Grimaldiite (α-CrOOH) Structure: ABC2_hR4_160_a_a_2a-002

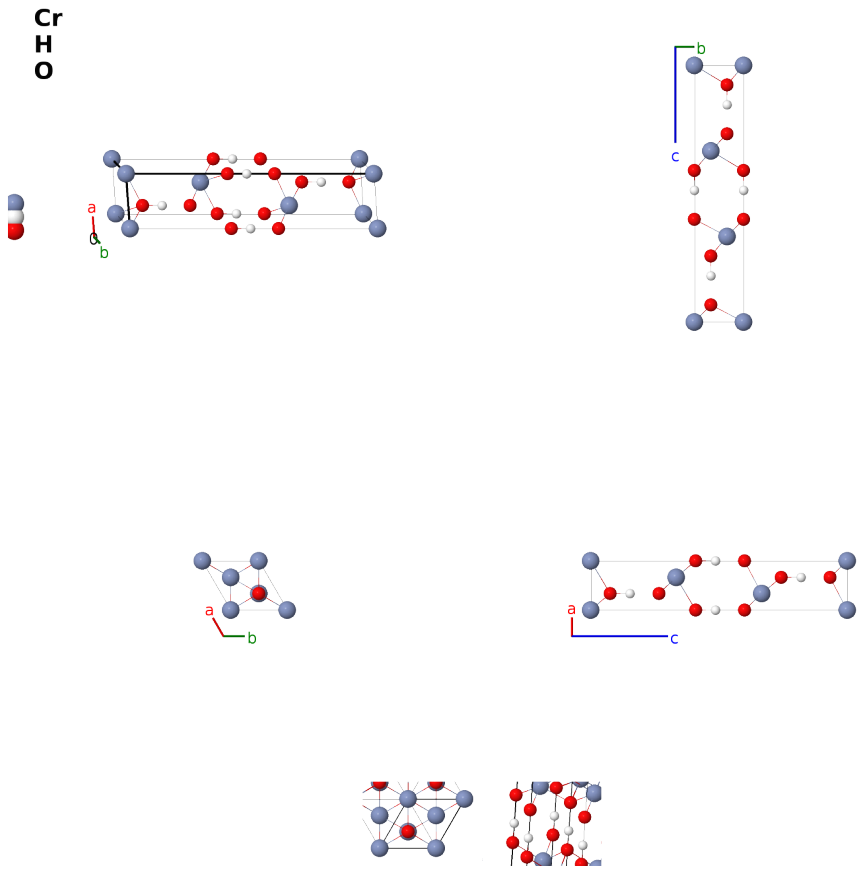
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/prototype-encyclopedia/LP35

https://aflow.org/prototype-encyclopedia/ABC2_hR4_160_a_a_2a-002



Prototype	$CrHO_2$
AFLOW prototype label	ABC2_hR4_160_a_a_2a-002
Mineral name	grimaldiite
ICSD	64754
CCDC	1626933
Pearson symbol	hR4
Space group number	160
Space group symbol	$R3m$

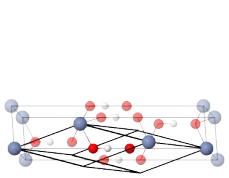
AFLOW prototype command `aflow --proto=ABC2_hR4_160_a_a_2a-002 --params=`$a, c/a, x_1, x_2, x_3, x_4$

Other compounds with this structure
$NaNiO_2$

- CrOOH is found naturally in three forms. They are usually found together with Cr_2O_3 in a mineral known as merumite (Milton, 1976):
  - Grimaldiite, rhombohedral α-CrOOH (this structure),
  - Guyanaite, orthorhombic β-CrOOH, and
  - Bracewellite, orthorhombic γ-CrOOH is in the Lepidocrocite (γ-FeOOH, $E0_4$) structure.
- We use the $R3m$ data from Table IIIa (Christensen,1977), which locates the hydrogen atoms.
- Space group $R3m$ #160 does not specify the origin of the z-axis. Here we choose $z_I = 0$ for the position of the chromium atom.
- α-CrOOH and $CrCuS_2$ have the AFLOW prototype label, ABC2_hR4_160_a_a_2a. They 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(1a)	Cr I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(1a)	H I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(1a)	O I
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(1a)	O II

References

[1] A. N. Christensen, P. Hansen, and M. S. Lehmann, *Isotope effects in the bonds of α-CrOOH and α-CrOOD*, J. Solid State Chem. **21**, 325–329 (1977), doi:10.1016/0022-4596(77)90130-X.

[2] C. Milton, D. E. Appleman, M. H. Appleman, E. C. T. Chao, F. Cuttitta, J. I. Dinnin, E. J. Dwornik, B. L. Ingram, and J. H. J. Rose, *Merumite – A Complex Assemblage of Chromium Minerals from Guyanna* (1976). Geological Survey Professional Paper 887.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.