Predicted Phase IV $Cd_2Re_2O_7$ Structure: A2B7C2_oF88_22_k_acefghij_k-001

This structure originally had the label `A2B7C2_oF88_22_k_bdefghij_k`. Calls to that address will be redirected here.

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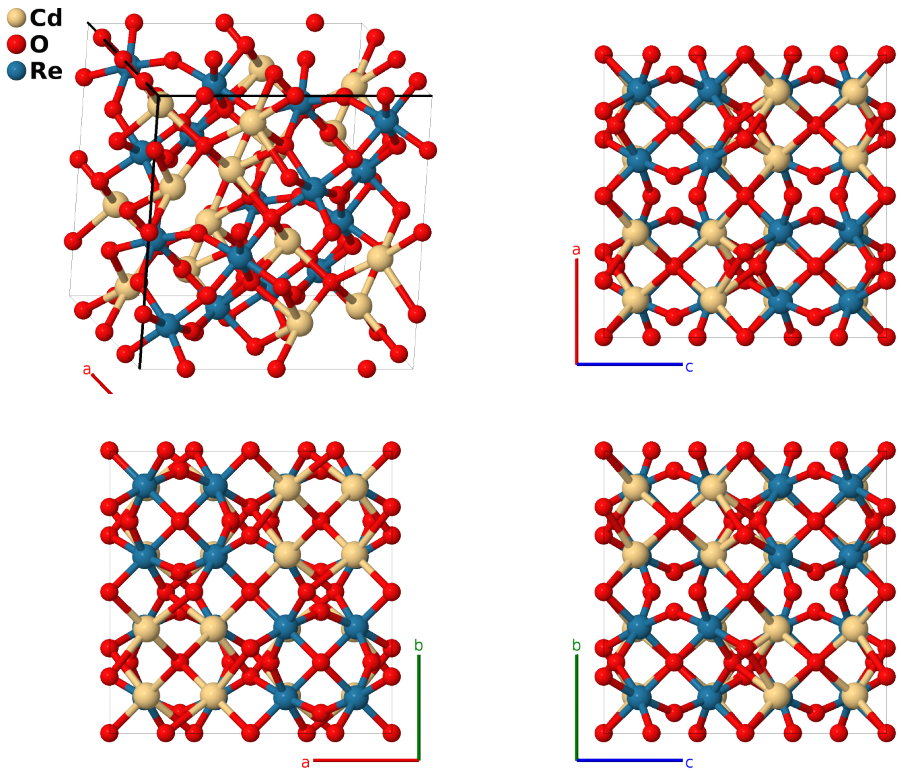
https://aflow.org/p/71CA

https://aflow.org/p/A2B7C2_oF88_22_k_acefghij_k-001



Prototype	$Cd_2O_7Re_2$
AFLOW prototype label	A2B7C2_oF88_22_k_acefghij_k-001
ICSD	none
Pearson symbol	oF88
Space group number	22
Space group symbol	$F222$
AFLOW prototype command	`aflow --proto=A2B7C2_oF88_22_k_acefghij_k-001 --params=`$a, b/a, c/a, x_3, y_4, z_5, z_6, y_7, x_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$

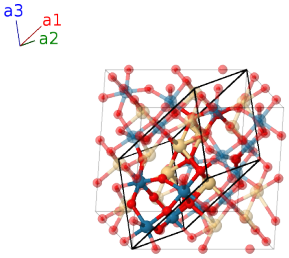
- $Cd_2Re_2O_7$ exhibits a number of phases. We will use the notation of (Kapcia, 2020) to describe them:
  - Phase I: Above 200K the system takes on the cubic pyrochlore ($E8_1$) structure.
  - Phase II: in the range 120-200K the system is in the tetragonal $I\bar{4}m2$ #119 structure.

  - Phase III: in the range 80-120K the system is in the tetragonal $I4_122$ #98 structure.
  - 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. (This 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.
- Although the default AFLOW tolerance makes this structure equivalent to Phase II, the published structure can be recovered using the command:
- aflow--proto=A2B7C2_oF88_22_k_acefghij_k:Cd:O:Re --params=a,c/a,z_3,z_4,x_5,x_6,x_7,z_7,x_8,z_8 --tolerance=0.001.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	O I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_3}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(8e)	O III
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(8e)	O III
$\mathbf{B_5}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}}$	(8f)	O IV
$\mathbf{B_6}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}}$	(8f)	O IV
$\mathbf{B_7}$	=	$z_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$cz_5\,\hat{\mathbf{z}}$	(8g)	O V
$\mathbf{B_8}$	=	$-z_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-cz_5\,\hat{\mathbf{z}}$	(8g)	O V
$\mathbf{B_9}$	=	$z_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8h)	O VI
$\mathbf{B_{10}}$	=	$-\left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8h)	O VI
$\mathbf{B_{11}}$	=	$y_7\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + y_7\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8i)	O VII
$\mathbf{B_{12}}$	=	$-\left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8i)	O VII
$\mathbf{B_{13}}$	=	$-\left(x_8 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8j)	O VIII
$\mathbf{B_{14}}$	=	$x_8\,\mathbf{a}_1 - \left(x_8 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_8 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8j)	O VIII
$\mathbf{B_{15}}$	=	$(-x_9 + y_9 + z_9)\,\mathbf{a}_1 + (x_9 - y_9 + z_9)\,\mathbf{a}_2 + (x_9 + y_9 - z_9)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(16k)	Cd I

$\mathbf{B_{16}}$	=	$(x_9 - y_9 + z_9)\ \mathbf{a}_1 +$ $(-x_9 + y_9 + z_9)\ \mathbf{a}_2 -$ $(x_9 + y_9 + z_9)\ \mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(16k)	Cd I
$\mathbf{B_{17}}$	=	$(x_9 + y_9 - z_9)\ \mathbf{a}_1 -$ $(x_9 + y_9 + z_9)\ \mathbf{a}_2 +$ $(-x_9 + y_9 + z_9)\ \mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(16k)	Cd I
$\mathbf{B_{18}}$	=	$-(x_9 + y_9 + z_9)\ \mathbf{a}_1 +$ $(x_9 + y_9 - z_9)\ \mathbf{a}_2 +$ $(x_9 - y_9 + z_9)\ \mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(16k)	Cd I
$\mathbf{B_{19}}$	=	$(-x_{10} + y_{10} + z_{10})\ \mathbf{a}_1 +$ $(x_{10} - y_{10} + z_{10})\ \mathbf{a}_2 +$ $(x_{10} + y_{10} - z_{10})\ \mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(16k)	Re I
$\mathbf{B_{20}}$	=	$(x_{10} - y_{10} + z_{10})\ \mathbf{a}_1 +$ $(-x_{10} + y_{10} + z_{10})\ \mathbf{a}_2 -$ $(x_{10} + y_{10} + z_{10})\ \mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(16k)	Re I
$\mathbf{B_{21}}$	=	$(x_{10} + y_{10} - z_{10})\ \mathbf{a}_1 -$ $(x_{10} + y_{10} + z_{10})\ \mathbf{a}_2 +$ $(-x_{10} + y_{10} + z_{10})\ \mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}}$	(16k)	Re I
$\mathbf{B_{22}}$	=	$-(x_{10} + y_{10} + z_{10})\ \mathbf{a}_1 +$ $(x_{10} + y_{10} - z_{10})\ \mathbf{a}_2 +$ $(x_{10} - y_{10} + z_{10})\ \mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}}$	(16k)	Re I

References

[1] 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.