Phase II $Cd_2Re_2O_7$ Structure: A2B7C2_tI44_119_i_acefgh_i-001

This structure originally had the label `A2B7C2_tI44_119_i_bdefgh_i`. Calls to that address will be redirected here.

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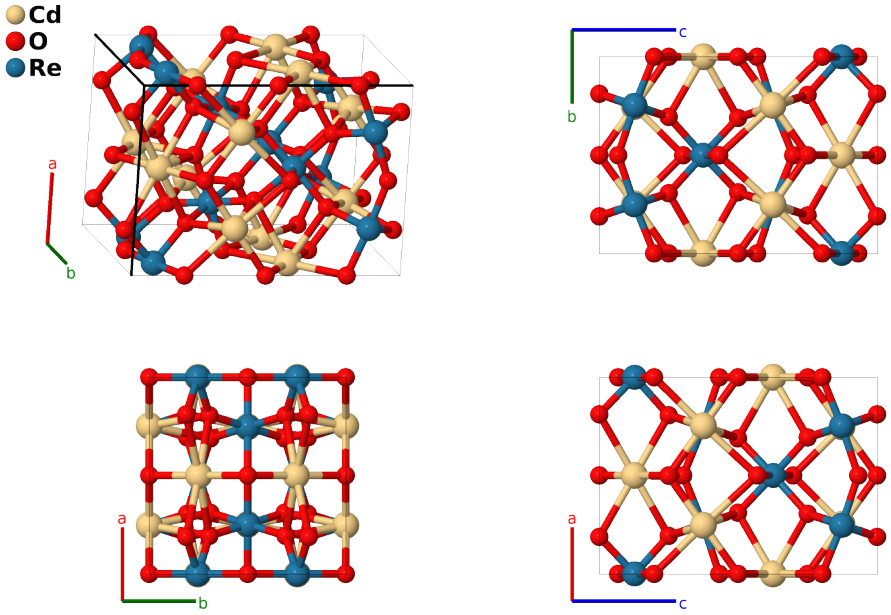
https://aflow.org/p/AZDB

https://aflow.org/p/A2B7C2_tI44_119_i_acefgh_i-001



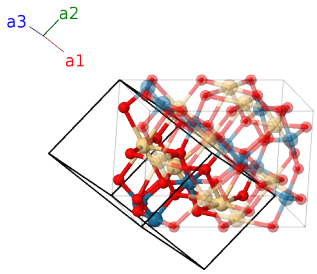
Prototype	$Cd_2O_7Re_2$
AFLOW prototype label	A2B7C2_tI44_119_i_acefgh_i-001
ICSD	none
Pearson symbol	tI44
Space group number	119
Space group symbol	$I\bar{4}m2$
AFLOW prototype command	`aflow --proto=A2B7C2_tI44_119_i_acefgh_i-001 --params=`$a, c/a, z_3, z_4, x_5, x_6, x_7, z_7, x_8, z_8$

- $Cd_2Re_2O_7$ 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. (this structure)
  - Phase III: in the range 80-120K the system is in the tetragonal $I4_122$ #98 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.
- Data for the Phase II structure was taken at 160K.

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	(2a)	O I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	O II
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_4}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_5}$	=	$\left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4f)	O IV
$\mathbf{B_6}$	=	$-z_4\,\mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_4\,\hat{\mathbf{z}}$	(4f)	O IV
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + 2x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}}$	(8g)	O V
$\mathbf{B_8}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - 2x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}}$	(8g)	O V
$\mathbf{B_9}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2$	=	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}}$	(8g)	O V
$\mathbf{B_{10}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$	=	$-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}}$	(8g)	O V
$\mathbf{B_{11}}$	=	$\left(x_6 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_6 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(2x_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8h)	O VI
$\mathbf{B_{12}}$	=	$-\left(x_6 - \frac{3}{4}\right)\,\mathbf{a}_1 - \left(x_6 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(2x_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8h)	O VI
$\mathbf{B_{13}}$	=	$-\left(x_6 - \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_6 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8h)	O VI
$\mathbf{B_{14}}$	=	$\left(x_6 + \frac{3}{4}\right)\,\mathbf{a}_1 - \left(x_6 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8h)	O VI
$\mathbf{B_{15}}$	=	$z_7\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + cz_7\,\hat{\mathbf{z}}$	(8i)	Cd I
$\mathbf{B_{16}}$	=	$z_7\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + cz_7\,\hat{\mathbf{z}}$	(8i)	Cd I
$\mathbf{B_{17}}$	=	$-(x_7 + z_7)\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8i)	Cd I
$\mathbf{B_{18}}$	=	$(x_7 - z_7)\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8i)	Cd I
$\mathbf{B_{19}}$	=	$z_8\,\mathbf{a}_1 + (x_8 + z_8)\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}}$	(8i)	Re I
$\mathbf{B_{20}}$	=	$z_8\,\mathbf{a}_1 - (x_8 - z_8)\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}}$	(8i)	Re I
$\mathbf{B_{21}}$	=	$-(x_8 + z_8)\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(8i)	Re I
$\mathbf{B_{22}}$	=	$(x_8 - z_8)\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(8i)	Re I

References

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[2] K. J. Kapcia, M. Reedyk, M. Hajialamdari, A. Ptok, P. Piekarz, A. Schulz, F. S. Razavi, R. K. Kremer, and A. M. Oleś, *Discovery of a low-temperature orthorhombic phase of the $Cd_2Re_2O_7$ superconductor*, Phys. Rev. Res. **2**, 033108 (2020), doi:10.1103/PhysRevResearch.2.033108.

Found in

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