High-pressure Te Structure: A_mP4_4_2a-001

This structure previously used the label(s) `A_mP4_4_2a`. Calls to these addresses will be redirected here.

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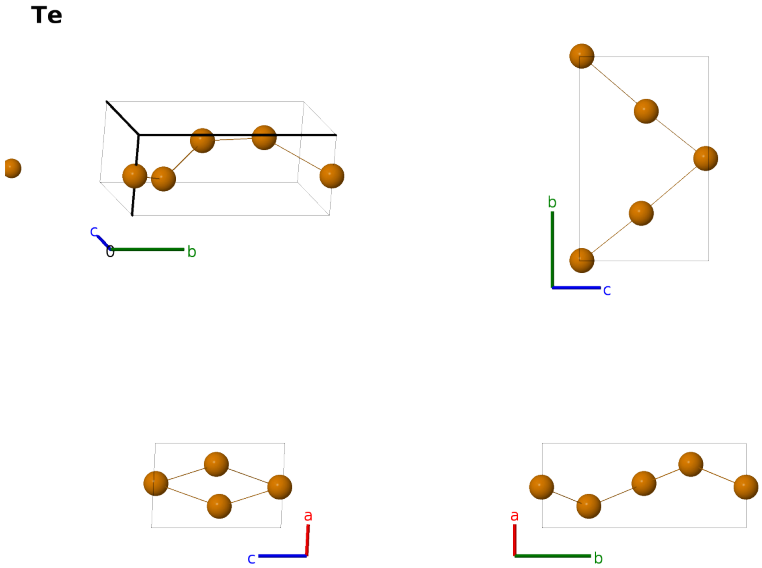
https://aflow.org/prototype-encyclopedia/H0F1

https://aflow.org/prototype-encyclopedia/A_mP4_4_2a-001



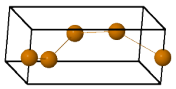
Prototype	Te
AFLOW prototype label	A_mP4_4_2a-001
ICSD	52501
CCDC	1617246
Pearson symbol	mP4
Space group number	4
Space group symbol	$P2_1$
AFLOW prototype command	`aflow --proto=A_mP4_4_2a-001 --params=`$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2$

- This is a high-pressure phase of tellurium, stable in the 4-7 GPa range. The ground state of Te appears to be in the γSe ($A8$) structure.

- We use the data taken by (Aoki, 1980) at 4.5 GPa.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(2a)	Te I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-\left(ax_1 + cz_1\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(2a)	Te I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(2a)	Te II
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-\left(ax_2 + cz_2\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(2a)	Te II

References

[1] K. Aoki, O. Shimomura, and S. Minomura, *Crystal Structure of the High-Pressure Phase of Tellurium*, J. Phys. Soc. Japan **48**, 551–556 (1980), doi:10.1143/JPSJ.48.551.

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