Tennantite ($Cu_{12}As_4S_{13}$) Structure: A4B24C13_cI82_217_c_deg_ag-001

This structure originally had the label `A4B24C13_cI82_217_c_deg_ag`. Calls to that address will be redirected here.

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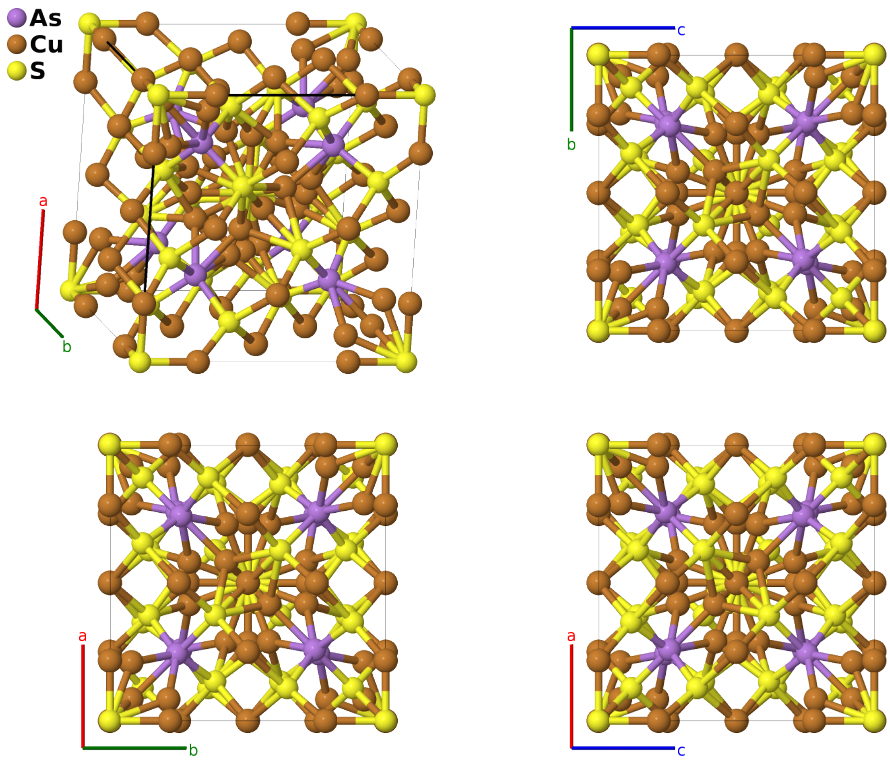
https://aflow.org/p/5PAV

https://aflow.org/p/A4B24C13_cI82_217_c_deg_ag-001



Prototype	$AsCu_{12}S_{13}$
AFLOW prototype label	A4B24C13_cI82_217_c_deg_ag-001
Mineral name	tennantite
ICSD	403458
Pearson symbol	cI82
Space group number	217
Space group symbol	$I\bar{4}3m$
AFLOW prototype command	`aflow --proto=A4B24C13_cI82_217_c_deg_ag-001 --params=`$a, x_2, x_4, x_5, z_5, x_6, z_6$

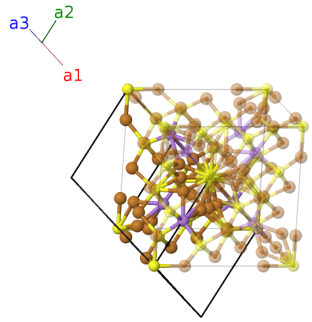
Other compounds with this structure

$Cu_{14}Sb_4S_{13}$ (tetrahedrite)

- The Cu-II (12e) site is only occupied 75.8% of the time, and the Cu-III site is occupied 12.1% of the time, so that these sites only contain twelve atoms between them.
- Searching (Downs, 2003) shows that natural samples often have antimony substituting for arsenic. The antimony structures (tetrahedrites) contain higher concentrations of copper.

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	S I
$\mathbf{B_2}$	=	$2x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	As I
$\mathbf{B_3}$	=	$-2x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	As I
$\mathbf{B_4}$	=	$-2x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	As I
$\mathbf{B_5}$	=	$-2x_2\,\mathbf{a}_1$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	As I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(12d)	Cu I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12d)	Cu I
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12d)	Cu I
$\mathbf{B_9}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(12d)	Cu I
$\mathbf{B_{10}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(12d)	Cu I
$\mathbf{B_{11}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(12d)	Cu I
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}$	(12e)	Cu II
$\mathbf{B_{13}}$	=	$-x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}$	(12e)	Cu II
$\mathbf{B_{14}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{y}}$	(12e)	Cu II
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{y}}$	(12e)	Cu II
$\mathbf{B_{16}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{z}}$	(12e)	Cu II
$\mathbf{B_{17}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{z}}$	(12e)	Cu II
$\mathbf{B_{18}}$	=	$(x_5 + z_5)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + 2x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(24g)	Cu III
$\mathbf{B_{19}}$	=	$-(x_5 - z_5)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - 2x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(24g)	Cu III
$\mathbf{B_{20}}$	=	$(x_5 - z_5)\,\mathbf{a}_1 - (x_5 + z_5)\,\mathbf{a}_2$	=	$-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(24g)	Cu III
$\mathbf{B_{21}}$	=	$-(x_5 + z_5)\,\mathbf{a}_1 + (x_5 - z_5)\,\mathbf{a}_2$	=	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(24g)	Cu III
$\mathbf{B_{22}}$	=	$2x_5\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + (x_5 + z_5)\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(24g)	Cu III

$\mathbf{B_{23}}$	=	$-2x_5\,\mathbf{a}_1 - (x_5 - z_5)\;\mathbf{a}_2 - (x_5 - z_5)\;\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(24g)	Cu III
$\mathbf{B_{24}}$	=	$(x_5 - z_5)\;\mathbf{a}_2 - (x_5 + z_5)\;\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(24g)	Cu III
$\mathbf{B_{25}}$	=	$-(x_5 + z_5)\;\mathbf{a}_2 + (x_5 - z_5)\;\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(24g)	Cu III
$\mathbf{B_{26}}$	=	$(x_5 + z_5)\;\mathbf{a}_1 + 2x_5\,\mathbf{a}_2 + (x_5 + z_5)\;\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(24g)	Cu III
$\mathbf{B_{27}}$	=	$-(x_5 - z_5)\;\mathbf{a}_1 - 2x_5\,\mathbf{a}_2 - (x_5 - z_5)\;\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(24g)	Cu III
$\mathbf{B_{28}}$	=	$-(x_5 + z_5)\;\mathbf{a}_1 + (x_5 - z_5)\;\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(24g)	Cu III
$\mathbf{B_{29}}$	=	$(x_5 - z_5)\;\mathbf{a}_1 - (x_5 + z_5)\;\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(24g)	Cu III
$\mathbf{B_{30}}$	=	$(x_6 + z_6)\;\mathbf{a}_1 + (x_6 + z_6)\;\mathbf{a}_2 + 2x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + az_6\,\hat{\mathbf{z}}$	(24g)	S II
$\mathbf{B_{31}}$	=	$-(x_6 - z_6)\;\mathbf{a}_1 - (x_6 - z_6)\;\mathbf{a}_2 - 2x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + az_6\,\hat{\mathbf{z}}$	(24g)	S II
$\mathbf{B_{32}}$	=	$(x_6 - z_6)\;\mathbf{a}_1 - (x_6 + z_6)\;\mathbf{a}_2$	=	$-ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - az_6\,\hat{\mathbf{z}}$	(24g)	S II
$\mathbf{B_{33}}$	=	$-(x_6 + z_6)\;\mathbf{a}_1 + (x_6 - z_6)\;\mathbf{a}_2$	=	$ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - az_6\,\hat{\mathbf{z}}$	(24g)	S II
$\mathbf{B_{34}}$	=	$2x_6\,\mathbf{a}_1 + (x_6 + z_6)\;\mathbf{a}_2 + (x_6 + z_6)\;\mathbf{a}_3$	=	$az_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(24g)	S II
$\mathbf{B_{35}}$	=	$-2x_6\,\mathbf{a}_1 - (x_6 - z_6)\;\mathbf{a}_2 - (x_6 - z_6)\;\mathbf{a}_3$	=	$az_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(24g)	S II
$\mathbf{B_{36}}$	=	$(x_6 - z_6)\;\mathbf{a}_2 - (x_6 + z_6)\;\mathbf{a}_3$	=	$-az_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(24g)	S II
$\mathbf{B_{37}}$	=	$-(x_6 + z_6)\;\mathbf{a}_2 + (x_6 - z_6)\;\mathbf{a}_3$	=	$-az_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(24g)	S II
$\mathbf{B_{38}}$	=	$(x_6 + z_6)\;\mathbf{a}_1 + 2x_6\,\mathbf{a}_2 + (x_6 + z_6)\;\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + az_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(24g)	S II
$\mathbf{B_{39}}$	=	$-(x_6 - z_6)\;\mathbf{a}_1 - 2x_6\,\mathbf{a}_2 - (x_6 - z_6)\;\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + az_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(24g)	S II
$\mathbf{B_{40}}$	=	$-(x_6 + z_6)\;\mathbf{a}_1 + (x_6 - z_6)\;\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - az_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(24g)	S II
$\mathbf{B_{41}}$	=	$(x_6 - z_6)\;\mathbf{a}_1 - (x_6 + z_6)\;\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - az_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(24g)	S II

References

[1] A. A. Yaroslavzev, A. V. Mironov, A. N. Kuznetsov, A. P. Dudka, and O. N. Khrykina, *Tennantite: multi-temperature crystal structure, phase transition and electronic structure of synthetic $Cu_{12}As_4S_{13}$*, Acta Crystallogr. Sect. B **75**, 634–642 (2019), doi:10.1107/S2052520619007595.

[2] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).