Ta_2H Structure: AB2_oC6_21_a_k-001

This structure originally had the label `AB2_oC6_21_a_k`. Calls to that address will be redirected here.

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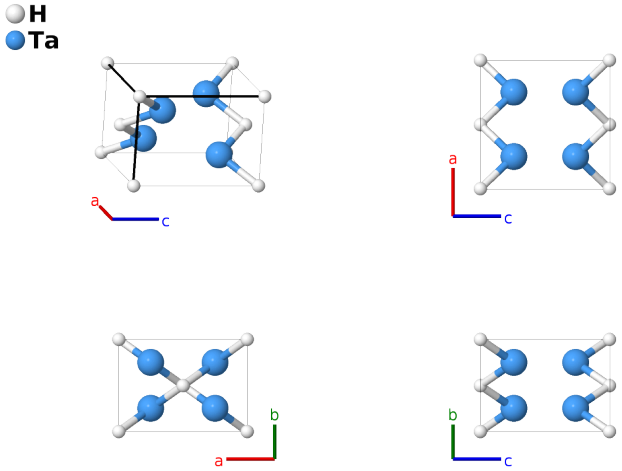
https://aflow.org/p/6XPU

https://aflow.org/p/AB2_oC6_21_a_k-001

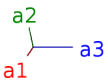


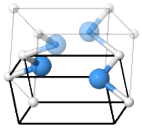
Prototype	HTa_2
AFLOW prototype label	AB2_oC6_21_a_k-001
ICSD	41774
Pearson symbol	oC6
Space group number	21
Space group symbol	$C222$
AFLOW prototype command	`aflow --proto=AB2_oC6_21_a_k-001 --params=`$a, b/a, c/a, z_2$

- Th_2H and $HoSb_2$ share the same AFLOW prototype label, AB2_oC6_21_a_k. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$





Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	H I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4k)	Ta I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4k)	Ta I

References

[1] H. Asano, Y. Ishikawa, and M. Hirabayashi, *Single-crystal X-ray diffraction study on the hydrogen ordering in Ta_2H*, J. Appl. Crystal. **11**, 681–683 (1978), doi:10.1107/S0021889878014260.

Found in

[1] P. Villars, *FeS Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database).