Mg$_3$TeO$_6$ Structure: A3B6C_hR20_148_f_2f_ab-001

https://aflow.org/p/K70X

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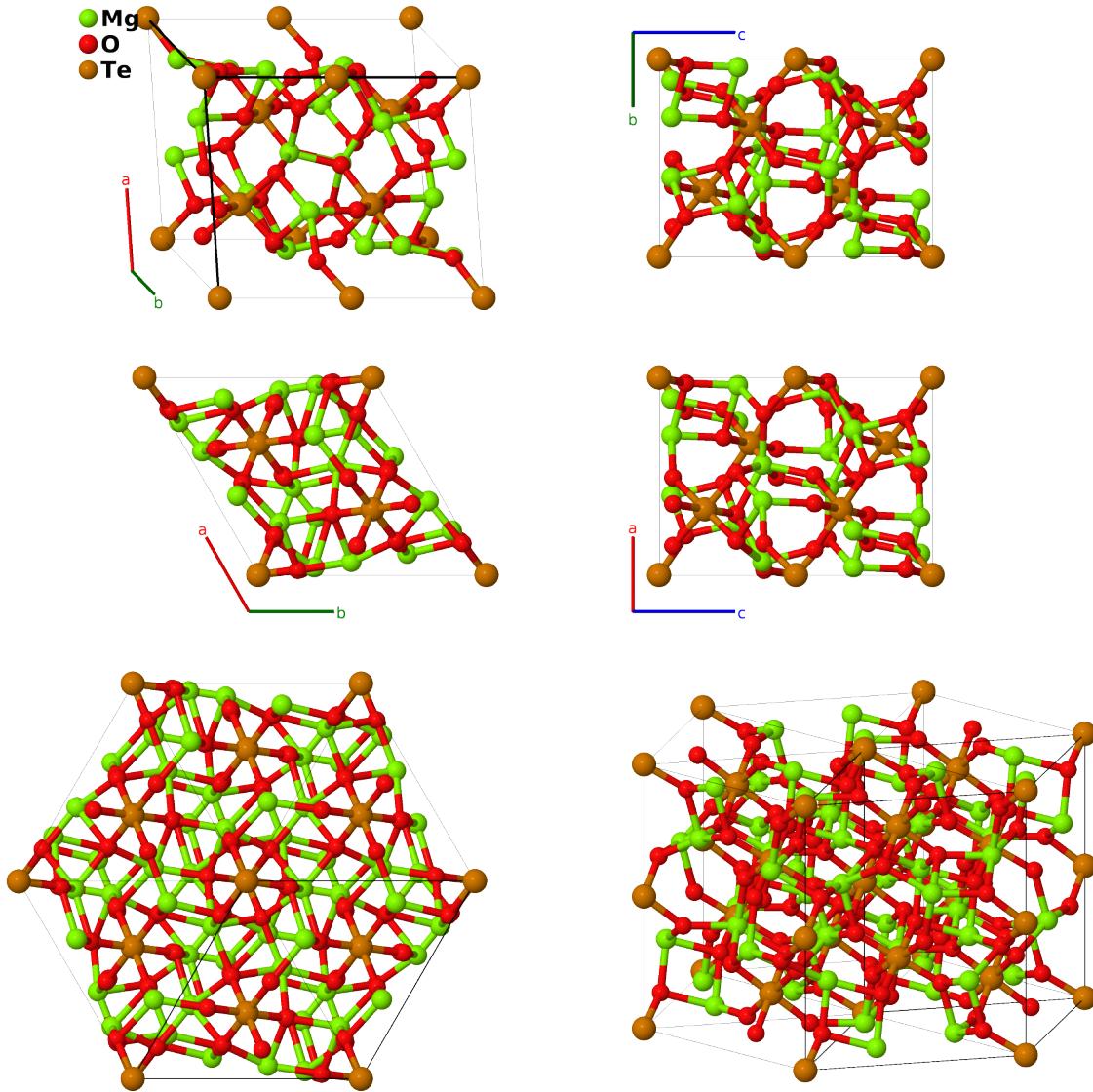
Prototype	Mg$_3$O$_6$Te
AFLOW prototype label	A3B6C_hR20_148_f_2f_ab-001
ICSD	23611
Pearson symbol	hR20
Space group number	148
Space group symbol	$R\bar{3}$

AFLOW prototype command `aflow --proto=A3B6C_hR20_148_f_2f_ab-001`
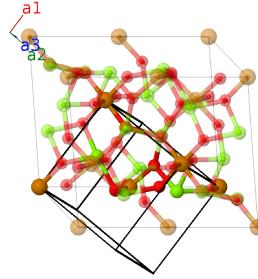$$\texttt{--params=}a, c/a, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$$

Other compounds with this structure

Bi_3DyO_6, Bi_3ErO_6, Bi_3LuO_6, Bi_3YO_6, Ca_3UO_6, La_3ScO_6, Li_3AlH_6, Li_3AlO_6, Li_3CuF_6, Li_3FeF_6, Li_3VF_6, Mg_3SbO_6, Mn_3TeO_6, Mn_3WO_6

- Hexagonal settings of this structure can be obtained with the option `--hex`.

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
$\mathbf{B_1}$	=	0	=	0	(1a)	Te I
$\mathbf{B_2}$	=	$\frac{1}{2}\mathbf{a_1} + \frac{1}{2}\mathbf{a_2} + \frac{1}{2}\mathbf{a_3}$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Te II
$\mathbf{B_3}$	=	$x_3\mathbf{a_1} + y_3\mathbf{a_2} + z_3\mathbf{a_3}$	=	$\frac{1}{2}a(x_3-z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3-2y_3+z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c(x_3+y_3+z_3)\,\hat{\mathbf{z}}$	(6f)	Mg I
$\mathbf{B_4}$	=	$z_3\mathbf{a_1} + x_3\mathbf{a_2} + y_3\mathbf{a_3}$	=	$-\frac{1}{2}a(y_3-z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3-y_3-z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c(x_3+y_3+z_3)\,\hat{\mathbf{z}}$	(6f)	Mg I
$\mathbf{B_5}$	=	$y_3\mathbf{a_1} + z_3\mathbf{a_2} + x_3\mathbf{a_3}$	=	$-\frac{1}{2}a(x_3-y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3+y_3-2z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c(x_3+y_3+z_3)\,\hat{\mathbf{z}}$	(6f)	Mg I
$\mathbf{B_6}$	=	$-x_3\mathbf{a_1} - y_3\mathbf{a_2} - z_3\mathbf{a_3}$	=	$-\frac{1}{2}a(x_3-z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3-2y_3+z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c(x_3+y_3+z_3)\,\hat{\mathbf{z}}$	(6f)	Mg I
$\mathbf{B_7}$	=	$-z_3\mathbf{a_1} - x_3\mathbf{a_2} - y_3\mathbf{a_3}$	=	$\frac{1}{2}a(y_3-z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_3-y_3-z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c(x_3+y_3+z_3)\,\hat{\mathbf{z}}$	(6f)	Mg I
$\mathbf{B_8}$	=	$-y_3\mathbf{a_1} - z_3\mathbf{a_2} - x_3\mathbf{a_3}$	=	$\frac{1}{2}a(x_3-y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3+y_3-2z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c(x_3+y_3+z_3)\,\hat{\mathbf{z}}$	(6f)	Mg I
$\mathbf{B_9}$	=	$x_4\mathbf{a_1} + y_4\mathbf{a_2} + z_4\mathbf{a_3}$	=	$\frac{1}{2}a(x_4-z_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4-2y_4+z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c(x_4+y_4+z_4)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{10}}$	=	$z_4\mathbf{a_1} + x_4\mathbf{a_2} + y_4\mathbf{a_3}$	=	$-\frac{1}{2}a(y_4-z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_4-y_4-z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c(x_4+y_4+z_4)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{11}}$	=	$y_4\mathbf{a_1} + z_4\mathbf{a_2} + x_4\mathbf{a_3}$	=	$-\frac{1}{2}a(x_4-y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4+y_4-2z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c(x_4+y_4+z_4)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{12}}$	=	$-x_4\mathbf{a_1} - y_4\mathbf{a_2} - z_4\mathbf{a_3}$	=	$-\frac{1}{2}a(x_4-z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4-2y_4+z_4)\,\hat{\mathbf{y}} - \frac{1}{3}c(x_4+y_4+z_4)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{13}}$	=	$-z_4\mathbf{a_1} - x_4\mathbf{a_2} - y_4\mathbf{a_3}$	=	$\frac{1}{2}a(y_4-z_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_4-y_4-z_4)\,\hat{\mathbf{y}} - \frac{1}{3}c(x_4+y_4+z_4)\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{14}}$	=	$-y_4\mathbf{a_1} - z_4\mathbf{a_2} - x_4\mathbf{a_3}$	=	$\frac{1}{2}a(x_4-y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4+y_4-2z_4)\,\hat{\mathbf{y}} - \frac{1}{3}c(x_4+y_4+z_4)\,\hat{\mathbf{z}}$	(6f)	O I

$$\mathbf{B_{15}} = x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3} = \tfrac{1}{2}a\left(x_5 - z_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_5 - 2y_5 + z_5\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_5 + y_5 + z_5\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{O II}$$

$$\mathbf{B_{16}} = z_5\,\mathbf{a_1} + x_5\,\mathbf{a_2} + y_5\,\mathbf{a_3} = -\tfrac{1}{2}a\left(y_5 - z_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_5 - y_5 - z_5\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_5 + y_5 + z_5\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{O II}$$

$$\mathbf{B_{17}} = y_5\,\mathbf{a_1} + z_5\,\mathbf{a_2} + x_5\,\mathbf{a_3} = -\tfrac{1}{2}a\left(x_5 - y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_5 + y_5 - 2z_5\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_5 + y_5 + z_5\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{O II}$$

$$\mathbf{B_{18}} = -x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} - z_5\,\mathbf{a_3} = -\tfrac{1}{2}a\left(x_5 - z_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_5 - 2y_5 + z_5\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_5 + y_5 + z_5\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{O II}$$

$$\mathbf{B_{19}} = -z_5\,\mathbf{a_1} - x_5\,\mathbf{a_2} - y_5\,\mathbf{a_3} = \tfrac{1}{2}a\left(y_5 - z_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(2x_5 - y_5 - z_5\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_5 + y_5 + z_5\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{O II}$$

$$\mathbf{B_{20}} = -y_5\,\mathbf{a_1} - z_5\,\mathbf{a_2} - x_5\,\mathbf{a_3} = \tfrac{1}{2}a\left(x_5 - y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_5 + y_5 - 2z_5\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_5 + y_5 + z_5\right)\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{O II}$$

References

[1] H. Schulz and G. Bayer, *A New Structure Type Mg₃TeO₆*, Naturwissenschaften **57**, 393 (1970), doi:10.1007/BF00599979.