



*hP*146

(176)  $P6_3/m - i^{10}h^3fda$



Structural features:  $\text{Cr}_3\text{O}(\text{H}_2\text{O})_3(\text{O}_2\text{CCF}_3)_6$  units (a ring of three vertex-linked  $\text{Cr}(\text{O}_5[\text{OH}_2])$  octahedra sharing vertices with three  $\text{O}_2\text{C-CF}_3$  units on each side; partial rotational disorder for  $\text{CF}_3$  in a Mg-type (h.c.p.) arrangement;  $\text{NO}_3$  trigonal units (partial orientational disorder) and additional  $\text{H}_2\text{O}$  between the units.

Glazunova T.Y. et al. (2004) [1]



$a = 0.9893$ ,  $c = 1.9366$  nm,  $c/a = 1.958$ ,  $V = 1.6414$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	12 <i>i</i>	1	0.099	0.374	0.0788	0.3	
F2	12 <i>i</i>	1	0.1244	0.3298	0.1008	0.7	
F3	12 <i>i</i>	1	0.174	0.048	0.088	0.3	
F4	12 <i>i</i>	1	0.2132	0.083	0.0657	0.7	
C5	12 <i>i</i>	1	0.2971	0.0277	0.08859		7-vertex polyhedron F <sub>6</sub> C
F6	12 <i>i</i>	1	0.386	0.111	0.0401	0.3	
F7	12 <i>i</i>	1	0.3892	0.0404	0.0383	0.7	
O8	12 <i>i</i>	1	0.38952	0.22632	0.17386		single atom C
C9	12 <i>i</i>	1	0.3918	0.1087	0.15414		non-coplanar triangle O <sub>2</sub> C
O10	12 <i>i</i>	1	0.46348	0.04679	0.17866		single atom C
O11	6 <i>h</i>	<i>m</i> ..	0.0295	0.1378	<sup>1</sup> / <sub>4</sub>		single atom N
O12	6 <i>h</i>	<i>m</i> ..	0.3096	0.4034	<sup>1</sup> / <sub>4</sub>		single atom Cr
Cr13	6 <i>h</i>	<i>m</i> ..	0.49678	0.37365	<sup>1</sup> / <sub>4</sub>		octahedron O <sub>6</sub>
O14	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1718		non-coplanar triangle O <sub>3</sub>
O15	2 <i>d</i>	-6..	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		coplanar triangle Cr <sub>3</sub>
N16	2 <i>a</i>	-6..	0	0	<sup>1</sup> / <sub>4</sub>		coplanar triangle O <sub>3</sub>
H17	12 <i>i</i>	1	0.304	0.591	0.1433	0.67	
H18	12 <i>i</i>	1	0.313	0.471	0.219	0.5	
H19	6 <i>h</i>	<i>m</i> ..	0.229	0.326	<sup>1</sup> / <sub>4</sub>		

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.036, T = 293 K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Short interatomic distances for partly occupied site(s). We assume that in [1] the chemical formula is misprinted as  $[\text{Cr}_3(\mu_3\text{-O})(\text{CF}_3\text{COO})_6(\text{H}_2\text{O})_3](\text{NO}_3)(\text{H}_2\text{O})$  instead of  $[\text{Cr}_3(\mu_3\text{-O})(\text{CF}_3\text{COO})_6(\text{H}_2\text{O})_3](\text{NO}_3)(\text{H}_2\text{O})_2$  (given in the cif file, in agreement with the refinement).

References: [1] Glazunova T.Y., Boltalin A.I., Troyanov S.I. (2004), Mendelev Comm. 14, 141-143.