$HoSb_2$ Structure: AB2_oC6_21_a_k-002

This structure originally had the label `AB2_oC6_21_a_k.HoSb2`. Calls to that address will be redirected here.

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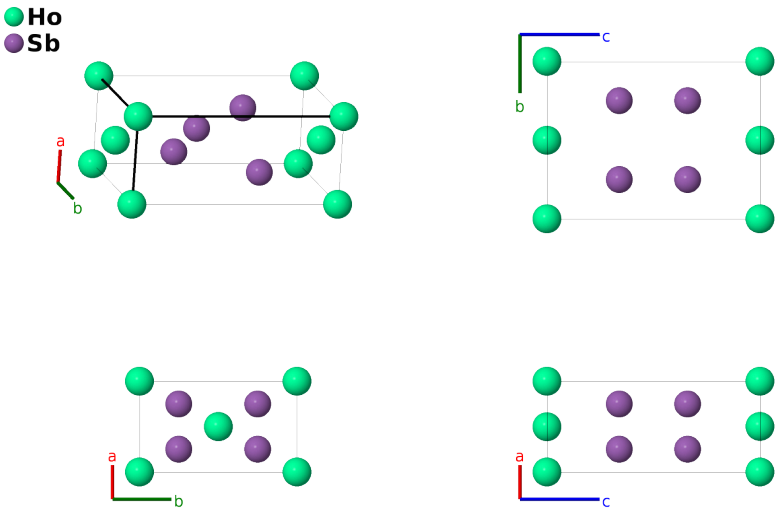
https://aflow.org/p/DD5U

https://aflow.org/p/AB2_oC6_21_a_k-002

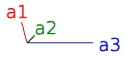


Prototype	$HoSb_2$
AFLOW prototype label	AB2_oC6_21_a_k-002
ICSD	26220
Pearson symbol	oC6
Space group number	21
Space group symbol	$C222$
AFLOW prototype command	`aflow --proto=AB2_oC6_21_a_k-002 --params=`$a, b/a, c/a, z_2$

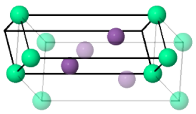
Other compounds with this structure
$LuSb_2$, YSb_2, $DySb_2$ (HT), $GdSb_2$ (HT), $TbSb_2$ (HT)

- Measurements were performed at a pressure of 65 kBar
- The primitive unit cell is nearly hexagonal
- The author states "We are well aware of the fact that the structure presented here may indeed be only a subcell of the true structure."
- $HoSb_2$ and Ta_2H 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



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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ho 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)	Sb 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)	Sb I

References

[1] Q. Johnson, *The Crystal Structure of High-Pressure Synthesized Holmium Diantimonde*, Inorg. Chem. **10**, 2089–2090 (1971), doi:10.1021/ic50103a059.

Found in

[1] M. N. Abdusaljamov, O. R. Burnashev, and K. E. Mironov, *The Ho-Sb Alloy System*, J. Less-Common Met. **102**, L19–L22 (1984), doi:10.1016/0022-5088(84)90403-X.