$CrCuS_2$ Structure: ABC2_hR4_160_a_a_2a-003

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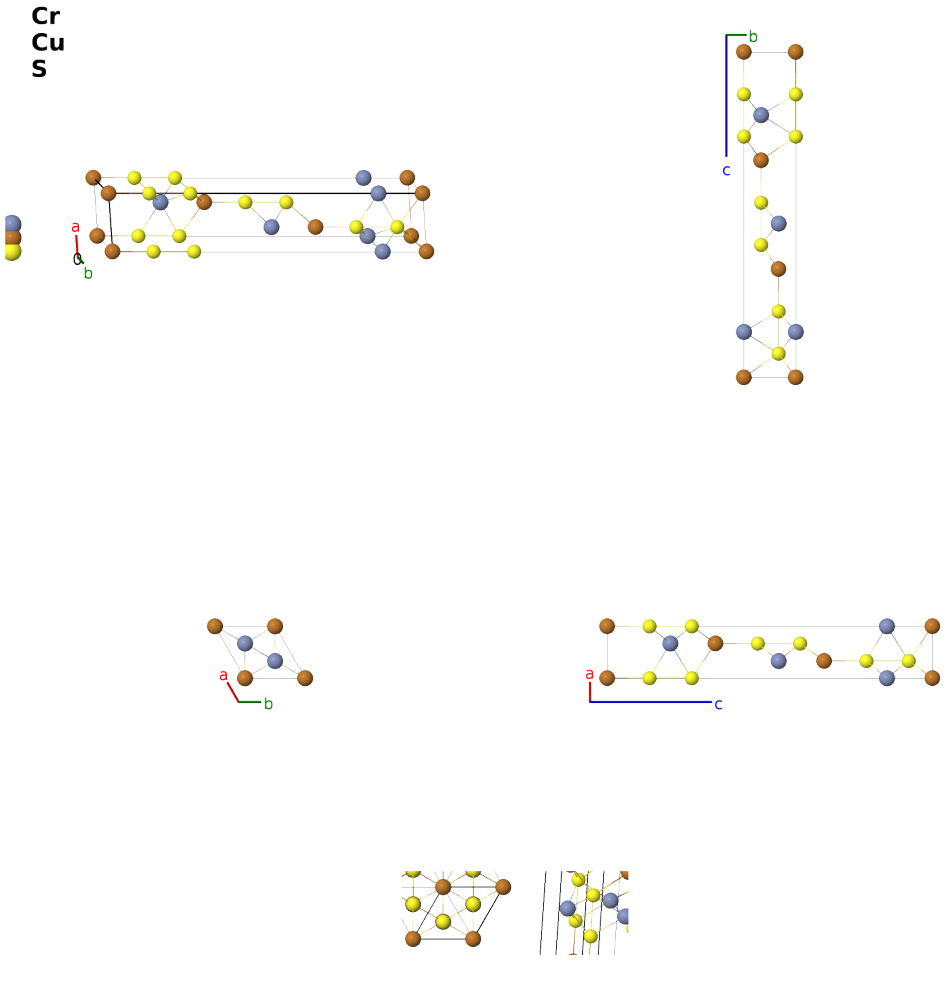
https://aflow.org/prototype-encyclopedia/BC9T

https://aflow.org/prototype-encyclopedia/ABC2_hR4_160_a_a_2a-003



Prototype	$CrCuS_2$
AFLOW prototype label	ABC2_hR4_160_a_a_2a-003
ICSD	25627
CCDC	1601277
Pearson symbol	hR4
Space group number	160
Space group symbol	$R3m$

AFLOW prototype command `aflow --proto=ABC2_hR4_160_a_a_2a-003 --params=`$a, c/a, x_1, x_2, x_3, x_4$

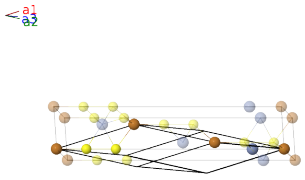
Other compounds with this structure

$AgCrS_2$, $AgCrSe_2$, $AgCuS_2$, $AgCuSe_2$, $AuCrS_2$, $CrCuSe_2$, $CrMoN_2$, $CrTlSe_2$, $CrWN_2$, $LiMoN_2$

- The ICSD uses $AgCrS_2$ to define the structure type.
- Space group $R3m$ #160 does not specify the origin of the z-axis. Here we choose $z_I = 0$ for the position of the chromium atom.
- α-CrOOH and $CrCuS_2$ have the same AFLOW prototype label, ABC2_hR4_160_a_a_2a. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(1a)	Cr I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(1a)	Cu I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(1a)	S I
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(1a)	S II

References

[1] H. Hahn and C. de Lorent, *Untersuchungen über ternäre Chalkogenide. XII. Über ternäre Chalkogenide des Chroms mit einwertigem Kupfer und Silber*, Z. Anorganische und Allgemeine Chemie **290**, 68–81 (1957), doi:10.1002/zaac.19572900108.

Found in

[1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).

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