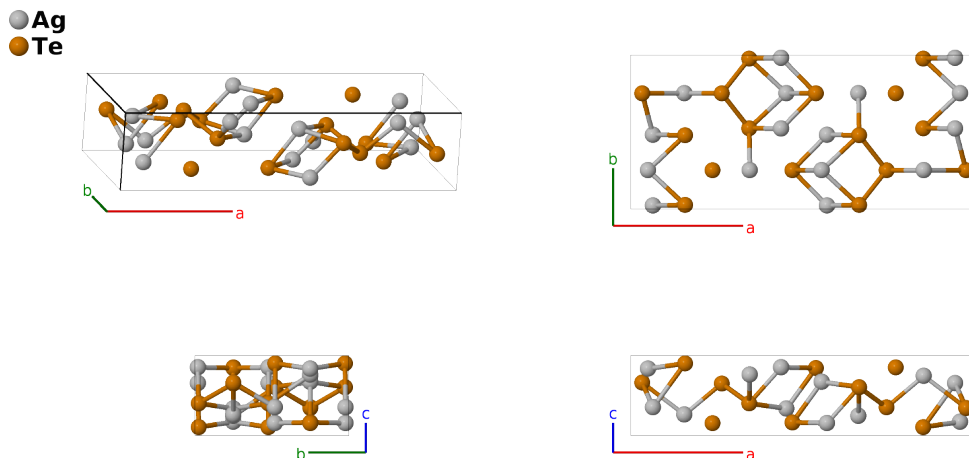


# Empressite (AgTe) Structure: AB\_oP32\_62\_2cd\_2cd-001

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.

<https://aflow.org/p/JH5H>

[https://aflow.org/p/AB\\_oP32\\_62\\_2cd\\_2cd-001](https://aflow.org/p/AB_oP32_62_2cd_2cd-001)



<b>Prototype</b>	AgTe
<b>AFLOW prototype label</b>	AB_oP32_62_2cd_2cd-001
<b>Mineral name</b>	empressite
<b>ICSD</b>	55237
<b>Pearson symbol</b>	oP32
<b>Space group number</b>	62
<b>Space group symbol</b>	<i>Pnma</i>
<b>AFLOW prototype command</b>	aflow --proto=AB_oP32_62_2cd_2cd-001 --params= <i>a, b/a, c/a, x<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub></i>

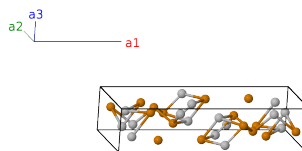
- (Bindi, 2004) give the structural information in the *Pmnb* setting of space group #62. We used FINDSYM to transform this to the standard *Pnma* setting.

## Simple Orthorhombic primitive vectors

$$\mathbf{a}_1 = a \hat{x}$$

$$\mathbf{a}_2 = b \hat{y}$$

$$\mathbf{a}_3 = c \hat{z}$$



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Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	Ag I
$\mathbf{B}_2$	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Ag I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	Ag I
$\mathbf{B}_4$	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Ag I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	Ag II
$\mathbf{B}_6$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Ag II
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	Ag II
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Ag II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	Te I
$\mathbf{B}_{10}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Te I
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	Te I
$\mathbf{B}_{12}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Te I
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	Te II
$\mathbf{B}_{14}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Te II
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c)	Te II
$\mathbf{B}_{16}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Te II
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8d)	Ag III
$\mathbf{B}_{18}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Ag III
$\mathbf{B}_{19}$	$= -x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8d)	Ag III
$\mathbf{B}_{20}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Ag III
$\mathbf{B}_{21}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8d)	Ag III
$\mathbf{B}_{22}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Ag III
$\mathbf{B}_{23}$	$= x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8d)	Ag III
$\mathbf{B}_{24}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Ag III
$\mathbf{B}_{25}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8d)	Te III
$\mathbf{B}_{26}$	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Te III
$\mathbf{B}_{27}$	$= -x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8d)	Te III
$\mathbf{B}_{28}$	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Te III
$\mathbf{B}_{29}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8d)	Te III
$\mathbf{B}_{30}$	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Te III
$\mathbf{B}_{31}$	$= x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8d)	Te III

$$\mathbf{B}_{32} = \begin{matrix} - (x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + \\ (z_6 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a (x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_6 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}} \quad (8d) \quad \text{Te III}$$

## References

- [1] L. Bindi, P. G. Spry, and C. Cipriani, *Empressite, AgTe, from the Empress-Josephine mine, Colorado, U.S.A.: Composition, physical properties, and determination of the crystal structure*, Am. Mineral. **89**, 1043–1047 (2004).

## Found in

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