

High-pressure Te Structure: A_mP4_4_2a-001

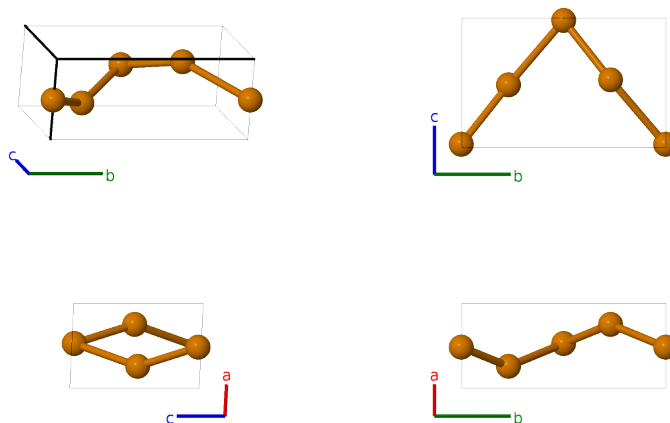
This structure originally had the label **A_mP4.4.2a**. Calls to that address will be redirected here.

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<https://aflow.org/p/H0F1>

https://aflow.org/p/A_mP4_4_2a-001

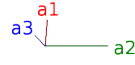
● Te



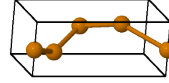
Prototype	Te
AFLOW prototype label	A_mP4.4.2a-001
ICSD	52501
Pearson symbol	mP4
Space group number	4
Space group symbol	$P2_1$
AFLOW prototype command	<code>aflow --proto=A_mP4_4_2a-001 --params=a,b/a,c/a,β,x_1,y_1,z_1,x_2,y_2,z_2</code>

- 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 γ Se (A8) structure.
- We use the data taken by (Aoki, 1980) at 4.5 GPa.

Simple Monoclinic primitive vectors



$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
 \end{aligned}$$



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	$-x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(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	$-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(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.