

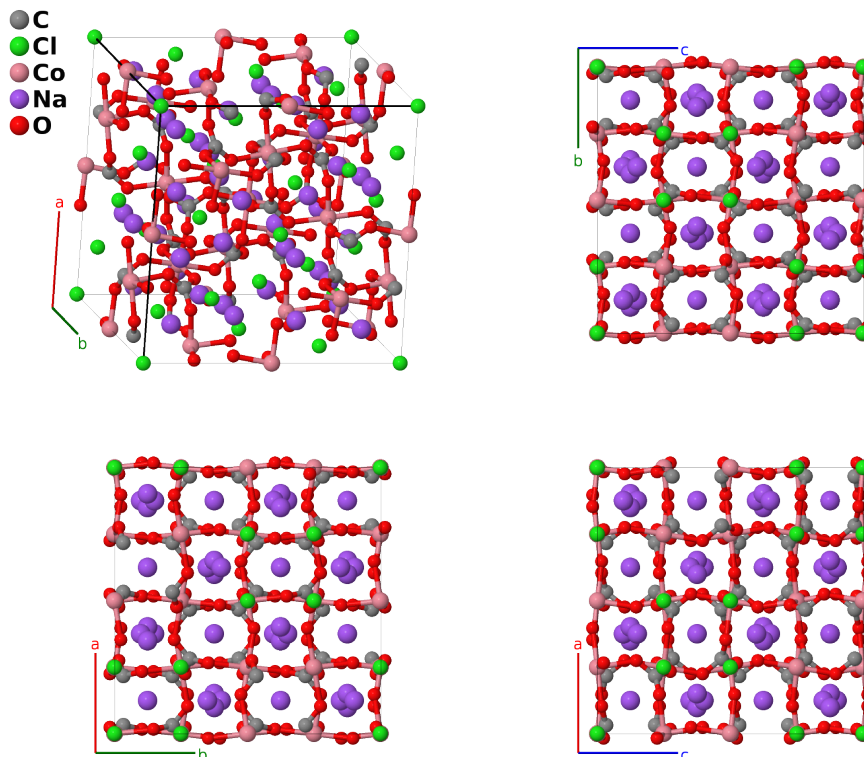
# Pyrochlore ( $\text{Na}_3\text{Co}(\text{CO}_3)_2\text{Cl}$ ) Structure: A2BCD3E6\_cF208\_203\_e\_c\_d\_f\_g-001

This structure originally had the label A2BCD3E6\_cF208\_203\_e\_c\_d\_f\_g. Calls to that address will be redirected here.

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<https://aflow.org/p/LH7J>

[https://aflow.org/p/A2BCD3E6\\_cF208\\_203\\_e\\_c\\_d\\_f\\_g-001](https://aflow.org/p/A2BCD3E6_cF208_203_e_c_d_f_g-001)



Prototype	$\text{C}_2\text{ClCoNa}_3\text{O}_6$
AFLOW prototype label	A2BCD3E6_cF208_203_e_c_d_f_g-001
Mineral name	pyrochlore
ICSD	none
Pearson symbol	cF208
Space group number	203
Space group symbol	$Fd\bar{3}$
AFLOW prototype command	<code>aflow --proto=A2BCD3E6_cF208_203_e_c_d_f_g-001 --params=a, x3, x4, x5, y5, z5</code>

## Other compounds with this structure

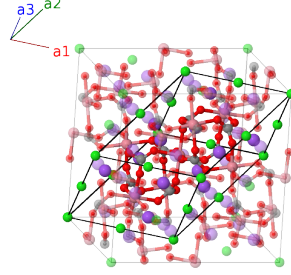
$\text{Na}_3\text{MgCl}(\text{CO}_3)_2$  (northupite),  $\text{Na}_3\text{MgBr}(\text{CO}_3)_2$

- This structure was suggested to us by Prof. Joel Helton, United States Naval Academy. This is a pyrochlore-like antiferromagnet, which we loosely define as a structure with magnetic ions on the corners of corner-sharing tetrahedra.
- We use the structural data taken by (Fu, 2013) at 3.7K

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### Face-centered Cubic primitive vectors

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




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### 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)	Co 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)	Co 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)	Co 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)	Co 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
$\mathbf{B}_{13}$	$-x_3\mathbf{a}_1 - x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-ax_3\hat{x} - ax_3\hat{y} - ax_3\hat{z}$	(32e)	C I
$\mathbf{B}_{14}$	$-x_3\mathbf{a}_1 - x_3\mathbf{a}_2 + (3x_3 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{4})\hat{x} + a(x_3 + \frac{1}{4})\hat{y} - ax_3\hat{z}$	(32e)	C I
$\mathbf{B}_{15}$	$-x_3\mathbf{a}_1 + (3x_3 + \frac{1}{2})\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{4})\hat{x} - ax_3\hat{y} + a(x_3 + \frac{1}{4})\hat{z}$	(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
$\mathbf{B}_{23}$	$(x_4 + \frac{3}{4})\mathbf{a}_1 - x_4\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$-ax_4\hat{x} + \frac{3}{8}a\hat{y} + \frac{3}{8}a\hat{z}$	(48f)	Na I



$$\begin{aligned}
\mathbf{B}_{43} &= \begin{aligned} &-(x_5 + y_5 - z_5) \mathbf{a}_1 + \\ &(x_5 + y_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + \\ &(x_5 - y_5 - z_5) \mathbf{a}_3 \end{aligned} &= a(x_5 + \frac{1}{4}) \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + a(z_5 + \frac{1}{4}) \hat{\mathbf{z}} &(96g) & \text{O I} \\
\mathbf{B}_{44} &= \begin{aligned} &(x_5 + y_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 - \\ &(x_5 + y_5 - z_5) \mathbf{a}_2 - \\ &(x_5 - y_5 + z_5) \mathbf{a}_3 \end{aligned} &= -ax_5 \hat{\mathbf{x}} + a(y_5 + \frac{1}{4}) \hat{\mathbf{y}} + a(z_5 + \frac{1}{4}) \hat{\mathbf{z}} &(96g) & \text{O I} \\
\mathbf{B}_{45} &= \begin{aligned} &-(x_5 + y_5 - z_5) \mathbf{a}_1 + \\ &(x_5 - y_5 - z_5) \mathbf{a}_2 - \\ &(x_5 - y_5 + z_5) \mathbf{a}_3 \end{aligned} &= -az_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}} &(96g) & \text{O I} \\
\mathbf{B}_{46} &= \begin{aligned} &(x_5 + y_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 - \\ &(x_5 - y_5 + z_5) \mathbf{a}_2 + \\ &(x_5 - y_5 - z_5) \mathbf{a}_3 \end{aligned} &= -az_5 \hat{\mathbf{x}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} + a(y_5 + \frac{1}{4}) \hat{\mathbf{z}} &(96g) & \text{O I} \\
\mathbf{B}_{47} &= \begin{aligned} &(x_5 - y_5 - z_5) \mathbf{a}_1 - \\ &(x_5 + y_5 - z_5) \mathbf{a}_2 + \\ &(x_5 + y_5 + z_5 + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= a(z_5 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}} &(96g) & \text{O I} \\
\mathbf{B}_{48} &= \begin{aligned} &-(x_5 - y_5 + z_5) \mathbf{a}_1 + \\ &(x_5 + y_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 - \\ &(x_5 + y_5 - z_5) \mathbf{a}_3 \end{aligned} &= a(z_5 + \frac{1}{4}) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + a(y_5 + \frac{1}{4}) \hat{\mathbf{z}} &(96g) & \text{O I} \\
\mathbf{B}_{49} &= \begin{aligned} &-(x_5 - y_5 + z_5) \mathbf{a}_1 - \\ &(x_5 + y_5 - z_5) \mathbf{a}_2 + \\ &(x_5 - y_5 - z_5) \mathbf{a}_3 \end{aligned} &= -ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}} &(96g) & \text{O I} \\
\mathbf{B}_{50} &= \begin{aligned} &(x_5 - y_5 - z_5) \mathbf{a}_1 + \\ &(x_5 + y_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 - \\ &(x_5 - y_5 + z_5) \mathbf{a}_3 \end{aligned} &= a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{z}} &(96g) & \text{O I} \\
\mathbf{B}_{51} &= \begin{aligned} &(x_5 + y_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 + \\ &(x_5 - y_5 - z_5) \mathbf{a}_2 - \\ &(x_5 + y_5 - z_5) \mathbf{a}_3 \end{aligned} &= -ay_5 \hat{\mathbf{x}} + a(z_5 + \frac{1}{4}) \hat{\mathbf{y}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{z}} &(96g) & \text{O I} \\
\mathbf{B}_{52} &= \begin{aligned} &-(x_5 + y_5 - z_5) \mathbf{a}_1 - \\ &(x_5 - y_5 + z_5) \mathbf{a}_2 + \\ &(x_5 + y_5 + z_5 + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} + a(z_5 + \frac{1}{4}) \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}} &(96g) & \text{O I}
\end{aligned}$$

## References

- [1] Z. Fu, Y. Zheng, Y. Xiao, S. Bedanta, A. Senyshyn, G. G. Simeoni, Y. Su, U. Rucker, P. Kögerler, and T. Brückel, *Coexistence of magnetic order and spin-glass-like phase in the pyrochlore antiferromagnet  $\text{Na}_3\text{Co}(\text{CO}_3)_2\text{Cl}$* , Phys. Rev. B **87**, 214406 (2013), doi:10.1103/PhysRevB.87.214406.