

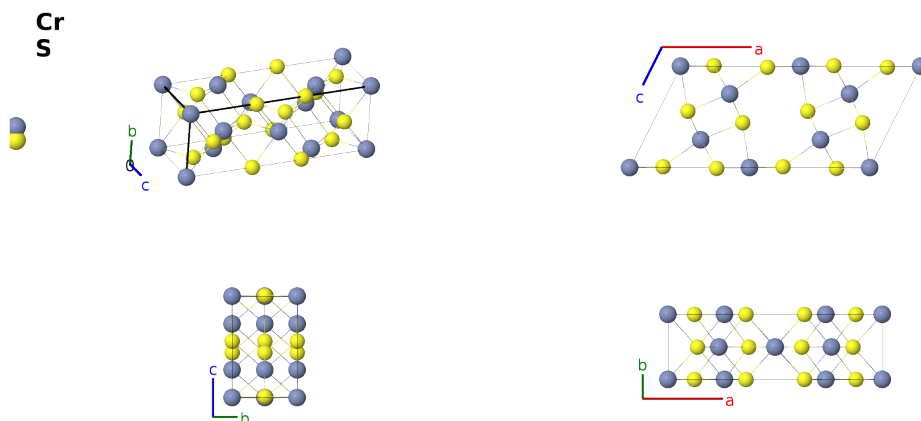
Brezinaite (Cr_3S_4) Structure: A3B4_mC14_12_ai_2i-002

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<https://aflow.org/prototype-encyclopedia/17US>

https://aflow.org/prototype-encyclopedia/A3B4_mC14_12_ai_2i-002



Prototype	Cr_3S_4
AFLOW prototype label	A3B4_mC14_12_ai_2i-002
Mineral name	brezinaite
ICSD	16722
CCDC	1597273
Pearson symbol	mC14
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<pre>aflow --proto=A3B4_mC14_12_ai_2i-002 --params=a, b/a, c/a, β, x_2, z_2, x_3, z_3, x_4, z_4</pre>

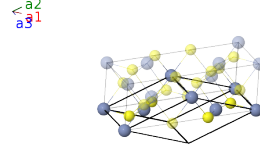
Other compounds with this structure

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_3S_4 and $\delta\text{-Ni}_3\text{Sn}_4$ ($D7_a$) 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

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



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).

First cited in

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