

$\text{Mn}_3[\text{CCl}_3\text{CO}_2]_6\text{O}[\text{H}_2\text{O}]_6$	$hP112$	$(176) P6_3/m - i^8h^2ca$
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$\text{Mn}_3\text{O}(\text{O}_2\text{CCCl}_3)_6(\text{H}_2\text{O})_3 \cdot 3\text{H}_2\text{O}$ [1]

Structural features: $\text{Mn}_3\text{O}(\text{H}_2\text{O})_3(\text{O}_2\text{CCCl}_3)_6$ units (a ring of three vertex-linked $\text{Mn}(\text{O}_5[\text{OH}_2])$ octahedra sharing vertices with three $\text{O}_2\text{C}-\text{CCl}_3$ units on each side) in a Mg-type (h.c.p.) arrangement; additional H_2O between the units (partial disorder).

Tsai H.L. et al. (2003) [1]

$\text{C}_{12}\text{Cl}_{18}\text{H}_{12}\text{Mn}_3\text{O}_{19}$

$a = 1.00741$, $c = 2.28668$ nm, $c/a = 2.270$, $V = 2.0098$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	12i	1	0.0184	0.3484	0.1023		tetrahedron CCl_3
O2	12i	1	0.0472	0.5037	0.1847		single atom C
C3	12i	1	0.085	0.4181	0.1636		coplanar triangle O_2C
O4	12i	1	0.1681	0.3776	0.185		single atom C
Cl5	12i	1	0.1708	0.397	0.05413		single atom C
Cl6	12i	1	0.2406	0.09332	0.10942		single atom C
Cl7	12i	1	0.51661	0.09841	0.07412		single atom C
(OH ₂)8	12i	1	0.5736	0.2914	0.2014	0.333	non-colinear (OH ₂) ₂
Mn9	6h	$m..$	0.33156	0.47484	$\frac{1}{4}$		octahedron $\text{O}_5(\text{OH}_2)$
(OH ₂)10	6h	$m..$	0.333	0.2754	$\frac{1}{4}$		single atom Mn
O11	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle Mn_3
(OH ₂)12	2a	-6..	0	0	$\frac{1}{4}$		coplanar triangle (OH ₂) ₃

Transformation from published data: $y, x, -z$; origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.066$, $T = 295$ K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Tsai H.L., Jwo T.Y., Yang C.I., Wur C.S., Lee G.H., Wang Y. (2003), J. Chin. Chem. Soc. Taipei 50, 1139-1146.