Na_2CrO_4 ($H1_8$) Structure: AB2C4_oC28_63_c_ac_fg-001

This structure previously used the label(s) `AB2C4_oC28_63_c_bc_fg`. Calls to these addresses will be redirected here.

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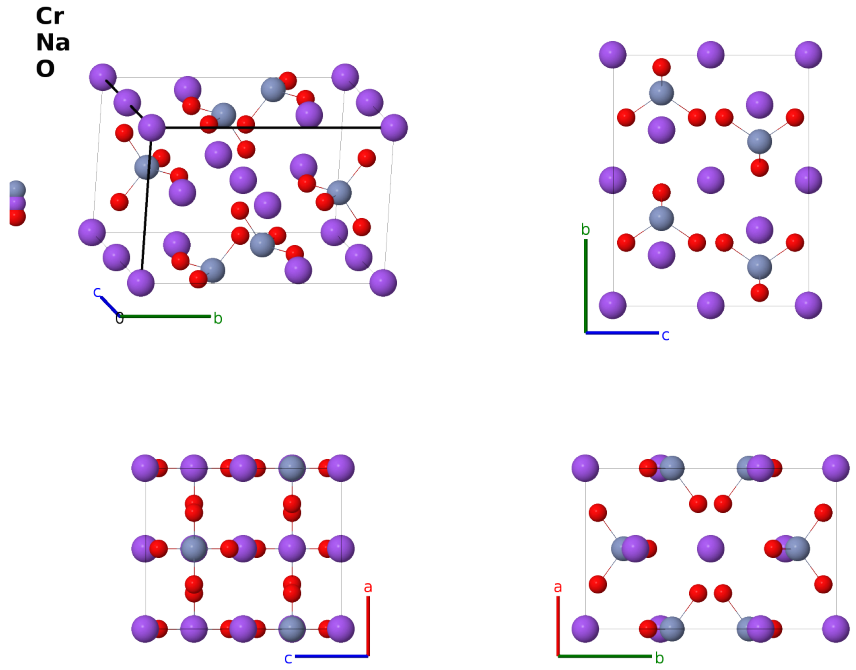
https://aflow.org/prototype-encyclopedia/A786

https://aflow.org/prototype-encyclopedia/AB2C4_oC28_63_c_ac_fg-001



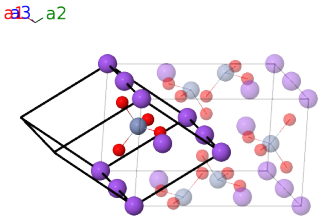
Prototype	$CrNa_2O_4$
AFLOW prototype label	AB2C4_oC28_63_c_ac_fg-001
***Strukturbericht* designation**	$H1_8$
ICSD	76001
CCDC	1636639
Pearson symbol	oC28
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=AB2C4_oC28_63_c_ac_fg-001 --params=`$a, b/a, c/a, y_2, y_3, y_4, z_4, x_5, y_5$

Other compounds with this structure
Li_2SO_4, $LiFeP_4$, Na_2FeO_4, Na_2SO_4 (III), $NaCaVO_4$, $NaMnPO_4$, $NaVCdO_4$, Tl_2SeO_4

- 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)
- AFLOW shifts the origin so that the Na I atoms, previously on th (4b) Wyckoff sites, are now on the (4a) sites, including an atom at the origin.
- β'-$LiFePO_4$ is the quaternary form of this structure.

Base-centered Orthorhombic primitive vectors

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



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
$\mathbf{B_8}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_9}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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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[2] J. J. Miller, *The Crystal Structure of Anhydrous Sodium Chromate, Na_2CrO_4*, Z. Kristallogr. **94**, 131–136 (1936), doi:10.1524/zkri.1936.94.1.131.

[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 Na_2CrO_4*, Thermochimica Acat **58**, 107–109 (1982), doi:10.1016/0040-6031(82)87145-1.

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