

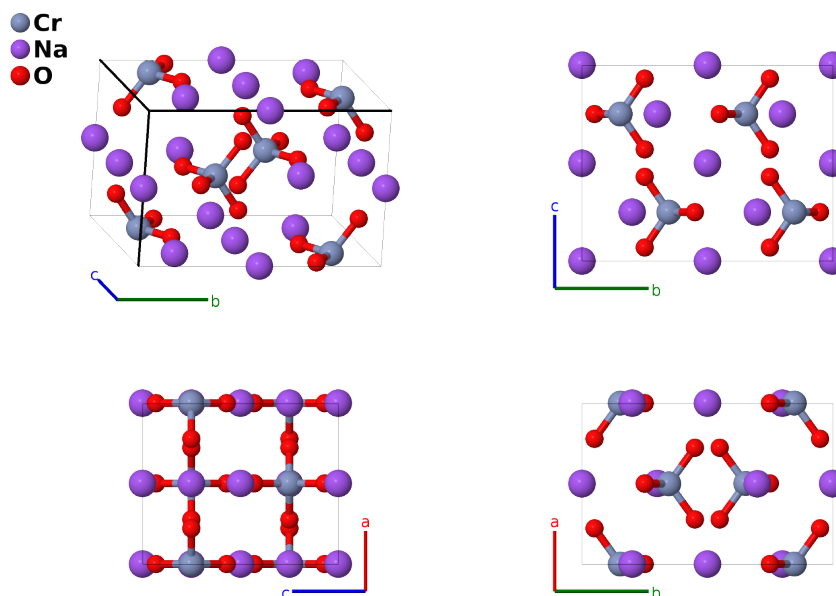
Na₂CrO₄ (*H1*₈) Structure: AB2C4_oC28_63_c_ac_fg-001

This structure originally had the label AB2C4_oC28_63_c.bc_fg. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/p/A786>

https://aflow.org/p/AB2C4_oC28_63_c_ac_fg-001



Prototype	CrNa ₂ O ₄
AFLOW prototype label	AB2C4_oC28_63_c_ac_fg-001
<i>Strukturbericht</i> designation	<i>H1</i> ₈
ICSD	76001
Pearson symbol	oC28
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=AB2C4_oC28_63_c_ac_fg-001 --params=a, b/a, c/a, y₂, y₃, y₄, z₄, x₅, y₅</code>

Other compounds with this structure

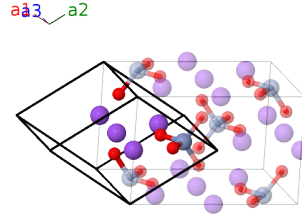
Li₂SO₄, LiFeP₄, Na₂FeO₄, Na₂SO₄ (III), NaCaVO₄, NaMnPO₄, NaVCdO₄, Tl₂SeO₄

- This structure was originally determined by (Miller, 1936), who placed it in space group *Pnna* #52, and (Gottfried, 1938) uses this data for *Strukturbericht H1*₈. Subsequently (Niggli, 1954) rather acerbically pointed out that Miller's coordinates were consistent with the more compact *Cmcm* #63 space group. This does not change the positions of the atoms in the conventional cell, so we use the compact structure as our prototype for *Strukturbericht* designation *H1*₈.

- This structure is stable up to 413°C. (Amirathanlingam, 1982)

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= 0$	$=$	0	(4a)	Na I
\mathbf{B}_2	$= \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}c\hat{\mathbf{z}}$	(4a)	Na I
\mathbf{B}_3	$= -y_2\mathbf{a}_1 + y_2\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$by_2\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4c)	Cr I
\mathbf{B}_4	$= y_2\mathbf{a}_1 - y_2\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$-by_2\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(4c)	Cr I
\mathbf{B}_5	$= -y_3\mathbf{a}_1 + y_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$by_3\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4c)	Na II
\mathbf{B}_6	$= y_3\mathbf{a}_1 - y_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$-by_3\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(4c)	Na II
\mathbf{B}_7	$= -y_4\mathbf{a}_1 + y_4\mathbf{a}_2 + z_4\mathbf{a}_3$	$=$	$by_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(8f)	O I
\mathbf{B}_8	$= y_4\mathbf{a}_1 - y_4\mathbf{a}_2 + (z_4 + \frac{1}{2})\mathbf{a}_3$	$=$	$-by_4\hat{\mathbf{y}} + c(z_4 + \frac{1}{2})\hat{\mathbf{z}}$	(8f)	O I
\mathbf{B}_9	$= -y_4\mathbf{a}_1 + y_4\mathbf{a}_2 - (z_4 - \frac{1}{2})\mathbf{a}_3$	$=$	$by_4\hat{\mathbf{y}} - c(z_4 - \frac{1}{2})\hat{\mathbf{z}}$	(8f)	O I
\mathbf{B}_{10}	$= y_4\mathbf{a}_1 - y_4\mathbf{a}_2 - z_4\mathbf{a}_3$	$=$	$-by_4\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(8f)	O I
\mathbf{B}_{11}	$= (x_5 - y_5)\mathbf{a}_1 + (x_5 + y_5)\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$ax_5\hat{\mathbf{x}} + by_5\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{12}	$= -(x_5 - y_5)\mathbf{a}_1 - (x_5 + y_5)\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$-ax_5\hat{\mathbf{x}} - by_5\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{13}	$= -(x_5 + y_5)\mathbf{a}_1 - (x_5 - y_5)\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$-ax_5\hat{\mathbf{x}} + by_5\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{14}	$= (x_5 + y_5)\mathbf{a}_1 + (x_5 - y_5)\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$ax_5\hat{\mathbf{x}} - by_5\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(8g)	O II

References

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- [3] C. Gottfried, ed., *Strukturbericht Band IV 1936* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1938).
- [4] V. Amirathanlingam and K. S. Venkateswarlu, *Te Thermal Expansion and Crystallographic Phase Transformation of Na₂CrO₄*, Thermochemica Acta **58**, 107–109 (1982), doi:10.1016/0040-6031(82)87145-1.