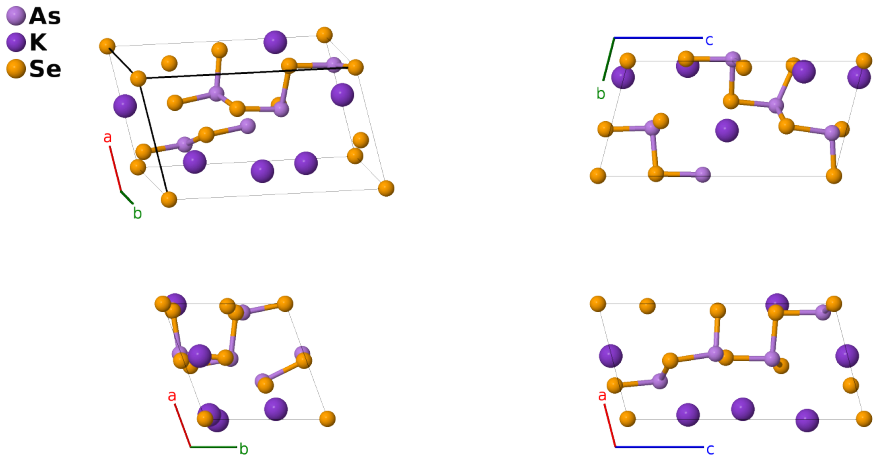
$AsKSe_2$ ($P1$) Structure: ABC2_aP16_1_4a_4a_8a-001

This structure originally had the label `ABC2_aP16_1_4a_4a_8a`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/GZNE

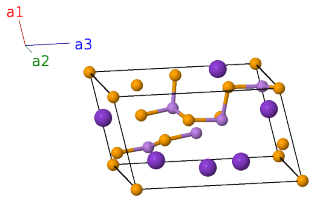
https://aflow.org/p/ABC2_aP16_1_4a_4a_8a-001



Prototype	$AsKSe_2$
AFLOW prototype label	ABC2_aP16_1_4a_4a_8a-001
ICSD	65297
Pearson symbol	aP16
Space group number	1
Space group symbol	$P1$
AFLOW prototype command	`aflow --proto=ABC2_aP16_1_4a_4a_8a-001 --params=`$a, b/a, c/a, \alpha, \beta, \gamma, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}$

Triclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\cos\gamma\,\hat{\mathbf{x}} + b\sin\gamma\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c_x\,\hat{\mathbf{x}} + c_y\,\hat{\mathbf{y}} + c_z\,\hat{\mathbf{z}}$$
$$c_x = c\cos\beta$$
$$c_y = c(\cos\alpha - \cos\beta\cos\gamma)/\sin\gamma$$
$$c_z = \sqrt{c^2 - c_x^2 - c_y^2}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + by_1\cos\gamma + c_x z_1)\,\hat{\mathbf{x}} + (by_1\sin\gamma + c_y z_1)\,\hat{\mathbf{y}} + c_z z_1\,\hat{\mathbf{z}}$	(1a)	As I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + by_2\cos\gamma + c_x z_2)\,\hat{\mathbf{x}} + (by_2\sin\gamma + c_y z_2)\,\hat{\mathbf{y}} + c_z z_2\,\hat{\mathbf{z}}$	(1a)	As II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + by_3\cos\gamma + c_x z_3)\,\hat{\mathbf{x}} + (by_3\sin\gamma + c_y z_3)\,\hat{\mathbf{y}} + c_z z_3\,\hat{\mathbf{z}}$	(1a)	As III
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + by_4\cos\gamma + c_x z_4)\,\hat{\mathbf{x}} + (by_4\sin\gamma + c_y z_4)\,\hat{\mathbf{y}} + c_z z_4\,\hat{\mathbf{z}}$	(1a)	As IV
$\mathbf{B_5}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + by_5\cos\gamma + c_x z_5)\,\hat{\mathbf{x}} + (by_5\sin\gamma + c_y z_5)\,\hat{\mathbf{y}} + c_z z_5\,\hat{\mathbf{z}}$	(1a)	K I
$\mathbf{B_6}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + by_6\cos\gamma + c_x z_6)\,\hat{\mathbf{x}} + (by_6\sin\gamma + c_y z_6)\,\hat{\mathbf{y}} + c_z z_6\,\hat{\mathbf{z}}$	(1a)	K II
$\mathbf{B_7}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + by_7\cos\gamma + c_x z_7)\,\hat{\mathbf{x}} + (by_7\sin\gamma + c_y z_7)\,\hat{\mathbf{y}} + c_z z_7\,\hat{\mathbf{z}}$	(1a)	K III
$\mathbf{B_8}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + by_8\cos\gamma + c_x z_8)\,\hat{\mathbf{x}} + (by_8\sin\gamma + c_y z_8)\,\hat{\mathbf{y}} + c_z z_8\,\hat{\mathbf{z}}$	(1a)	K IV
$\mathbf{B_9}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + by_9\cos\gamma + c_x z_9)\,\hat{\mathbf{x}} + (by_9\sin\gamma + c_y z_9)\,\hat{\mathbf{y}} + c_z z_9\,\hat{\mathbf{z}}$	(1a)	Se I
$\mathbf{B_{10}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + by_{10}\cos\gamma + c_x z_{10})\,\hat{\mathbf{x}} + (by_{10}\sin\gamma + c_y z_{10})\,\hat{\mathbf{y}} + c_z z_{10}\,\hat{\mathbf{z}}$	(1a)	Se II
$\mathbf{B_{11}}$	=	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + by_{11}\cos\gamma + c_x z_{11})\,\hat{\mathbf{x}} + (by_{11}\sin\gamma + c_y z_{11})\,\hat{\mathbf{y}} + c_z z_{11}\,\hat{\mathbf{z}}$	(1a)	Se III
$\mathbf{B_{12}}$	=	$x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$(ax_{12} + by_{12}\cos\gamma + c_x z_{12})\,\hat{\mathbf{x}} + (by_{12}\sin\gamma + c_y z_{12})\,\hat{\mathbf{y}} + c_z z_{12}\,\hat{\mathbf{z}}$	(1a)	Se IV
$\mathbf{B_{13}}$	=	$x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$(ax_{13} + by_{13}\cos\gamma + c_x z_{13})\,\hat{\mathbf{x}} + (by_{13}\sin\gamma + c_y z_{13})\,\hat{\mathbf{y}} + c_z z_{13}\,\hat{\mathbf{z}}$	(1a)	Se V
$\mathbf{B_{14}}$	=	$x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$	=	$(ax_{14} + by_{14}\cos\gamma + c_x z_{14})\,\hat{\mathbf{x}} + (by_{14}\sin\gamma + c_y z_{14})\,\hat{\mathbf{y}} + c_z z_{14}\,\hat{\mathbf{z}}$	(1a)	Se VI
$\mathbf{B_{15}}$	=	$x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	=	$(ax_{15} + by_{15}\cos\gamma + c_x z_{15})\,\hat{\mathbf{x}} + (by_{15}\sin\gamma + c_y z_{15})\,\hat{\mathbf{y}} + c_z z_{15}\,\hat{\mathbf{z}}$	(1a)	Se VII
$\mathbf{B_{16}}$	=	$x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3$	=	$(ax_{16} + by_{16}\cos\gamma + c_x z_{16})\,\hat{\mathbf{x}} + (by_{16}\sin\gamma + c_y z_{16})\,\hat{\mathbf{y}} + c_z z_{16}\,\hat{\mathbf{z}}$	(1a)	Se VIII

References

[1] W. S. Sheldrick and H.-J. Häusler, *Zur Kenntnis von Alkalimetaselenoarseniten Darstellung und Kristallstrukturen von $MAsSe_2$, M = K, Rb, Cs*, Z. Anorganische und Allgemeine Chemie **561**, 139–148 (1988), doi:10.1002/zaac.19885610115.

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.