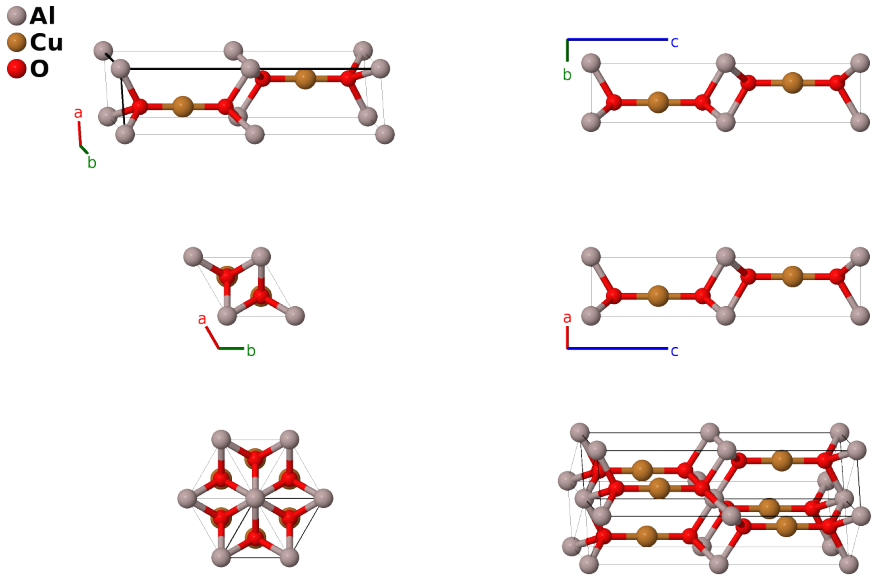
Hexagonal Delafossite ($CuFeO_2$) Structure: ABC2_hP8_194_a_c_f-005

This structure originally had the label `ABC2_hP8_194_a_c_f`. 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/Y6AL

https://aflow.org/p/ABC2_hP8_194_a_c_f-005



Prototype	$CuFeO_2$
AFLOW prototype label	ABC2_hP8_194_a_c_f-005
Mineral name	delafossite
ICSD	60845
Pearson symbol	hP8
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=ABC2_hP8_194_a_c_f-005 --params=`$a, c/a, z_3$

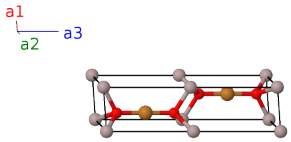
Other compounds with this structure

$AlCCr_2$, $AlCNb_2$, $AlCTa_2$, $AlCTi_2$, $AlCV_2$, $AsCNb_2$, $AsCV_2$, $AlCuO_2$, $BBiHf_2$, $BPbHf_2$, $CdCTi_2$, $CuAlO_2$, $CuGaO_2$, $CuScO_2$, $CuYO_2$, $GaCCr_2$, $GaCMo_2$, $GaCNb_2$, $GaCTa_2$, $GaCTi_2$, $GaCV_2$, $GaNTi_2$, $GeCCr_2$, $GeCTi_2$, $GeCV_2$, $InCHf_2$, $InCNb_2$, $InCTi_2$, $InCZr_2$, $InNTi_2$, $InNZr_2$, $PbCHf_2$, $PbCTi_2$, $PbCZr_2$, $SCNb_2$, $SCTi_2$, $SCZr_2$, $SCZr_2$, $SeCZr_2$, $SnCHf_2$, $SnCNb_2$, $SnCZr_2$, $TlCHf_2$, $TlCTi_2$, $TlCZr_2$

- Delafossite appears in two forms which differ in the stacking of the layers: rhombohedral, prototype $CuFeO_2$, and hexagonal, shown here. Most of the structures found in the hexagonal phase can also be found in the rhombohedral structure (Marquardt, 2006).

Hexagonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Cu I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Cu I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4f)	O I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	O I
$\mathbf{B_7}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4f)	O I
$\mathbf{B_8}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	O I

References

[1] B. U. Köhler and M. Jansen, *Darstellung und Strukturdaten von „Delafossiten" $CuMO_2$ (M = Al, Ga, Sc, Y)*, Z. Anorganische und Allgemeine Chemie **543**, 73–80 (1986), doi:10.1002/zaac.19865431209.

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.