Brezinaite (Cr_3S_4) Structure: A3B4_mC14_12_ai_2i-002

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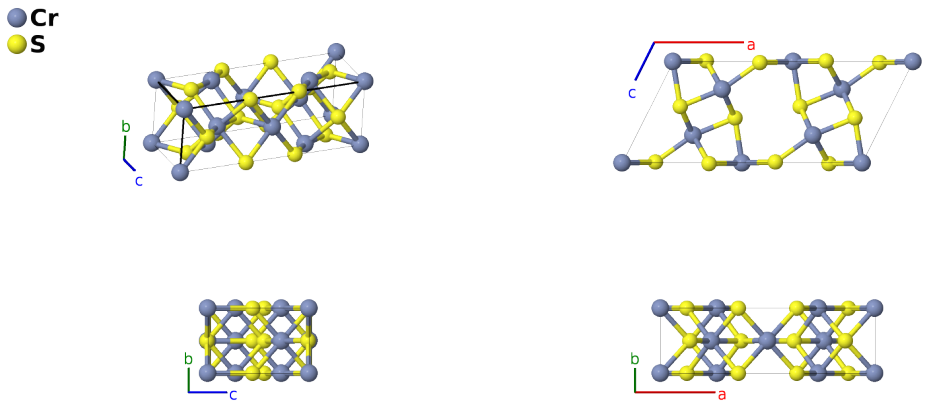
https://aflow.org/p/17US

https://aflow.org/p/A3B4_mC14_12_ai_2i-002



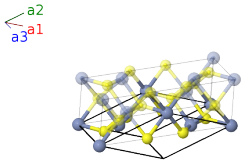
Prototype	Cr_3S_4
AFLOW prototype label	A3B4_mC14_12_ai_2i-002
Mineral name	brezinaite
ICSD	16722
Pearson symbol	mC14
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A3B4_mC14_12_ai_2i-002 --params=`$a, b/a, c/a, \beta, x_2, z_2, x_3, z_3, x_4, z_4$

Other compounds with this structure
Co_3Se_4, Cr_3Te_4, Fe_3Se_4, Re_3P_4, V_3S_4, V_3Te_4, $FeCr_2Se_4$, $MnCr_2Se_4$, $NiCr_2S_4$, $NiTi_2Se_4$, VCr_2S_4

- (Jellinek, 1957) gives this structure in the $I2/m$ setting of space group #12. We used FINDSYM to change this to the standard $C2/m$ setting. When doing this the shape of the conventional cell changes from that found in the original paper, but of course the Wigner-Seitz cells are identical.
- Cr_3Sn_4 and δ-Ni_3Sn_4 ($D7_a$) have the same AFLOW prototype label, A3B4_mC14_12_ai_2i. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Cr I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Cr II
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Cr II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	S I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	S I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	S II
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	S II

References

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

Found in

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