

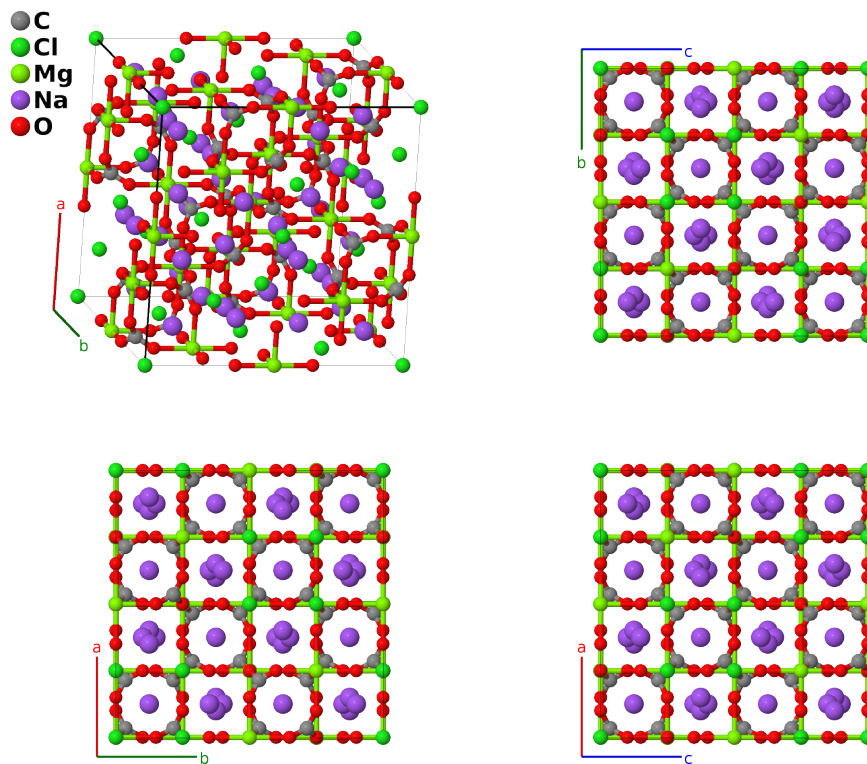
$G7_3$ $[\text{Na}_3\text{MgCl}(\text{CO}_3)_2]$ Structure (*Obsolete*): A2BCD3E6_cF208_227_e_c_d_f_g-001

This structure originally had the label A2BCD3E6_cF208_227_e_c_d_f_g. 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/8XP6>

https://afLOW.org/p/A2BCD3E6_cF208_227_e_c_d_f_g-001

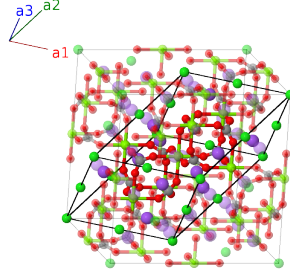


Prototype	$\text{C}_2\text{ClMgNa}_3\text{O}_6$
AFLOW prototype label	A2BCD3E6_cF208_227_e_c_d_f_g-001
<i>Strukturbericht</i> designation	$G7_3$
Mineral name	northupite
ICSD	27790
Pearson symbol	cF208
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	<code>afLOW --proto=A2BCD3E6_cF208_227_e_c_d_f_g-001 --params=a, x3, x4, x5, z5</code>

- This is the original structure determined by (Shiba, 1931) and given the designation $G7_3$ in (Hermann, 1937). (Negro, 1975) showed that the correct structure was actually related to cubic pyrochlore. The two structures are very similar, and a displacement of the oxygen atoms by less than 1\AA brings the two structures into agreement.

Face-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$=$	0	$=$	0	(16c) Cl I
\mathbf{B}_2	$=$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} + \frac{1}{4}a\hat{y}$	(16c) Cl I
\mathbf{B}_3	$=$	$\frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{x} + \frac{1}{4}a\hat{z}$	(16c) Cl I
\mathbf{B}_4	$=$	$\frac{1}{2}\mathbf{a}_1$	$=$	$\frac{1}{4}a\hat{y} + \frac{1}{4}a\hat{z}$	(16c) Cl I
\mathbf{B}_5	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z}$	(16d) Mg I
\mathbf{B}_6	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{x} + \frac{1}{4}a\hat{y} + \frac{1}{2}a\hat{z}$	(16d) Mg I
\mathbf{B}_7	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} + \frac{1}{2}a\hat{y} + \frac{1}{4}a\hat{z}$	(16d) Mg I
\mathbf{B}_8	$=$	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{x} + \frac{1}{4}a\hat{y} + \frac{1}{4}a\hat{z}$	(16d) Mg I
\mathbf{B}_9	$=$	$x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{x} + ax_3\hat{y} + ax_3\hat{z}$	(32e) C I
\mathbf{B}_{10}	$=$	$x_3\mathbf{a}_1 + x_3\mathbf{a}_2 - (3x_3 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{4})\hat{x} - a(x_3 - \frac{1}{4})\hat{y} + ax_3\hat{z}$	(32e) C I
\mathbf{B}_{11}	$=$	$x_3\mathbf{a}_1 - (3x_3 - \frac{1}{2})\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{4})\hat{x} + ax_3\hat{y} - a(x_3 - \frac{1}{4})\hat{z}$	(32e) C I
\mathbf{B}_{12}	$=$	$-(3x_3 - \frac{1}{2})\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{x} - a(x_3 - \frac{1}{4})\hat{y} - a(x_3 - \frac{1}{4})\hat{z}$	(32e) C I
\mathbf{B}_{13}	$=$	$-x_3\mathbf{a}_1 - x_3\mathbf{a}_2 + (3x_3 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{4})\hat{x} + a(x_3 + \frac{1}{4})\hat{y} - ax_3\hat{z}$	(32e) C I
\mathbf{B}_{14}	$=$	$-x_3\mathbf{a}_1 - x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-ax_3\hat{x} - ax_3\hat{y} - ax_3\hat{z}$	(32e) C I
\mathbf{B}_{15}	$=$	$-x_3\mathbf{a}_1 + (3x_3 + \frac{1}{2})\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{4})\hat{x} - ax_3\hat{y} + a(x_3 + \frac{1}{4})\hat{z}$	(32e) C I
\mathbf{B}_{16}	$=$	$(3x_3 + \frac{1}{2})\mathbf{a}_1 - x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-ax_3\hat{x} + a(x_3 + \frac{1}{4})\hat{y} + a(x_3 + \frac{1}{4})\hat{z}$	(32e) C I
\mathbf{B}_{17}	$=$	$-(x_4 - \frac{1}{4})\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{x} + \frac{1}{8}a\hat{y} + \frac{1}{8}a\hat{z}$	(48f) Na I
\mathbf{B}_{18}	$=$	$x_4\mathbf{a}_1 - (x_4 - \frac{1}{4})\mathbf{a}_2 - (x_4 - \frac{1}{4})\mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{4})\hat{x} + \frac{1}{8}a\hat{y} + \frac{1}{8}a\hat{z}$	(48f) Na I
\mathbf{B}_{19}	$=$	$x_4\mathbf{a}_1 - (x_4 - \frac{1}{4})\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{x} + ax_4\hat{y} + \frac{1}{8}a\hat{z}$	(48f) Na I
\mathbf{B}_{20}	$=$	$-(x_4 - \frac{1}{4})\mathbf{a}_1 + x_4\mathbf{a}_2 - (x_4 - \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{x} - a(x_4 - \frac{1}{4})\hat{y} + \frac{1}{8}a\hat{z}$	(48f) Na I
\mathbf{B}_{21}	$=$	$x_4\mathbf{a}_1 + x_4\mathbf{a}_2 - (x_4 - \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{x} + \frac{1}{8}a\hat{y} + ax_4\hat{z}$	(48f) Na I
\mathbf{B}_{22}	$=$	$-(x_4 - \frac{1}{4})\mathbf{a}_1 - (x_4 - \frac{1}{4})\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{x} + \frac{1}{8}a\hat{y} - a(x_4 - \frac{1}{4})\hat{z}$	(48f) Na I
\mathbf{B}_{23}	$=$	$(x_4 + \frac{3}{4})\mathbf{a}_1 - x_4\mathbf{a}_2 + (x_4 + \frac{3}{4})\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{x} + a(x_4 + \frac{3}{4})\hat{y} + \frac{3}{8}a\hat{z}$	(48f) Na I
\mathbf{B}_{24}	$=$	$-x_4\mathbf{a}_1 + (x_4 + \frac{3}{4})\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{x} - ax_4\hat{y} + \frac{3}{8}a\hat{z}$	(48f) Na I

References

- [1] H. Shiba and T. Watanabé, *Les structures des cristaux de northupite, de northupite bromée et de tychite*, Compt. Rend. **193**, 1421–1423 (1931).
- [2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

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- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).