Trigonal Cr_5S_6 Structure: A5B6_hP22_163_abcf_i-001
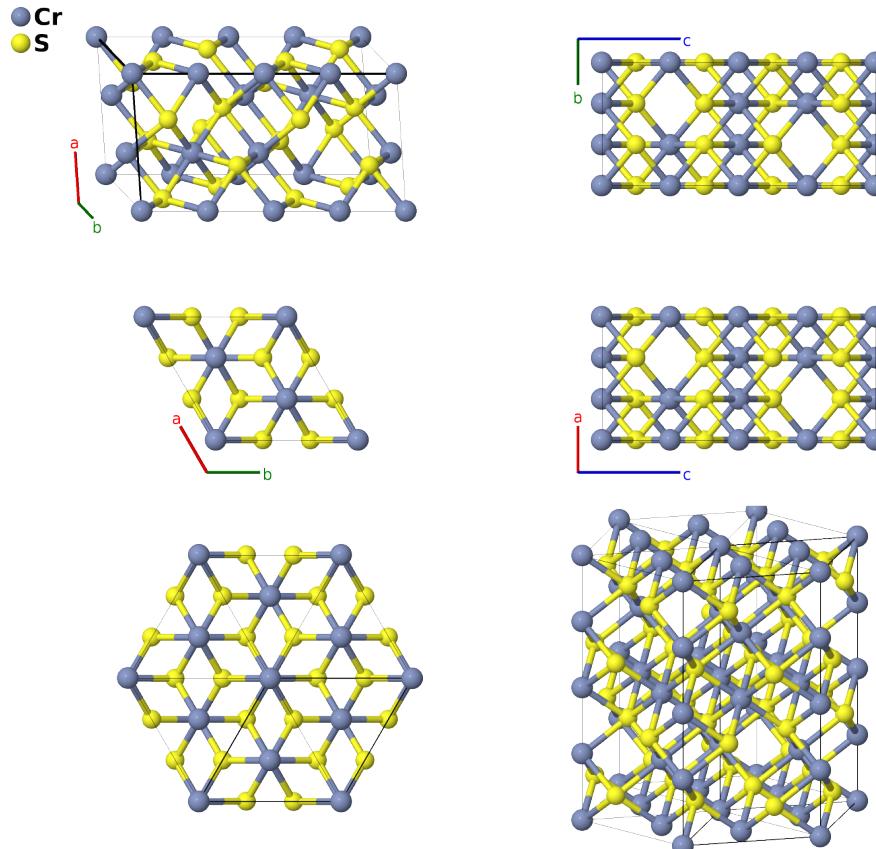
Prototype	Cr_5S_6
AFLOW prototype label	A5B6_hP22_163_abcf_i-001
ICSD	16719
Pearson symbol	hP22
Space group number	163
Space group symbol	$P\bar{3}1c$
AFLOW prototype command	aflow --proto=A5B6_hP22_163_abcf_i-001 --params=$a, c/a, z_4, x_5, y_5, z_5$

- (Jellinek, 1957) also has data for trigonal Cr_2S_3, which is generated from this structure by removing the Chromium atoms from the (2a) sites. (Venkatraman, 1990) lists the structure Cr_2S_3Cr, which is likely the same structure with possible vacancies on the (2a) sites. There is also a rhombohedral Cr_2S_3 structure found in both references.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
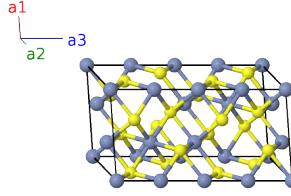
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$\tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{4}c\,\hat{\mathbf{z}}$	(2a)	Cr I
$\mathbf{B_2}$	$=$	$\tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{3}{4}c\,\hat{\mathbf{z}}$	(2a)	Cr I
$\mathbf{B_3}$	$=$	0	$=$	0	(2b)	Cr II
$\mathbf{B_4}$	$=$	$\tfrac{1}{2}\mathbf{a_3}$	$=$	$\tfrac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Cr II
$\mathbf{B_5}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Cr III
$\mathbf{B_6}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Cr III
$\mathbf{B_7}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + z_4\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4f)	Cr IV
$\mathbf{B_8}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	Cr IV
$\mathbf{B_9}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} - z_4\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4f)	Cr IV
$\mathbf{B_{10}}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	Cr IV
$\mathbf{B_{11}}$	$=$	$x_5\mathbf{a_1} + y_5\mathbf{a_2} + z_5\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_5 + y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B_{12}}$	$=$	$-y_5\mathbf{a_1} + \left(x_5 - y_5\right)\mathbf{a_2} + z_5\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_5 - 2y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B_{13}}$	$=$	$-\left(x_5 - y_5\right)\mathbf{a_1} - x_5\mathbf{a_2} + z_5\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(2x_5 - y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B_{14}}$	$=$	$-y_5\mathbf{a_1} - x_5\mathbf{a_2} - \left(z_5 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_5 + y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B_{15}}$	$=$	$-\left(x_5 - y_5\right)\mathbf{a_1} + y_5\mathbf{a_2} - \left(z_5 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(-x_5 + 2y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B_{16}}$	$=$	$x_5\mathbf{a_1} + \left(x_5 - y_5\right)\mathbf{a_2} - \left(z_5 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(2x_5 - y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B_{17}}$	$=$	$-x_5\mathbf{a_1} - y_5\mathbf{a_2} - z_5\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_5 + y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B_{18}}$	$=$	$y_5\mathbf{a_1} - \left(x_5 - y_5\right)\mathbf{a_2} - z_5\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(-x_5 + 2y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B_{19}}$	$=$	$\left(x_5 - y_5\right)\mathbf{a_1} + x_5\mathbf{a_2} - z_5\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(2x_5 - y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B_{20}}$	$=$	$y_5\mathbf{a_1} + x_5\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_5 + y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B_{21}}$	$=$	$\left(x_5 - y_5\right)\mathbf{a_1} - y_5\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_5 - 2y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	S I
$\mathbf{B_{22}}$	$=$	$-x_5\mathbf{a_1} - \left(x_5 - y_5\right)\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(2x_5 - y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	S I

References

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

[2] 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).