α-monoclinic Selenium Structure: A_mP32_14_8e-002

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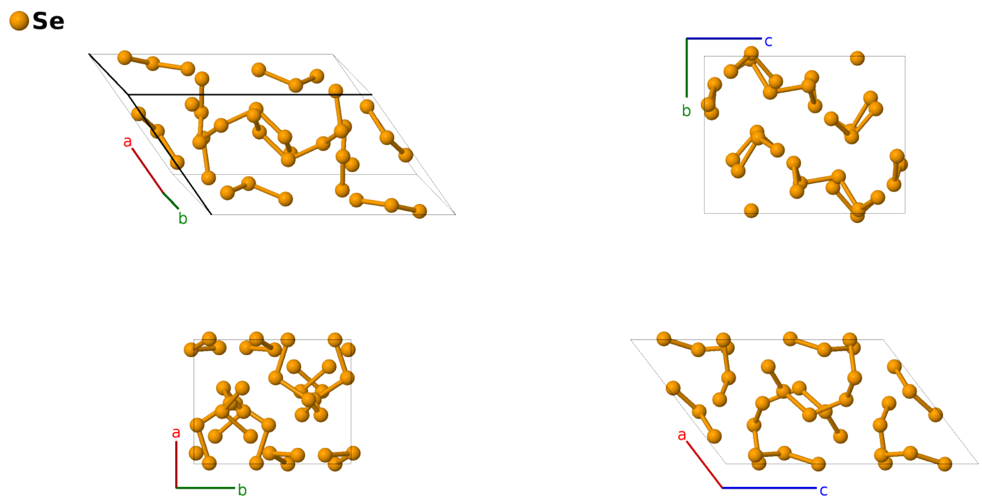
https://aflow.org/p/VEFR

https://aflow.org/p/A_mP32_14_8e-002

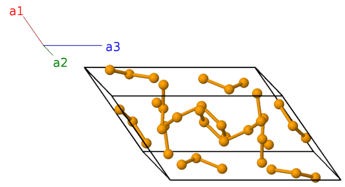


Prototype	Se
AFLOW prototype label	A_mP32_14_8e-002
ICSD	2718
Pearson symbol	mP32
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	`aflow --proto=A_mP32_14_8e-002` `--params=`$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

- There is no consistency in the naming convention of selenium structures, and we have generally tried to avoid the Greek-letter-monoclinic form in favor of something less confusing. This structure, however, has no other name that we are aware of, so we follow (Cherin, 1972) and call it α-monoclinic selenium, a designation followed by (Donohue, 1974).
- Although this structure has the same AFLOW prototype label, A_mP32_14_e, as β-Se (A_l), the two structures are distinct. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_1 + c\left(z_1-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se I
$\mathbf{B_4}$	=	$x_1\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_1 + c\left(z_1+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_2 + c\left(z_2-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se II
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se II
$\mathbf{B_8}$	=	$x_2\,\mathbf{a}_1 - \left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_2 + c\left(z_2+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se III
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_3 + c\left(z_3-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se III
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se III
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1 - \left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se III
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se IV
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_4-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se IV
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se IV
$\mathbf{B_{16}}$	=	$x_4\,\mathbf{a}_1 - \left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se IV
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se V
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 + \left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5 + c\left(z_5-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_5-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se V
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se V
$\mathbf{B_{20}}$	=	$x_5\,\mathbf{a}_1 - \left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5 + c\left(z_5+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se V
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se VI
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 + \left(y_6+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_6 + c\left(z_6-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_6-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se VI
$\mathbf{B_{23}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se VI

$\mathbf{B_{24}}$	=	$x_6\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se VI
$\mathbf{B_{25}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se VII
$\mathbf{B_{26}}$	=	$-x_7\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_7 + c\left(z_7 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se VII
$\mathbf{B_{27}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se VII
$\mathbf{B_{28}}$	=	$x_7\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_7 + c\left(z_7 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se VII
$\mathbf{B_{29}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se VIII
$\mathbf{B_{30}}$	=	$-x_8\,\mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_8 + c\left(z_8 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se VIII
$\mathbf{B_{31}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se VIII
$\mathbf{B_{32}}$	=	$x_8\,\mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_8 + c\left(z_8 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Se VIII

References

[1] P. Cherin and P. Unger, *Refinement of the Crystal Structure of α-Monoclinic Se*, Acta Crystallogr. Sect. B **28**, 313–317 (1927), doi:10.1107/S0567740872002249.

Found in

[1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).