

CrPS₄ Structure:

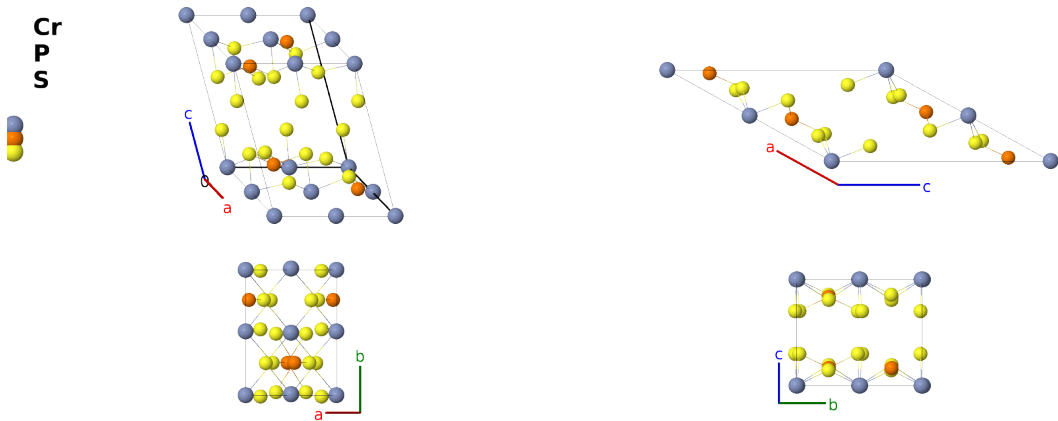
ABC4_mC24_5_2a_c_4c-001

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<https://aflow.org/prototype-encyclopedia/VB2Y>

https://aflow.org/prototype-encyclopedia/ABC4_mC24_5_2a_c_4c-001



Prototype	CrPS ₄
AFLOW prototype label	ABC4_mC24_5_2a_c_4c-001
ICSD	937
CCDC	1591155
Pearson symbol	mC24
Space group number	5
Space group symbol	<i>C</i> 2
AFLOW prototype command	<pre>aflow --proto=ABC4_mC24_5_2a_c_4c-001 --params=a,b/a,c/a,β,y₁,y₂,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇,y₇,z₇</pre>

- Space group *C*2 #5 does not specify the origin of the *y*-axis. Here we follow (Diehl, 1977) and set *y*_I = 0 for the Cr-I atom.

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
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	$=$	$by_1 \hat{\mathbf{y}}$	(2a)	Cr I
$\mathbf{B}_2$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$by_2 \hat{\mathbf{y}}$	(2a)	Cr II
$\mathbf{B}_3$	$= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B}_4$	$= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B}_5$	$= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B}_6$	$= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B}_7$	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4c)	S II
$\mathbf{B}_8$	$= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4c)	S II
$\mathbf{B}_9$	$= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4c)	S III
$\mathbf{B}_{10}$	$= -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4c)	S III
$\mathbf{B}_{11}$	$= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4c)	S IV
$\mathbf{B}_{12}$	$= -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4c)	S IV

References

- [1] R. Diehl and C.-D. Carpentier, *The crystal structure of chromium thiophosphate, CrPS₄*, Acta Crystallogr. Sect. B **33**, 1399–1404 (1977), doi:10.1107/S0567740877006165.

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