Rhombohedral $CuTi_2S_4$ Structure: AB4C2_hR28_166_2c_2c2h_abh-001

This structure previously used the label(s) `AB4C2_hR28_166_2c_2c2h_abh`. Calls to these addresses will be redirected here.

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- 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.

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https://aflow.org/prototype-encyclopedia/8BYU

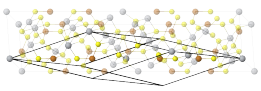
https://aflow.org/prototype-encyclopedia/AB4C2_hR28_166_2c_2c2h_abh-001

Prototype	CuS_4Ti_2
AFLOW prototype label	AB4C2_hR28_166_2c_2c2h_abh-001
ICSD	170228
CCDC	1685824
Pearson symbol	hR28
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=AB4C2_hR28_166_2c_2c2h_abh-001 --params=`$a, c/a, x_3, x_4, x_5, x_6, x_7, z_7, x_8, z_8, x_9, z_9$

- $CuTi_2S_4$ can also be found in a spinel phase.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Ti I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Ti II

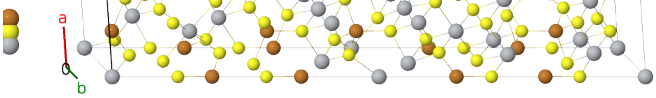
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	Cu I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Cu I
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	Cu II
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	Cu II
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$cx_5\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_8}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-cx_5\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_9}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$cx_6\,\hat{\mathbf{z}}$	(2c)	S II
$\mathbf{B_{10}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-cx_6\,\hat{\mathbf{z}}$	(2c)	S II
$\mathbf{B_{11}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	S III
$\mathbf{B_{12}}$	=	$z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	S III
$\mathbf{B_{13}}$	=	$x_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	S III
$\mathbf{B_{14}}$	=	$-z_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	S III
$\mathbf{B_{15}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	S III
$\mathbf{B_{16}}$	=	$-x_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_7 - z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	S III
$\mathbf{B_{17}}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - z_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_8 - z_8)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_8 + z_8)\,\hat{\mathbf{z}}$	(6h)	S IV
$\mathbf{B_{18}}$	=	$z_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_8 - z_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_8 - z_8)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_8 + z_8)\,\hat{\mathbf{z}}$	(6h)	S IV
$\mathbf{B_{19}}$	=	$x_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_8 - z_8)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_8 + z_8)\,\hat{\mathbf{z}}$	(6h)	S IV
$\mathbf{B_{20}}$	=	$-z_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - z_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_8 - z_8)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_8 + z_8)\,\hat{\mathbf{z}}$	(6h)	S IV
$\mathbf{B_{21}}$	=	$-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_8 - z_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_8 - z_8)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_8 + z_8)\,\hat{\mathbf{z}}$	(6h)	S IV
$\mathbf{B_{22}}$	=	$-x_8\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_8 - z_8)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_8 + z_8)\,\hat{\mathbf{z}}$	(6h)	S IV
$\mathbf{B_{23}}$	=	$x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_9 - z_9)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_9 - z_9)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_9 + z_9)\,\hat{\mathbf{z}}$	(6h)	Ti III
$\mathbf{B_{24}}$	=	$z_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + x_9\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_9 - z_9)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_9 - z_9)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_9 + z_9)\,\hat{\mathbf{z}}$	(6h)	Ti III
$\mathbf{B_{25}}$	=	$x_9\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + x_9\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_9 - z_9)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_9 + z_9)\,\hat{\mathbf{z}}$	(6h)	Ti III
$\mathbf{B_{26}}$	=	$-z_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - x_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_9 - z_9)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_9 - z_9)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_9 + z_9)\,\hat{\mathbf{z}}$	(6h)	Ti III
$\mathbf{B_{27}}$	=	$-x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_9 - z_9)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_9 - z_9)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_9 + z_9)\,\hat{\mathbf{z}}$	(6h)	Ti III
$\mathbf{B_{28}}$	=	$-x_9\,\mathbf{a}_1 - z_9\,\mathbf{a}_2 - x_9\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_9 - z_9)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_9 + z_9)\,\hat{\mathbf{z}}$	(6h)	Ti III

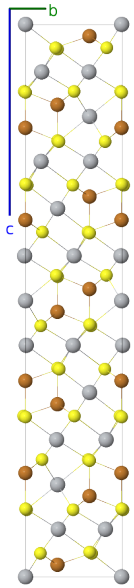
References

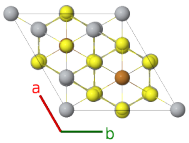
[1] N. Soheilnia, K. M. Kleinke, E. Dashjav, H. L. Cuthbert, J. E. Greedan, and H. Kleinke, *Crystal Structure and Physical Properties of a New $CuTi_2S_4$ Modification in Comparison to the Thiospinel*, Inorg. Chem. **43**, 6473–6478 (2004), doi:10.1021/ic0495113.

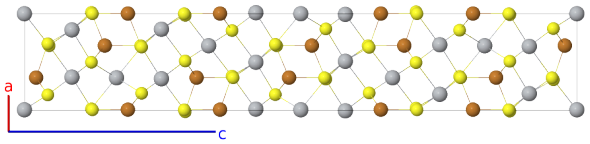
First cited in

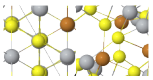
Cu
S
Ti











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