High-pressure CdTe Structure: AB_oP2_25_a_b-001

This structure previously used the label(s) `AB_oP2_25_b_a`. Calls to these addresses will be redirected here.

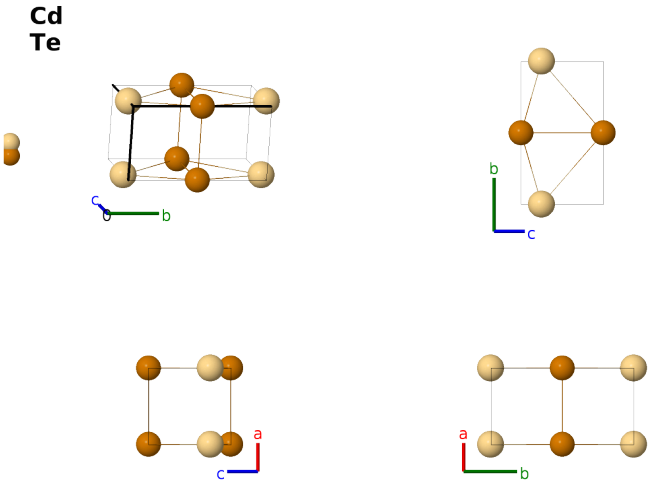
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

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

https://aflow.org/prototype-encyclopedia/AB_oP2_25_a_b-001



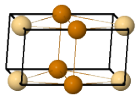
Prototype	CdTe
AFLOW prototype label	AB_oP2_25_a_b-001
ICSD	108237
CCDC	1665901
Pearson symbol	oP2
Space group number	25
Space group symbol	$Pmm2$
AFLOW prototype command	`aflow --proto=AB_oP2_25_a_b-001 --params=`$a, b/a, c/a, z_1, z_2$

Other compounds with this structure
GaAs (HP)

- This is a high-pressure phase of CdTe. We use the data given for a pressure of 19.3 GPa.
- Space group $Pmm2$ #25 allows are arbitary origin in the z-direction. Here we chose it to put the tellurium atom at the origin.

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(1a)	Cd I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(1b)	Te I

References

[1] J. Z. Hu, *A New High Pressure Phase of CdTe*, Solid State Commun. **63**, 471–474 (1987), doi:10.1016/0038-1098(87)90273-0.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. 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