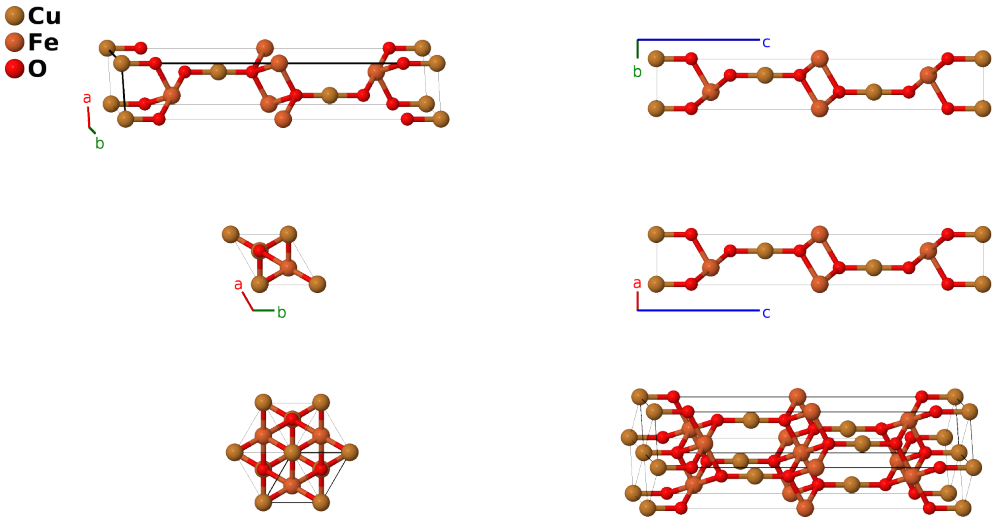
Rhombohedral Delafossite ($CuFeO_2$) Structure: ABC2_hR4_166_a_b_c-004

This structure originally had the label `ABC2_hR4_166_a_b_c.CuFeO2`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

https://aflow.org/p/Y8C3

https://aflow.org/p/ABC2_hR4_166_a_b_c-004



Prototype	$CuFeO_2$
AFLOW prototype label	ABC2_hR4_166_a_b_c-004
Mineral name	delafossite
ICSD	31918
Pearson symbol	hR4
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=ABC2_hR4_166_a_b_c-004 --params=`$a, c/a, x_3$

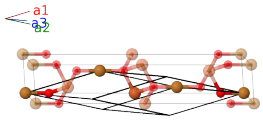
Other compounds with this structure
$AgAlO_2$, $AgCoO_2$, $AgCrO_2$, $AgFeO_2$, $AgGaO_2$, $AgInO_2$, $AgNiO_2$, $AgRhO_2$, $AgScO_2$, $AgTlO_2$, $CuAlO_2$, $CuCoO_2$, $CuCrO_2$, $CuEuO_2$, $CuGaO_2$, $CuInO_2$, $CuLaO_2$, $CuPrO_2$, $CuRhO_2$, $CuScO_2$, $CuYO_2$, $NiLaO_2$, $NiPrO_2$, $PdCoO_2$, $PdCrO_2$, $PdRhO_2$, $PtCoO_2$

- Delafossite appears in two forms which differ in the stacking of the layers: rhombohedral, shown here, and hexagonal, prototype $CuAlO_2$. Most of the structures found in the hexagonal phase can also be found in the rhombohedral structure (Marquardt, 2006).

- Rhombohedral delafossite has the same AFLOW label, ABC2_hR4_166_a_b_c, as caswellsilverite $CrNaS_2$, $F5_1$ and α-$NaFeO_2$.
- The difference in the internal parameter z_3 between $CuFeO_2$ and $CrNaS_2$ causes a large change in the bonding of the two crystals, so we present them as different structures.
- The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Fe I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	O I

References

[1] C. T. Prewitt, R. D. Shannon, and D. B. Rogers, *Chemistry of noble metal oxides. II. Crystal structures of platinum cobalt dioxide, palladium cobalt dioxide, coppper iron dioxide, and silver iron dioxide*, Inorg. Chem. **10**, 719–723 (1971), doi:10.1021/ic50098a012.

Found in

[1] M. A. Marquardt, N. A. Ashmore, and D. P. Cann, *Crystal chemistry and electrical properties of the delafossite structure*, Thin Solid Films **496**, 146–156 (2006), doi:10.1016/j.tsf.2005.08.316.