Phase III $Cd_2Re_2O_7$ Structure: A2B7C2_tI44_98_f_acde_f-001

This structure previously used the label(s) `A2B7C2_tI44_98_f_bcde_f`. Calls to these addresses will be redirected here.

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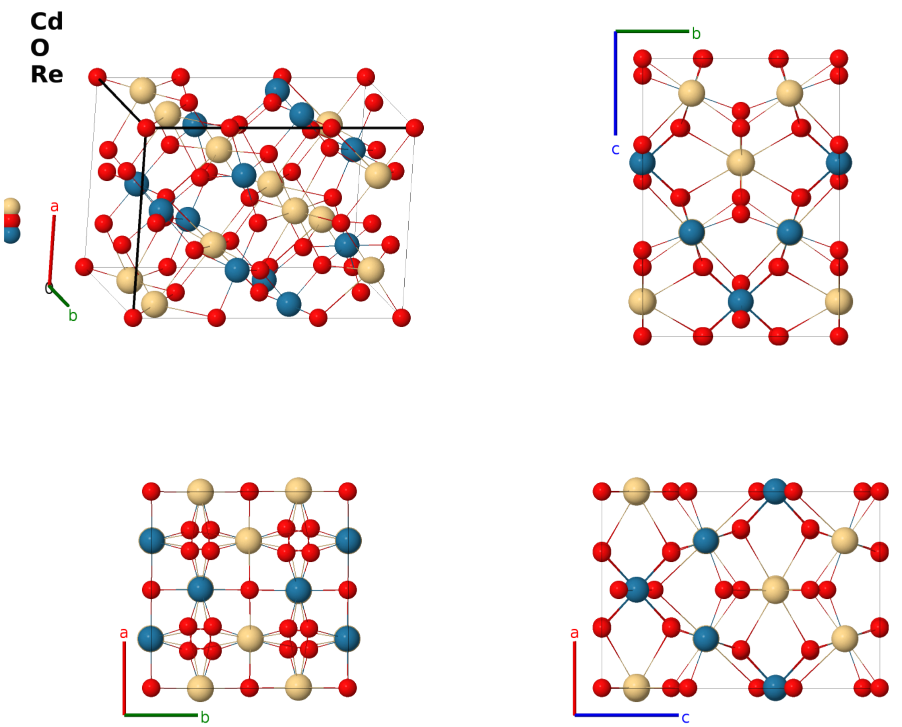
https://aflow.org/prototype-encyclopedia/XLYF

https://aflow.org/prototype-encyclopedia/A2B7C2_tI44_98_f_acde_f-001



Prototype	$Cd_2O_7Re_2$
AFLOW prototype label	A2B7C2_tI44_98_f_acde_f-001
Pearson symbol	tI44
Space group number	98
Space group symbol	$I4_122$
AFLOW prototype command	`aflow --proto=A2B7C2_tI44_98_f_acde_f-001` `--params=`$a, c/a, z_2, x_3, x_4, x_5, x_6$

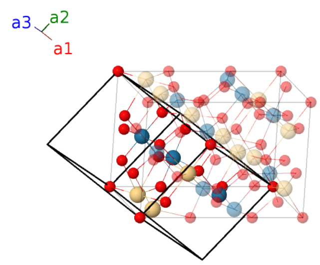
- $Cd_2Re_2O_7$ exhibits a number of phases. We will use the notation of (Kapcia, 2020) to describe them:

- Phase I: Above 200K the system takes on the cubic pyrochlore ($E8_1$) structure.
- Phase II: in the range 120-200K the system is in the tetragonal $I\bar{4}m2$ #119 structure.
- Phase III: in the range 80-120K the system is in the tetragonal $I4_122$ #98 structure (this structure).
- Phase IV: (Kapcia, 2020) did a first-principles study of this system and found that below 80K Phase III develops a soft phonon mode which transforms the system into an orthorhombic $F222$ #22 structure.

- There are many issues with all of these structures (Norman, 2020):
  - Phases II, III, and IV are all close to phase I. If we loosen the tolerance using AFLOW-SYM or FINDSYM the structures are seen to be equivalent to cubic pyrochlore.
  - Using the default tolerance, Phase II and Phase IV are equivalent.

Body-centered Tetragonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	O I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_4}$	=	$\left(z_2 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_5}$	=	$-\left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - \left(z_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_6}$	=	$-z_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2$	=	$-cz_2\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + 2x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8d)	O III
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - 2x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8d)	O III
$\mathbf{B_9}$	=	$\left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(8e)	O IV
$\mathbf{B_{12}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(8e)	O IV
$\mathbf{B_{13}}$	=	$-\left(x_4 - \frac{3}{4}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(2x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	O IV
$\mathbf{B_{14}}$	=	$\left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_4 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(2x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	O IV
$\mathbf{B_{15}}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \left(x_5 + \frac{1}{8}\right)\,\mathbf{a}_2 + \left(x_5 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8f)	Cd I
$\mathbf{B_{16}}$	=	$\frac{7}{8}\,\mathbf{a}_1 - \left(x_5 - \frac{1}{8}\right)\,\mathbf{a}_2 - \left(x_5 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8f)	Cd I

$$\begin{array}{lllllll}
\mathbf{B_{17}} & = & \left(x_5+\frac{7}{8}\right)\,\mathbf{a}_1+\frac{1}{8}\,\mathbf{a}_2+\left(x_5+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -\frac{1}{4}a\,\mathbf{\hat{x}}+a\left(x_5+\frac{1}{2}\right)\,\mathbf{\hat{y}}+\frac{3}{8}c\,\mathbf{\hat{z}} & \text{(8f)} & \text{Cd I} \\
\mathbf{B_{18}} & = & -\left(x_5-\frac{7}{8}\right)\,\mathbf{a}_1+\frac{5}{8}\,\mathbf{a}_2-\left(x_5-\frac{3}{4}\right)\,\mathbf{a}_3 & = & \frac{1}{4}a\,\mathbf{\hat{x}}-a\left(x_5-\frac{1}{2}\right)\,\mathbf{\hat{y}}+\frac{3}{8}c\,\mathbf{\hat{z}} & \text{(8f)} & \text{Cd I} \\
\mathbf{B_{19}} & = & \frac{3}{8}\,\mathbf{a}_1+\left(x_6+\frac{1}{8}\right)\,\mathbf{a}_2+\left(x_6+\frac{1}{4}\right)\,\mathbf{a}_3 & = & ax_6\,\mathbf{\hat{x}}+\frac{1}{4}a\,\mathbf{\hat{y}}+\frac{1}{8}c\,\mathbf{\hat{z}} & \text{(8f)} & \text{Re I} \\
\mathbf{B_{20}} & = & \frac{7}{8}\,\mathbf{a}_1-\left(x_6-\frac{1}{8}\right)\,\mathbf{a}_2-\left(x_6-\frac{3}{4}\right)\,\mathbf{a}_3 & = & -ax_6\,\mathbf{\hat{x}}+\frac{3}{4}a\,\mathbf{\hat{y}}+\frac{1}{8}c\,\mathbf{\hat{z}} & \text{(8f)} & \text{Re I} \\
\mathbf{B_{21}} & = & \left(x_6+\frac{7}{8}\right)\,\mathbf{a}_1+\frac{1}{8}\,\mathbf{a}_2+\left(x_6+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -\frac{1}{4}a\,\mathbf{\hat{x}}+a\left(x_6+\frac{1}{2}\right)\,\mathbf{\hat{y}}+\frac{3}{8}c\,\mathbf{\hat{z}} & \text{(8f)} & \text{Re I} \\
\mathbf{B_{22}} & = & -\left(x_6-\frac{7}{8}\right)\,\mathbf{a}_1+\frac{5}{8}\,\mathbf{a}_2-\left(x_6-\frac{3}{4}\right)\,\mathbf{a}_3 & = & \frac{1}{4}a\,\mathbf{\hat{x}}-a\left(x_6-\frac{1}{2}\right)\,\mathbf{\hat{y}}+\frac{3}{8}c\,\mathbf{\hat{z}} & \text{(8f)} & \text{Re I}
\end{array}$$

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First cited in

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