Modderite (CoAs) Structure: AB_oP8_33_a_a-001

This structure originally had the label `AB_oP8_33_a_a`. Calls to that address will be redirected here.

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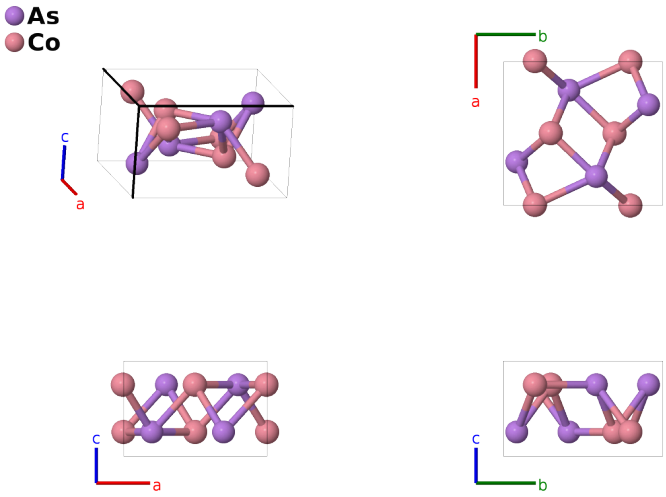
https://aflow.org/p/8Z7Q

https://aflow.org/p/AB_oP8_33_a_a-001



Prototype	AsCo
AFLOW prototype label	AB_oP8_33_a_a-001
Mineral name	modderite
ICSD	48027
Pearson symbol	oP8
Space group number	33
Space group symbol	$Pna2_1$
AFLOW prototype command	`aflow --proto=AB_oP8_33_a_a-001 --params=`$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2$

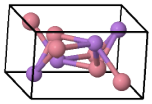
Other compounds with this structure
FeAs

- Space group $Pna2_1$ #33 allows an arbitrary origin for the z-axis, which is set here by taking $z_2 = 1/4$.
- When $z_1 = z_2 = 1/4$, the space group becomes $Pnma$ #62 and the structure is equivalent to MnP ($B31$).
- (Lyman, 1984) sets $z_1 = 0.2506$, so this condition is almost fulfilled.
- (Lyman, 1984) lists both space groups for both CoAs and FeAs, and prefers the MnP structure for these compounds.

- AFLOW also places this structure in space group *Pnma*, and only predicts the lower symmetry structure if we lower the native tolerance using
- aflow --proto=AB_oP8_33_a_a --tolerance=0.001 --params=a,b/,c/a,x_1,y_1,z_1,x_2,y_2,z_2 .

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	As I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	As I
$\mathbf{B_3}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	As I
$\mathbf{B_4}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	As I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	Co I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Co I
$\mathbf{B_7}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	Co I
$\mathbf{B_8}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Co I

References

[1] P. S. Lyman and C. T. Prewitt, *Room- and high-pressure crystal chemistry of CoAs and FeAs*, Acta Crystallogr. Sect. B **40**, 14–20 (1984), doi:10.1107/S0108768184001695.