

CrP₄ Structure:

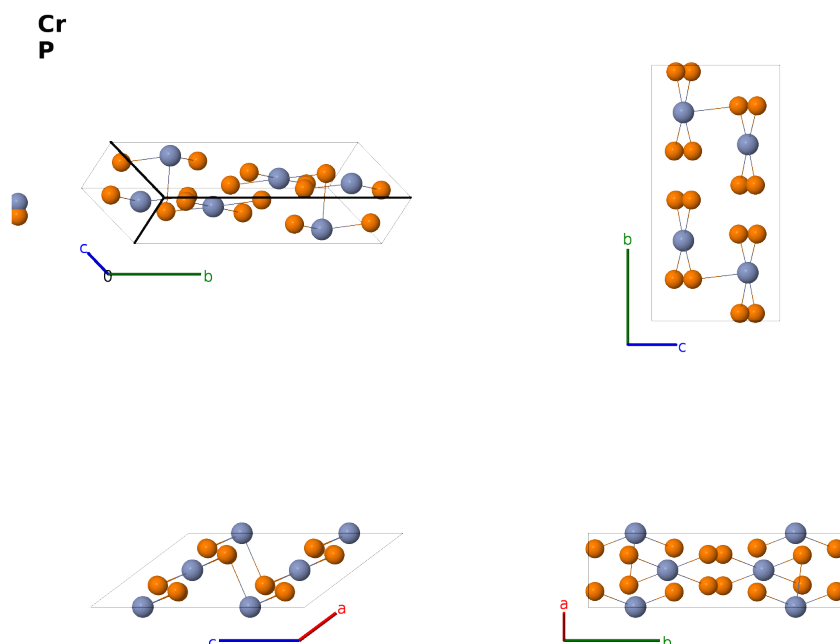
AB4_mC20_15_e_2f-001

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<https://aflow.org/prototype-encyclopedia/2S3X>

https://aflow.org/prototype-encyclopedia/AB4_mC20_15_e_2f-001



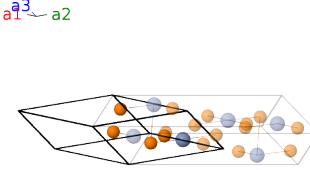
Prototype	CrP ₄
AFLOW prototype label	AB4_mC20_15_e_2f-001
ICSD	2790
CCDC	1592594
Pearson symbol	mC20
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	<code>aflow --proto=AB4_mC20_15_e_2f-001</code> <code>--params=a, b/a, c/a, β, y_1, x_2, y_2, z_2, x_3, y_3, z_3</code>

Other compounds with this structure

MoP₄, OsP₄, RuP₄

- This is the high temperature form OsP₄ and RuP₄ (Flörke, 1982). For the low temperature form see the CdP₄ structure.
- OsO₄, A4B_mC20_15_2f_e-001, and CrP₄, AB4_mC20_15_e_2f-001, occupy the same Wyckoff positions in space group C2/c #15. The structures are generated by the same symmetry operations with their own AFLOW labels and 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
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Cr I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Cr I
$\mathbf{B}_3$	$= (x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(8f)	P I
$\mathbf{B}_4$	$= -(x_2 + y_2) \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_2 + c(z_2 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	P I
$\mathbf{B}_5$	$= -(x_2 - y_2) \mathbf{a}_1 - (x_2 + y_2) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(8f)	P I
$\mathbf{B}_6$	$= (x_2 + y_2) \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	P I
$\mathbf{B}_7$	$= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(8f)	P II
$\mathbf{B}_8$	$= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	P II
$\mathbf{B}_9$	$= -(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(8f)	P II
$\mathbf{B}_{10}$	$= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	P II

References

- [1] W. Jeitschko and P. C. Donohue, *The high pressure synthesis, crystal structure, and properties of CrP₄ and MoP₄*, Acta Crystallogr. Sect. B **28**, 1893–1898 (1972), doi:10.1107/S0567740872005187.
- [2] U. Flörke and W. Jeitscho, *Preparation and properties of new modifications of RuP₄ and OsP₄ with CdP₄-type structure*, J. Less-Common Met. **86**, 247–253 (1982), doi:10.1016/0022-5088(82)90210-7.

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