

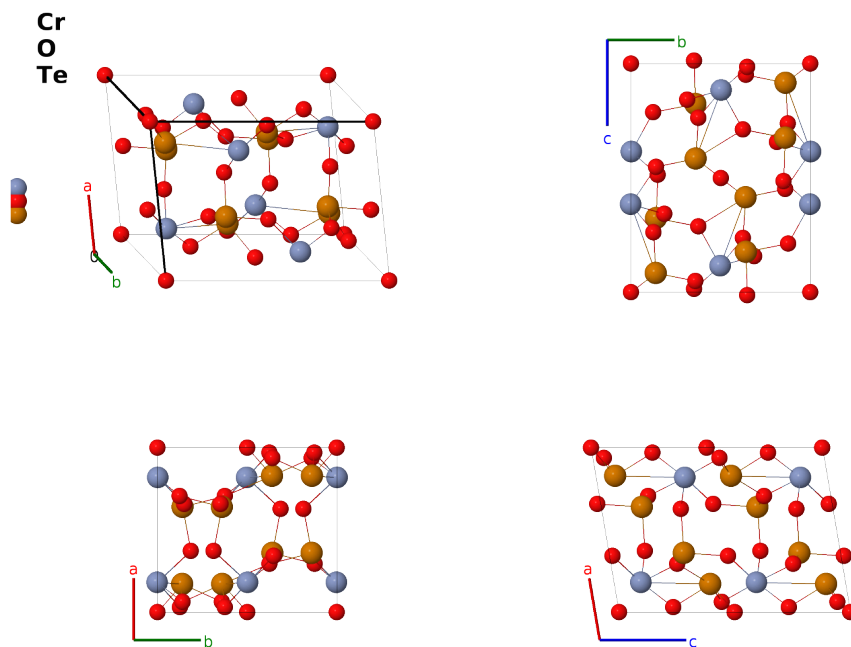
Cr₂Te₄O₁₁ Structure: A2B11C4_mP34_14_e_a5e_2e-001

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<https://aflow.org/prototype-encyclopedia/1LFJ>

https://aflow.org/prototype-encyclopedia/A2B11C4_mP34_14_e_a5e_2e-001



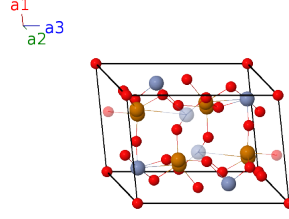
Prototype	Cr ₂ O ₁₁ Te ₄
AFLOW prototype label	A2B11C4_mP34_14_e_a5e_2e-001
ICSD	1
CCDC	1590636
Pearson symbol	mP34
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	<pre>aflow --proto=A2B11C4_mP34_14_e_a5e_2e-001 --params=a, b/a, c/a, β, $x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$</pre>

- (Meunier, 1976) set $z_6 = 0.624$, but the ICSD entry sets $z_6 = 0.644$. The former choice agrees with the values in the paper, so we use it.

- (Meunier, 1976) put what we call the O I atom on the (2d) Wyckoff position, $(1/2 \ 0 \ 1/2)$. The AFLOW label scheme moves this to the (2a) site.

Simple Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(2a)	O I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \cos \beta \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	Cr I
$\mathbf{B}_4$	$-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_2 + c(z_2 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Cr I
$\mathbf{B}_5$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	Cr I
$\mathbf{B}_6$	$x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Cr I
$\mathbf{B}_7$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_8$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_9$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{10}$	$x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{11}$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{12}$	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{13}$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{14}$	$x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{15}$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B}_{16}$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B}_{17}$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B}_{18}$	$x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B}_{19}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4e)	O V
$\mathbf{B}_{20}$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_6 + c(z_6 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O V

$$\begin{aligned}
\mathbf{B}_{21} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= - (ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}} &(4e) &\text{O V} \\
\mathbf{B}_{22} &= x_6 \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= \begin{aligned} &(ax_6 + c \left(z_6 + \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} - \\ &b \left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \end{aligned} &(4e) &\text{O V} \\
\mathbf{B}_{23} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= (ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}} &(4e) &\text{O VI} \\
\mathbf{B}_{24} &= -x_7 \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= \begin{aligned} &- (ax_7 + c \left(z_7 - \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} + \\ &b \left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \end{aligned} &(4e) &\text{O VI} \\
\mathbf{B}_{25} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= - (ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}} &(4e) &\text{O VI} \\
\mathbf{B}_{26} &= x_7 \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= \begin{aligned} &(ax_7 + c \left(z_7 + \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} - \\ &b \left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \end{aligned} &(4e) &\text{O VI} \\
\mathbf{B}_{27} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= (ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}} &(4e) &\text{Te I} \\
\mathbf{B}_{28} &= -x_8 \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 &= \begin{aligned} &- (ax_8 + c \left(z_8 - \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} + \\ &b \left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \end{aligned} &(4e) &\text{Te I} \\
\mathbf{B}_{29} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= - (ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}} &(4e) &\text{Te I} \\
\mathbf{B}_{30} &= x_8 \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= \begin{aligned} &(ax_8 + c \left(z_8 + \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} - \\ &b \left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \end{aligned} &(4e) &\text{Te I} \\
\mathbf{B}_{31} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 &= (ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}} &(4e) &\text{Te II} \\
\mathbf{B}_{32} &= -x_9 \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= \begin{aligned} &- (ax_9 + c \left(z_9 - \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} + \\ &b \left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \end{aligned} &(4e) &\text{Te II} \\
\mathbf{B}_{33} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 &= - (ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}} &(4e) &\text{Te II} \\
\mathbf{B}_{34} &= x_9 \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= \begin{aligned} &(ax_9 + c \left(z_9 + \frac{1}{2}\right) \cos \beta) \hat{\mathbf{x}} - \\ &b \left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \end{aligned} &(4e) &\text{Te II}
\end{aligned}$$

References

- [1] G. Meunier, B. Frit, and J. Galy, *Cr₂Te₄O₁₁: une structure à anions complexes (Cr₂O₁₀)¹⁴⁻*, Acta Crystallogr. Sect. B **32**, 175–180 (1976), doi:10.1107/S0567740876002549.

Found in

- [1] ICSD, Inorganic Crystal Structure Database. ID 1.

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