Adamite [$Zn_2(AsO_4)(OH)$, $H2_7$] Structure: ABC5D2_oP36_58_g_g_3gh_eg-001

This structure originally had the label `ABC5D2_oP36_58_g_g_3gh_eg`. Calls to that address will be redirected here.

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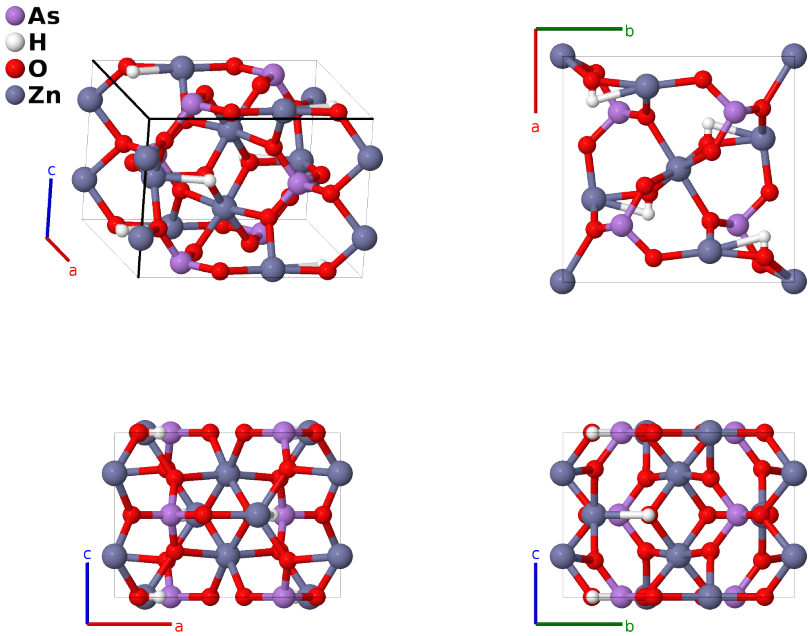
https://aflow.org/p/YE34

https://aflow.org/p/ABC5D2_oP36_58_g_g_3gh_eg-001



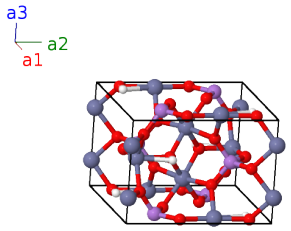
Prototype	$AsHO_5Zn_2$
AFLOW prototype label	ABC5D2_oP36_58_g_g_3gh_eg-001
***Strukturbericht* designation**	$H2_7$
Mineral name	adamite
ICSD	34868
Pearson symbol	oP36
Space group number	58
Space group symbol	$Pnnm$
AFLOW prototype command	`aflow --proto=ABC5D2_oP36_58_g_g_3gh_eg-001 --params=`$a, b/a, c/a, z_1, x_2, y_2, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, x_8, y_8, z_8$

Other compounds with this structure
$Cu_2(AsO_4)(OH)$, $Cu_2(PO_4)(OH)$

- This structure was originally determined by (Kokorous, 1937) and designated $H2_7$ by (Gottfried, 1940). (Hill, 1976) refined the structure, including the positions of the hydrogen atoms in the OH radical.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(4e)	Zn I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Zn I
$\mathbf{B_3}$	=	$-z_1\,\mathbf{a}_3$	=	$-cz_1\,\hat{\mathbf{z}}$	(4e)	Zn I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Zn I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}}$	(4g)	As I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}}$	(4g)	As I
$\mathbf{B_7}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	As I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	As I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}}$	(4g)	H I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}}$	(4g)	H I
$\mathbf{B_{11}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	H I
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	H I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B_{15}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B_{19}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	O II
$\mathbf{B_{20}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	O II
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}}$	(4g)	O III
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}}$	(4g)	O III
$\mathbf{B_{23}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	O III

$\mathbf{B_{24}}$	=	$\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	O III
$\mathbf{B_{25}}$	=	$x_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2$	=	$ax_7\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}$	(4g)	Zn II
$\mathbf{B_{26}}$	=	$-x_7\,\mathbf{a}_1-y_7\,\mathbf{a}_2$	=	$-ax_7\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}$	(4g)	Zn II
$\mathbf{B_{27}}$	=	$-\left(x_7-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_7+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	Zn II
$\mathbf{B_{28}}$	=	$\left(x_7+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_7-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	Zn II
$\mathbf{B_{29}}$	=	$x_8\,\mathbf{a}_1+y_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8h)	O IV
$\mathbf{B_{30}}$	=	$-x_8\,\mathbf{a}_1-y_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8h)	O IV
$\mathbf{B_{31}}$	=	$-\left(x_8-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_8+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_8-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_8+\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8h)	O IV
$\mathbf{B_{32}}$	=	$\left(x_8+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_8-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_8+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_8-\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8h)	O IV
$\mathbf{B_{33}}$	=	$-x_8\,\mathbf{a}_1-y_8\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(8h)	O IV
$\mathbf{B_{34}}$	=	$x_8\,\mathbf{a}_1+y_8\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(8h)	O IV
$\mathbf{B_{35}}$	=	$\left(x_8+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_8-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_8+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_8-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8h)	O IV
$\mathbf{B_{36}}$	=	$-\left(x_8-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_8+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_8-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_8+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8h)	O IV

References

[1] R. J. Hill, *The crystal structure and infrared properties of adamite*, Am. Mineral. **61**, 979–986 (1976).

[2] P. Kokorous, *Über die Struktur von Adamin*, Z. Kristallgr. **96**, 417–434 (1937), doi:10.1524/zkri.1937.96.1.417.

[3] C. Gottfried, ed., *Strukturbericht Band V 1937* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1940).