

Mg₃TeO₆ Structure:

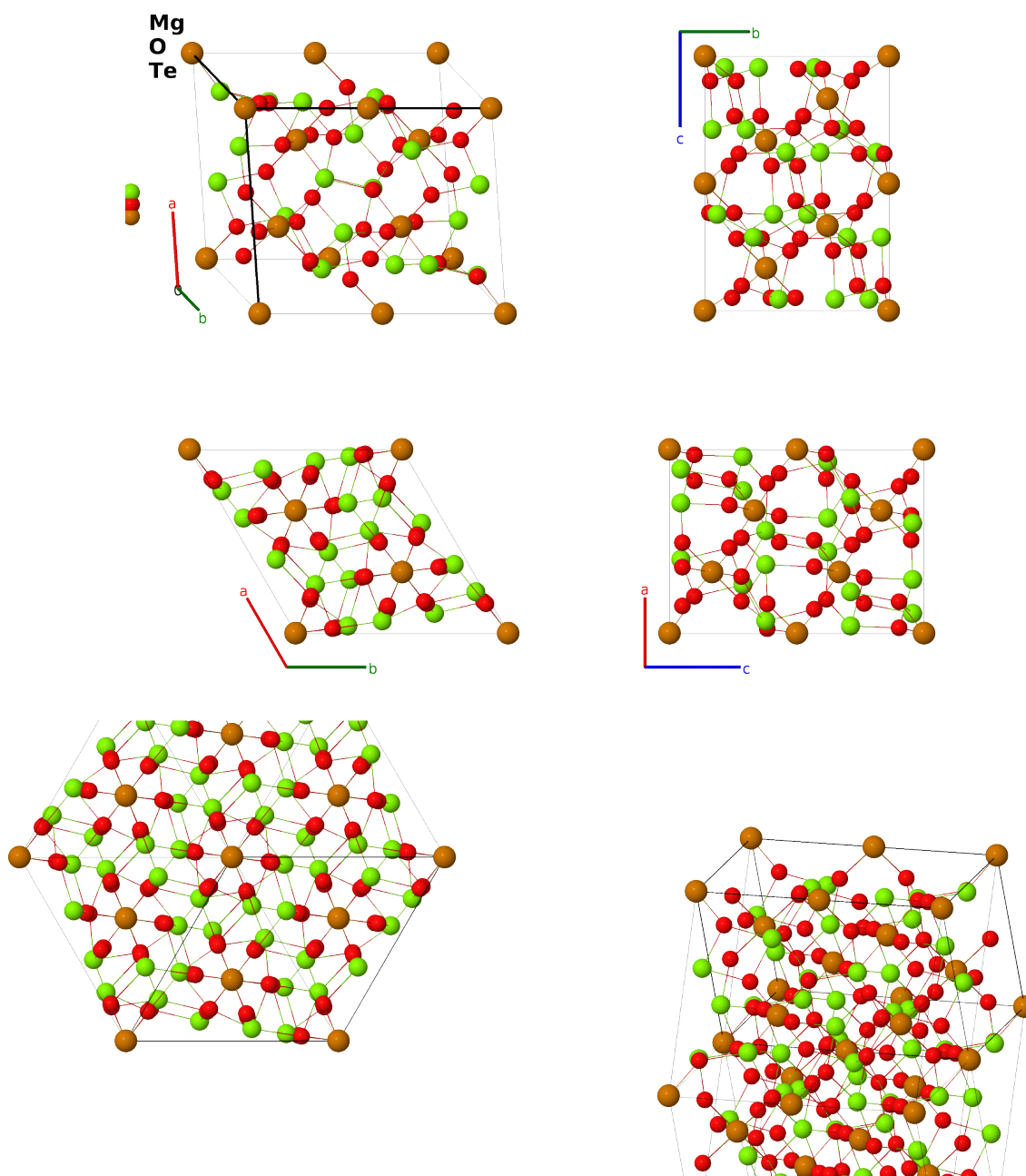
A3B6C_hR20_148_f_2f_ab-001

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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/K70X>

https://aflow.org/prototype-encyclopedia/A3B6C_hR20_148_f_2f_ab-001



Prototype

Mg₃O₆Te

AFLOW prototype label	A3B6C_hR20_148_f_2f_ab-001
ICSD	23611
CCDC	1599711
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 --params= $a, c/a, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

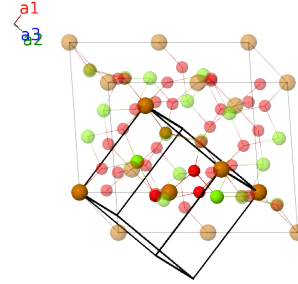
Other compounds with this structure

Bi₃DyO₆, Bi₃ErO₆, Bi₃LuO₆, Bi₃YO₆, Ca₃UO₆, La₃ScO₆, Li₃AlH₆, Li₃AlO₆, Li₃CuF₆, Li₃FeF₆, Li₃VF₆, Mg₃SbO₆, Mn₃TeO₆, Mn₃WO₆

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

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
$\mathbf{B}_1$	$= 0$	$=$	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

$$\begin{aligned}
\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) &\quad \text{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) &\quad \text{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) &\quad \text{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) &\quad \text{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) &\quad \text{O I} \\
\mathbf{B}_{15} &= 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) &\quad \text{O II} \\
\mathbf{B}_{16} &= 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) &\quad \text{O II} \\
\mathbf{B}_{17} &= 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) &\quad \text{O II} \\
\mathbf{B}_{18} &= -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) &\quad \text{O II} \\
\mathbf{B}_{19} &= -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) &\quad \text{O II} \\
\mathbf{B}_{20} &= -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) &\quad \text{O II}
\end{aligned}$$

References

- [1] H. Schulz and G. Bayer, *A New Structure Type Mg_3TeO_6* , *Naturwissenschaften* **57**, 393 (1970), doi:10.1007/BF00599979.

First cited in

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