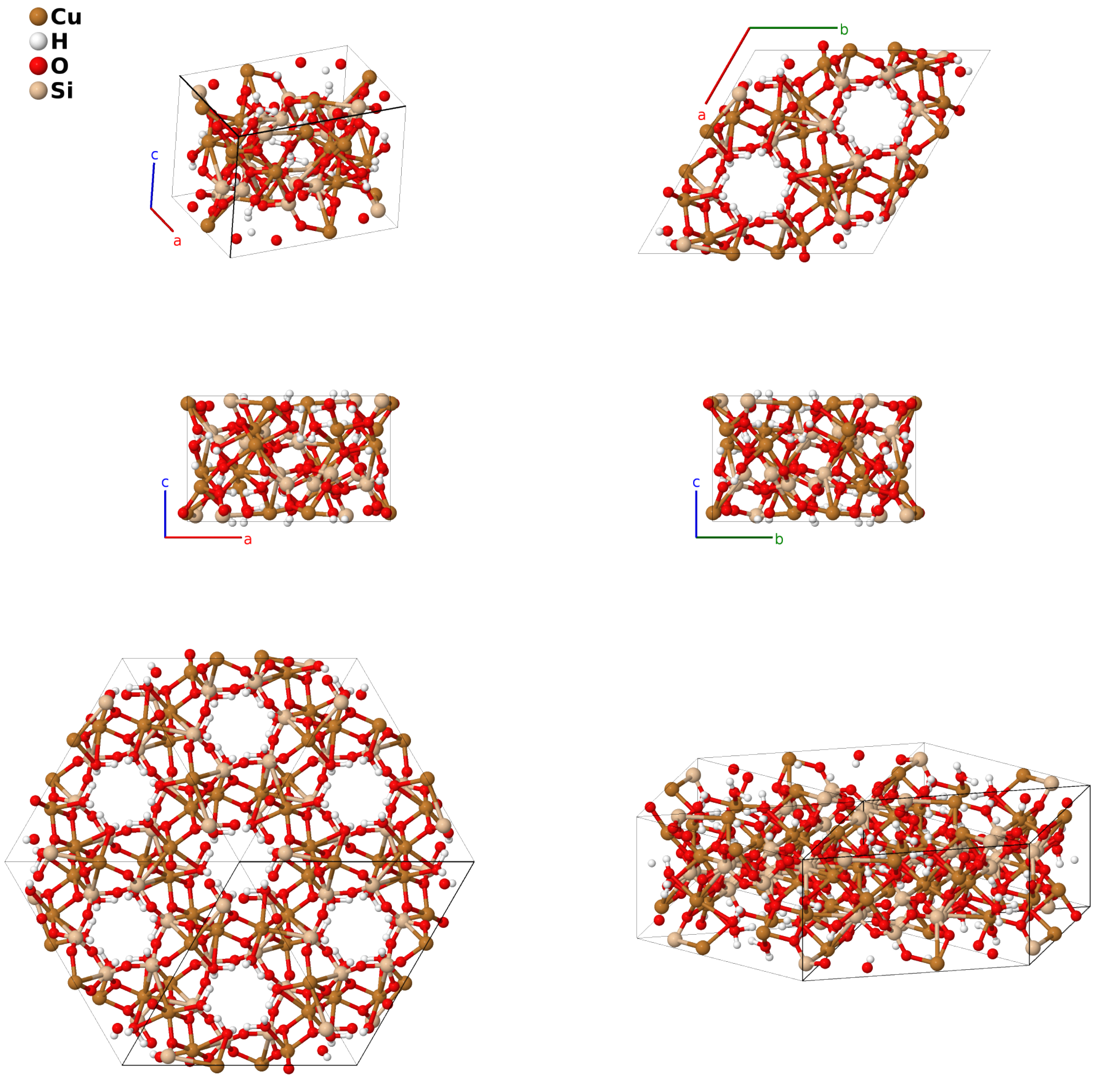
https://aflow.org/p/4C7V

https://aflow.org/p/AB2C4D_hR48_148_f_2f_4f_f-001



Prototype $Cu_6H_{12}O_{24}Si_6$

AFLOW prototype label AB2C4D_hR48_148_f_2f_4f_f-001

Mineral name dioptase

ICSD 100077

Pearson symbol hR48

Space group number 148

Space group symbol $R\bar{3}$

AFLOW prototype command `aflow --proto=AB2C4D_hR48_148_f_2f_4f_f-001`
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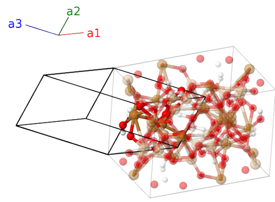
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

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



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)	Cu 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)	Cu 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)	Cu 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)	Cu 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)	Cu 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)	Cu 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)	H I
$\mathbf{B_8}$	=	$z_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_2 - y_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	H I
$\mathbf{B_9}$	=	$y_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 + y_2 - 2z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	H I
$\mathbf{B_{10}}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 - 2y_2 + z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	H I
$\mathbf{B_{11}}$	=	$-z_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_2 - z_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_2 - y_2 - z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	H I
$\mathbf{B_{12}}$	=	$-y_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 + y_2 - 2z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	H I
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	H II

$\mathbf{B_{14}}$	$=$	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(y_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	H II
$\mathbf{B_{15}}$	$=$	$y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	H II
$\mathbf{B_{16}}$	$=$	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	H II
$\mathbf{B_{17}}$	$=$	$-z_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(y_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	H II
$\mathbf{B_{18}}$	$=$	$-y_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	H II
$\mathbf{B_{19}}$	$=$	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{20}}$	$=$	$z_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(y_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{21}}$	$=$	$y_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{22}}$	$=$	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{23}}$	$=$	$-z_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(y_4 - z_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{24}}$	$=$	$-y_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_4 - y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{25}}$	$=$	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_5 - 2y_5 + z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B_{26}}$	$=$	$z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(y_5 - z_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_5 - y_5 - z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B_{27}}$	$=$	$y_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B_{28}}$	$=$	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_5 - 2y_5 + z_5)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B_{29}}$	$=$	$-z_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - y_5\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(y_5 - z_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_5 - y_5 - z_5)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B_{30}}$	$=$	$-y_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_5 - y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B_{31}}$	$=$	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B_{32}}$	$=$	$z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B_{33}}$	$=$	$y_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B_{34}}$	$=$	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B_{35}}$	$=$	$-z_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - y_6\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B_{36}}$	$=$	$-y_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B_{37}}$	$=$	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 - 2y_7 + z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(6f)	O IV

$\mathbf{B_{38}}$	=	$z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + y_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_7 - y_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(6f)	O IV
$\mathbf{B_{39}}$	=	$y_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 + y_7 - 2z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(6f)	O IV
$\mathbf{B_{40}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 - 2y_7 + z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(6f)	O IV
$\mathbf{B_{41}}$	=	$-z_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - y_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_7 - y_7 - z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(6f)	O IV
$\mathbf{B_{42}}$	=	$-y_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 + y_7 - 2z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(6f)	O IV
$\mathbf{B_{43}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - z_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_8 - 2y_8 + z_8)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_8 + y_8 + z_8)\,\hat{\mathbf{z}}$	(6f)	Si I
$\mathbf{B_{44}}$	=	$z_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + y_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_8 - z_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_8 - y_8 - z_8)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_8 + y_8 + z_8)\,\hat{\mathbf{z}}$	(6f)	Si I
$\mathbf{B_{45}}$	=	$y_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_8 - y_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_8 + y_8 - 2z_8)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_8 + y_8 + z_8)\,\hat{\mathbf{z}}$	(6f)	Si I
$\mathbf{B_{46}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_8 - z_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_8 - 2y_8 + z_8)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_8 + y_8 + z_8)\,\hat{\mathbf{z}}$	(6f)	Si I
$\mathbf{B_{47}}$	=	$-z_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - y_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_8 - z_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_8 - y_8 - z_8)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_8 + y_8 + z_8)\,\hat{\mathbf{z}}$	(6f)	Si I
$\mathbf{B_{48}}$	=	$-y_8\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - y_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_8 + y_8 - 2z_8)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_8 + y_8 + z_8)\,\hat{\mathbf{z}}$	(6f)	Si I

References

[1] P. H. Ribbe, G. V. Gibbs, and M. M. Hamil, *A refinement of the structure of dioptase, $Cu_6[Si_6O_{18}]\cdot 6H_2O$*, Am. Mineral. **62**, 807–188 (1977).

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).