CrS Structure: AB_mC8_15_a_e-003

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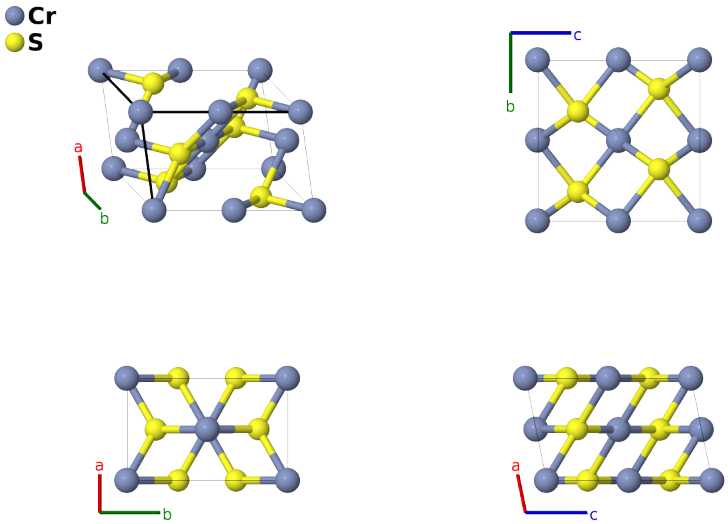
https://aflow.org/p/H6Z8

https://aflow.org/p/AB_mC8_15_a_e-003

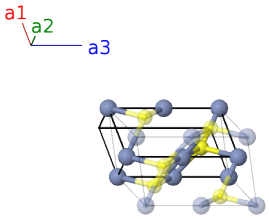


Prototype	CrS
AFLOW prototype label	AB_mC8_15_a_e-003
ICSD	16723
Pearson symbol	mC8
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=AB_mC8_15_a_e-003 --params=`$a, b/a, c/a, \beta, y_2$

- (Wyckoff, 1963) lists two structures for CrS. The first is this structure, where the sulfur (4e) site has 3% vacancies. The second is the NiAs ($B8_1$) structure. (Venkatraman, 1990) list this structure as the ground state and $B8_1$ has the high-temperature phase, with the transition occuring at 297K.

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Cr I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4a)	Cr I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	S I

References

[1] F. Jellinek, *The Structures of the Chromium Sulphides*, Acta Cryst. **10**, 620–628 (1957), doi:10.1107/S0365110X57002200.

[2] R. W. G. Wyckoff, *The Structure of Crystals*, vol. I (John Wiley & Sons, 1963), 2nd edn.

[3] M. Venkatraman and J. P. Neumann, *Binary Alloy Phase Diagrams* (ASM International, 1990), vol. 2, chap. Cr-S (Chromium-Sulfur), ii edn. T. B. Massalski, Ed.

Found in

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