Predicted Phase IV $Cd_2Re_2O_7$ Structure: A2B7C2_oF88_22_k_acefghij_k-001

This structure previously used the label(s) `A2B7C2_oF88_22_k_bdefghij_k`. Calls to these addresses will be redirected here.

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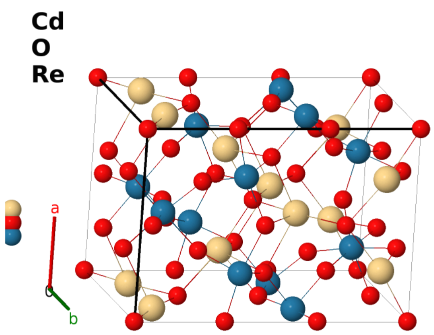
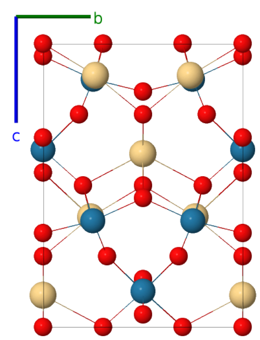
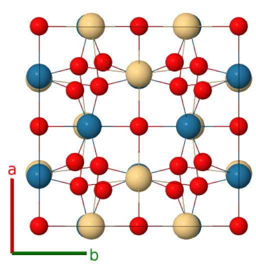
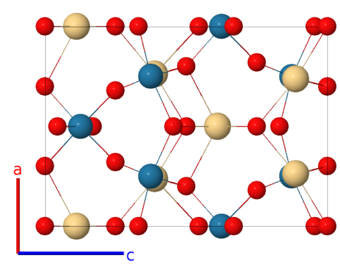
https://aflow.org/prototype-encyclopedia/71CA

https://aflow.org/prototype-encyclopedia/A2B7C2_oF88_22_k_acefghij_k-001









Prototype	$Cd_2O_7Re_2$
AFLOW prototype label	A2B7C2_oF88_22_k_acefghij_k-001
Pearson symbol	tI44
Space group number	82
Space group symbol	$I\bar{4}$
AFLOW prototype command	`aflow --proto=A2B7C2_oF88_22_k_acefghij_k-001` `--params=`$a, c/a, z_3, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

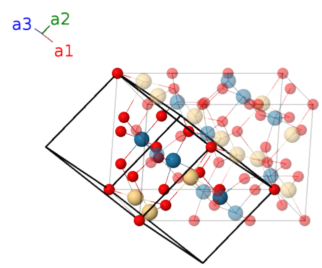
- $Cd_2Re_2O_7$ exhibits a number of phases. We will use the notation of (Kapcia, 2020) to describe them:

- 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.
- 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 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
$\mathbf{B_7}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8g)	Cd I
$\mathbf{B_8}$	=	$-(y_5 - z_5)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8g)	Cd I
$\mathbf{B_9}$	=	$-(x_5 + z_5)\,\mathbf{a}_1 + (y_5 - z_5)\,\mathbf{a}_2 - (x_5 - y_5)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8g)	Cd I
$\mathbf{B_{10}}$	=	$(x_5 - z_5)\,\mathbf{a}_1 - (y_5 + z_5)\,\mathbf{a}_2 + (x_5 - y_5)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8g)	Cd I
$\mathbf{B_{11}}$	=	$(y_6 + z_6)\,\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + (x_6 + y_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8g)	O V
$\mathbf{B_{12}}$	=	$-(y_6 - z_6)\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8g)	O V

$\mathbf{B_{13}}$	=	$-\left(x_6+z_6\right)\,\mathbf{a}_1+\left(y_6-z_6\right)\,\mathbf{a}_2-\left(x_6-y_6\right)\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}}$	(8g)	O V
$\mathbf{B_{14}}$	=	$\left(x_6-z_6\right)\,\mathbf{a}_1-\left(y_6+z_6\right)\,\mathbf{a}_2+\left(x_6-y_6\right)\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}}+ax_6\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}}$	(8g)	O V
$\mathbf{B_{15}}$	=	$\left(y_7+z_7\right)\,\mathbf{a}_1+\left(x_7+z_7\right)\,\mathbf{a}_2+\left(x_7+y_7\right)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}}+ay_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(8g)	O VI
$\mathbf{B_{16}}$	=	$-\left(y_7-z_7\right)\,\mathbf{a}_1-\left(x_7-z_7\right)\,\mathbf{a}_2-\left(x_7+y_7\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}}-ay_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(8g)	O VI
$\mathbf{B_{17}}$	=	$-\left(x_7+z_7\right)\,\mathbf{a}_1+\left(y_7-z_7\right)\,\mathbf{a}_2-\left(x_7-y_7\right)\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{x}}-ax_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$	(8g)	O VI
$\mathbf{B_{18}}$	=	$\left(x_7-z_7\right)\,\mathbf{a}_1-\left(y_7+z_7\right)\,\mathbf{a}_2+\left(x_7-y_7\right)\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{x}}+ax_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$	(8g)	O VI
$\mathbf{B_{19}}$	=	$\left(y_8+z_8\right)\,\mathbf{a}_1+\left(x_8+z_8\right)\,\mathbf{a}_2+\left(x_8+y_8\right)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}+ay_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8g)	Re I
$\mathbf{B_{20}}$	=	$-\left(y_8-z_8\right)\,\mathbf{a}_1-\left(x_8-z_8\right)\,\mathbf{a}_2-\left(x_8+y_8\right)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}-ay_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8g)	Re I
$\mathbf{B_{21}}$	=	$-\left(x_8+z_8\right)\,\mathbf{a}_1+\left(y_8-z_8\right)\,\mathbf{a}_2-\left(x_8-y_8\right)\,\mathbf{a}_3$	=	$ay_8\,\hat{\mathbf{x}}-ax_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(8g)	Re I
$\mathbf{B_{22}}$	=	$\left(x_8-z_8\right)\,\mathbf{a}_1-\left(y_8+z_8\right)\,\mathbf{a}_2+\left(x_8-y_8\right)\,\mathbf{a}_3$	=	$-ay_8\,\hat{\mathbf{x}}+ax_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(8g)	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.

First cited in

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