Guyanaite (β-CrOOH) Structure: ABC2_oP8_31_a_a_2a-001

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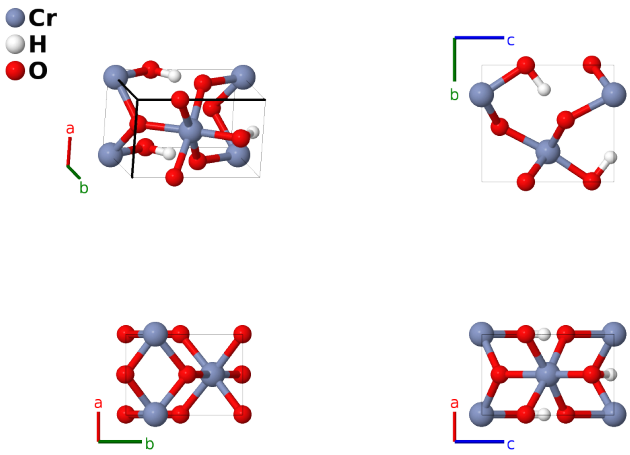
https://aflow.org/p/TZ68

https://aflow.org/p/ABC2_oP8_31_a_a_2a-001



Prototype	$CrHO_2$
AFLOW prototype label	ABC2_oP8_31_a_a_2a-001
Mineral name	guyanaite
ICSD	none
Pearson symbol	oP8
Space group number	31
Space group symbol	$Pmn2_1$
AFLOW prototype command	`aflow --proto=ABC2_oP8_31_a_a_2a-001 --params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3, y_4, z_4$

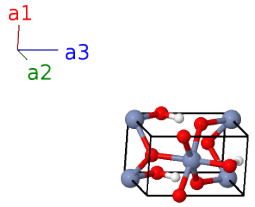
Other compounds with this structure
InOOH

- 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,
  - Guyanaite, orthorhombic β-CrOOH (this structure), and
  - Bracewellite, orthorhombic γ-CrOOH is in the Lepidocrocite (γ-FeOOH, $E0_4$) 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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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.