

Muthmannite (AuAgTe₂) Structure: ABC2_mP8_10_ac_eh_mn-001

This structure previously used the label(s) `ABC2_mP8_10_ac_eh_mn`. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/ALSR>

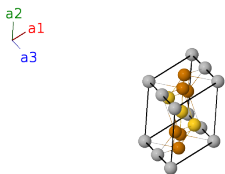
https://aflow.org/prototype-encyclopedia/ABC2_mP8_10_ac_eh_mn-001



Prototype	AgAuTe ₂
AFLOW prototype label	ABC2_mP8_10_ac_eh_mn-001
Mineral name	muthmannite
ICSD	55250
CCDC	1619567
Pearson symbol	mP8
Space group number	10
Space group symbol	$P2/m$
AFLOW prototype command	<code>aflow --proto=ABC2_mP8_10_ac_eh_mn-001</code> <code>--params=$a, b/a, c/a, \beta, x_5, z_5, x_6, z_6$</code>

Simple Monoclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	Ag I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \cos \beta \hat{\mathbf{x}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	Ag II
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	Au I
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} (a + c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	Au II
$\mathbf{B}_5$	$=$	$x_5 \mathbf{a}_1 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	Te I
$\mathbf{B}_6$	$=$	$-x_5 \mathbf{a}_1 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	Te I
$\mathbf{B}_7$	$=$	$x_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	Te II
$\mathbf{B}_8$	$=$	$-x_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	Te II

References

- [1] L. Bindi and C. Cipriani, *Ordered distribution of Au and Ag in the crystal structure of muthmannite, AuAgTe₂, a rare telluride from Sacarîmb, western Romania*, Am. Mineral. **89**, 1505–1509 (2004).

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043