$CrPS_4$ Structure: ABC4_mC24_5_2a_c_4c-001

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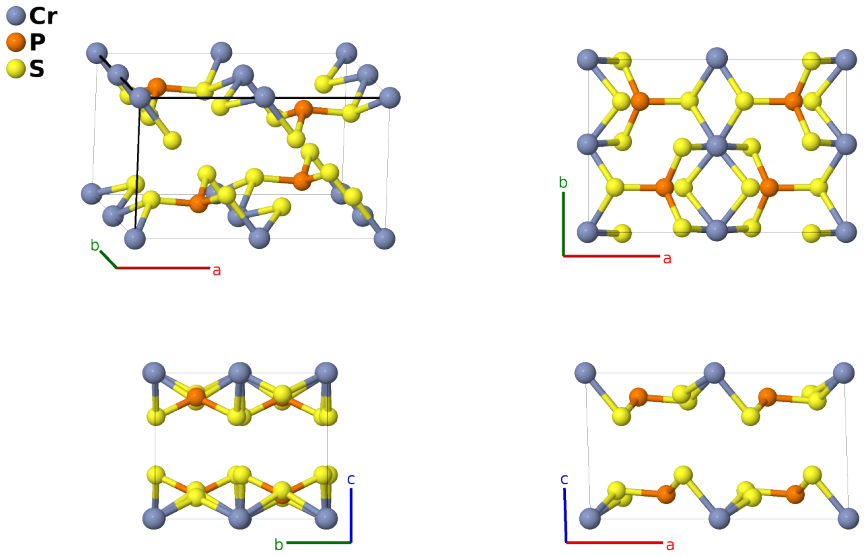
https://aflow.org/p/VB2Y

https://aflow.org/p/ABC4_mC24_5_2a_c_4c-001

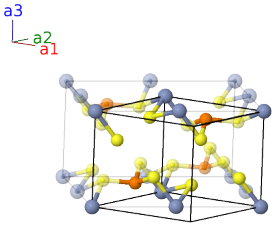


Prototype	$CrPS_4$
AFLOW prototype label	ABC4_mC24_5_2a_c_4c-001
ICSD	937
Pearson symbol	mC24
Space group number	5
Space group symbol	$C2$
AFLOW prototype command	`aflow --proto=ABC4_mC24_5_2a_c_4c-001 --params=`$a, b/a, c/a, \beta, y_1, y_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

- Space group $C2$ #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

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



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, $CrPS_4$*, Acta Crystallogr. Sect. B **33**, 1399–1404 (1977), doi:10.1107/S0567740877006165.