

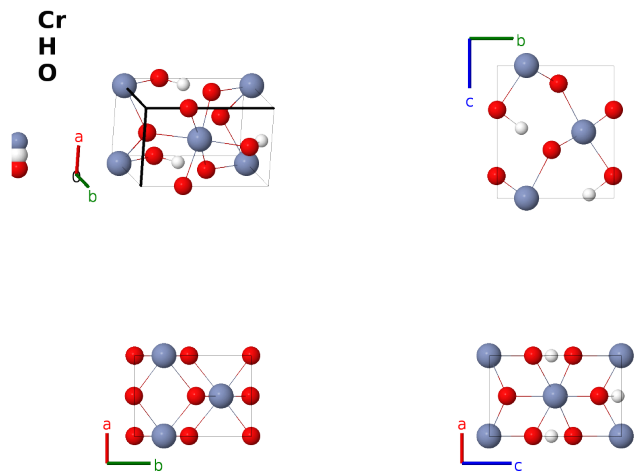
Guyanaite (β -CrOOH) Structure: ABC2_oP8_31_a_a_2a-001

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/TZ68>

https://aflow.org/prototype-encyclopedia/ABC2_oP8_31_a_a_2a-001



Prototype	CrHO ₂
AFLOW prototype label	ABC2_oP8_31_a_a_2a-001
Mineral name	guyanaite
Pearson symbol	oP8
Space group number	31
Space group symbol	<i>Pmn</i> 2 ₁
AFLOW prototype command	<code>aflow --proto=ABC2_oP8_31_a_a_2a-001</code> <code>--params=a, b/a, c/a, y₁, z₁, y₂, z₂, y₃, z₃, y₄, z₄</code>

Other compounds with this structure

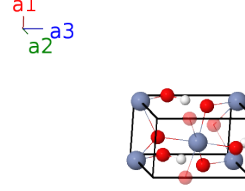
InOOH

- CrOOH is found naturally in three forms. They are usually found together with Cr₂O₃ in a mineral known as merumite (Milton, 1976):
 - Grimaldiite, rhombohedral α -CrOOH,
 - Guyanaite, orthorhombic β -CrOOH (this structure), and
 - Bracewellite, orthorhombic γ -CrOOH is in the Lepidocrocite (γ -FeOOH, *E*0₄) structure.

- (Jahn, 2012) give the data for this structure in the $P2_1nm$ setting of space group #31. We use FINDSYM to transform this to the standard $Pmn2_1$ setting.
- Space group $Pmn2_1$ #31 does not specify the origin of the z -axis. We choose it by setting $z_1 = 0$ for the position of the chromium atom.

Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2a)	Cr I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Cr I
$\mathbf{B}_3$	$= y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2a)	H I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	H I
$\mathbf{B}_5$	$= y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_7$	$= y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	O II

References

- [1] S. Jahn, B. Wunder, M. Koch-Müller, L. Tarrieu, M. Pöhle, A. Watenphul, and M. N. Taran, *Pressure-induced hydrogen bond symmetrisation in guyanaite, β -CrOOH: evidence from spectroscopy and ab initio simulations*, Eur. J. Mineral. **24**, 839–850 (2012), doi:10.1127/0935-1221/2012/0024-2228.
- [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.

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.