Henryite [$(Ag_{1.48}Cu_{1.44}Fe_{0.32})Te_2$] Structure: AB3C2_cP12_224_a_d_b-001

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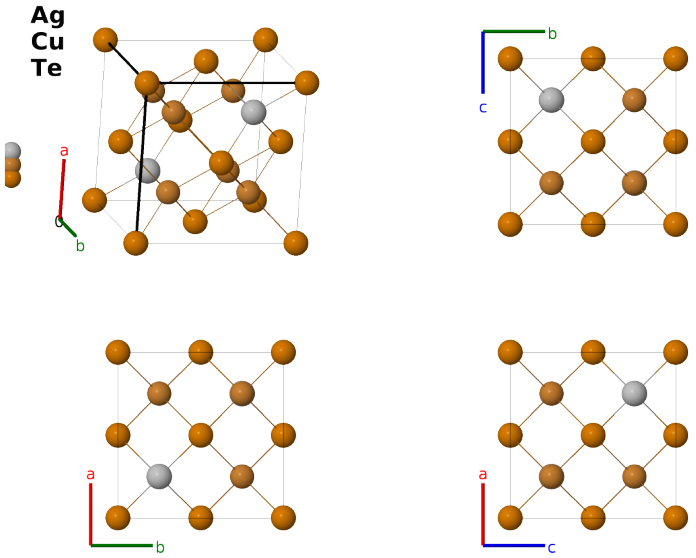
https://aflow.org/prototype-encyclopedia/SDL9

https://aflow.org/prototype-encyclopedia/AB3C2_cP12_224_a_d_b-001



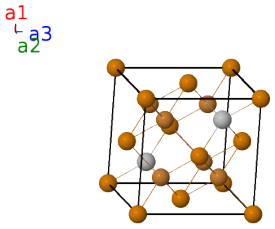
Prototype	$(Ag_{1.48}Cu_{1.44}Fe_{0.32})Te_2$
AFLOW prototype label	AB3C2_cP12_224_a_d_b-001
Mineral name	henryite
ICSD	239361
CCDC	1710367
Pearson symbol	cP12
Space group number	224
Space group symbol	$Pn\bar{3}m$
AFLOW prototype command	`aflow --proto=AB3C2_cP12_224_a_d_b-001 --params=`a

- The ICSD entries for (Bindi, 2014, ICSD 23936) and (Cohen-Addad, 1971 ICSD 5165) are identical except for the rounding of the site occupation. We reference the newer version as it is more accessible to the user.
- The (2a) and (6d) sites are 37% silver, 48% copper, and 0.8% iron, giving the observed stoichiometry.
- We arbitrarily assign silver to the (2a) site and copper to the (6c) cite.

- Both papers put the structure in space group $Fd\bar{3}c$ #228, with the atoms occupying the (16a), (32c), and (48d) sites, however these sites are identical to the (2a), (4b) and (6d) sites of space group $Pn\bar{3}m$ #224 with $a_{224} = 1/2a_{228}$. AFLOW favors the smaller unit cell, so we assign this structure to space group #224.
- In addtion, if the (2a) and (6c) sites are fully alloyed, this becomes the fluorite ($C1$) structure.
- The reported structure can be viewed by clicking the "load block" button and entering a value of 12.2 Ångström.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(2a)	Ag I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(2a)	Ag I
$\mathbf{B_3}$	=	0	=	0	(4b)	Te I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(4b)	Te I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	Te I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	Te I
$\mathbf{B_7}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(6d)	Cu I
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(6d)	Cu I
$\mathbf{B_9}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(6d)	Cu I
$\mathbf{B_{10}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(6d)	Cu I
$\mathbf{B_{11}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(6d)	Cu I
$\mathbf{B_{12}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(6d)	Cu I

References

[1] L. Bindi, *Chemical and structural characterization of henryite, $(Cu,Ag)_{3+x}Te_2$ (x 0.40): A new structure type in the (Ag)-Cu-Te system*, Solid State Sciences **38**, 108–111 (2014), doi:10.1016/j.solidstatesciences.2014.10.008.

[2] C. Cohen-Addad, *Etude du compose Te (O H)6 par diffraction des neutrons*, Bull. Soc. Franc. Mineral. Cristall. **94**, 172–174 (1971).

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