

Table S1. Crystal data and structure refinement for Tm(OAc)2Cl·x_3H2O.

Identification code	Ha2019_92_0m_a
Empirical formula	C4 H12 Cl O7 Tm
Formula weight	376.52
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.7747(2) Å b = 7.8392(2) Å β = 97.552(1) deg. c = 17.1517(5) Å
Volume	1036.28(5) Å ³
Z, Calculated density	4, 2.413 Mg/m ³
Absorption coefficient	8.823 mm ⁻¹
F(000)	712
Crystal size	0.465 x 0.120 x 0.074 mm
Theta range for data collection	2.755 to 27.994 deg.
Limiting indices	-10 ≤ h ≤ 10, -10 ≤ k ≤ 10, -22 ≤ l ≤ 22
Reflections collected / unique	108715 / 2504 [R(int) = 0.0397]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.753 and 0.389
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2504 / 0 / 126
Goodness-of-fit on F ²	1.132
Final R indices [I > 2σ(I)]	R1 = 0.0108, wR2 = 0.0240
R indices (all data)	R1 = 0.0113, wR2 = 0.0241
Extinction coefficient	n/a
Largest diff. peak and hole	0.386 and -0.579 e.Å ⁻³

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Tm}(\text{OAc})_2\text{Cl} \cdot 3\text{H}_2\text{O}$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U (eq)
Tm(1)	2752(1)	4481(1)	5413(1)	8(1)
Cl(1)	3757(1)	9578(1)	6839(1)	15(1)
O(11)	207(2)	3216(2)	5434(1)	17(1)
O(12)	-2622(2)	2902(2)	5255(1)	13(1)
C(11)	-1125(2)	2358(2)	5511(1)	10(1)
C(12)	-962(3)	646(3)	5900(1)	19(1)
O(21)	5419(2)	5634(2)	5745(1)	11(1)
O(22)	8153(2)	6319(2)	5911(1)	12(1)
C(21)	6789(2)	6010(2)	6209(1)	10(1)
C(22)	6766(3)	6067(3)	7075(1)	17(1)
O(1W)	4106(2)	1824(2)	5374(1)	13(1)
O(2W)	1650(2)	6399(2)	6251(1)	12(1)
O(3W)	3197(2)	3458(2)	6718(1)	16(1)

Table S3. Bond lengths [Å] and angles [deg] for Tm(OAc)2Cl_x_3H2O.

Tm(1)-O(11)	2.218(1)
Tm(1)-O(21)	2.265(1)
Tm(1)-O(2W)	2.320(1)
Tm(1)-O(1W)	2.339(1)
Tm(1)-O(12)#1	2.346(1)
Tm(1)-O(3W)	2.360(1)
Tm(1)-O(22)#2	2.373(1)
Tm(1)-O(21)#2	2.592(1)
Tm(1)-O(11)#1	3.128(2)
Tm(1)-Tm(1)#2	4.0237(2)
Tm(1)-Tm(1)#1	4.4037(2)
O(11)-C(11)	1.257(2)
O(12)-C(11)	1.263(2)
C(11)-C(12)	1.497(3)
O(21)-C(21)	1.278(2)
O(22)-C(21)	1.260(2)
C(21)-C(22)	1.487(3)
O(11)-Tm(1)-O(21)	164.53(5)
O(11)-Tm(1)-O(2W)	82.94(5)
O(21)-Tm(1)-O(2W)	89.22(5)
O(11)-Tm(1)-O(1W)	90.45(5)
O(21)-Tm(1)-O(1W)	87.83(5)
O(2W)-Tm(1)-O(1W)	143.07(5)
O(11)-Tm(1)-O(12)#1	114.67(5)
O(21)-Tm(1)-O(12)#1	75.71(5)
O(2W)-Tm(1)-O(12)#1	74.94(5)
O(1W)-Tm(1)-O(12)#1	139.07(5)
O(11)-Tm(1)-O(3W)	81.55(5)
O(21)-Tm(1)-O(3W)	83.23(5)
O(2W)-Tm(1)-O(3W)	69.70(5)
O(1W)-Tm(1)-O(3W)	73.40(5)
O(12)#1-Tm(1)-O(3W)	138.80(5)
O(11)-Tm(1)-O(22)#2	75.15(5)
O(21)-Tm(1)-O(22)#2	119.51(4)
O(2W)-Tm(1)-O(22)#2	132.61(5)
O(1W)-Tm(1)-O(22)#2	79.32(5)
O(12)#1-Tm(1)-O(22)#2	76.99(5)
O(3W)-Tm(1)-O(22)#2	143.73(5)
O(11)-Tm(1)-O(21)#2	125.23(5)
O(21)-Tm(1)-O(21)#2	68.29(5)
O(2W)-Tm(1)-O(21)#2	141.41(4)
O(1W)-Tm(1)-O(21)#2	69.68(4)
O(12)#1-Tm(1)-O(21)#2	69.43(4)
O(3W)-Tm(1)-O(21)#2	133.49(4)
O(22)#2-Tm(1)-O(21)#2	51.72(4)
O(11)-Tm(1)-O(11)#1	70.25(5)
O(21)-Tm(1)-O(11)#1	118.66(4)
O(2W)-Tm(1)-O(11)#1	66.69(4)
O(1W)-Tm(1)-O(11)#1	143.80(4)
O(12)#1-Tm(1)-O(11)#1	44.47(4)
O(3W)-Tm(1)-O(11)#1	130.07(4)
O(22)#2-Tm(1)-O(11)#1	66.46(4)
O(21)#2-Tm(1)-O(11)#1	96.22(4)
Tm(1)#2-Tm(1)-Tm(1)#1	134.557(4)

C (11)-O (11)-Tm (1)	172.1 (1)
C (11)-O (12)-Tm (1) #1	116.4 (1)
O (11)-C (11)-O (12)	121.1 (2)
O (11)-C (11)-C (12)	120.3 (2)
O (12)-C (11)-C (12)	118.6 (2)
C (21)-O (21)-Tm (1)	155.4 (1)
C (21)-O (21)-Tm (1) #2	89.4 (1)
Tm (1)-O (21)-Tm (1) #2	111.7 (1)
C (21)-O (22)-Tm (1) #2	100.3 (1)
O (22)-C (21)-O (21)	117.9 (2)
O (22)-C (21)-C (22)	121.4 (2)
O (21)-C (21)-C (22)	120.7 (2)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z+1 #2 -x+1,-y+1,-z+1

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Tm(OAc)₂Cl₂·3H₂O.

The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Tm(1)	6(1)	9(1)	10(1)	0(1)	1(1)	-1(1)
Cl(1)	18(1)	12(1)	16(1)	1(1)	2(1)	-2(1)
O(11)	12(1)	19(1)	20(1)	-5(1)	6(1)	-6(1)
O(12)	8(1)	14(1)	16(1)	3(1)	2(1)	1(1)
C(11)	9(1)	12(1)	9(1)	-2(1)	2(1)	0(1)
C(12)	19(1)	15(1)	22(1)	6(1)	1(1)	3(1)
O(21)	6(1)	13(1)	12(1)	0(1)	0(1)	-1(1)
O(22)	7(1)	15(1)	14(1)	0(1)	1(1)	-1(1)
C(21)	10(1)	7(1)	14(1)	0(1)	1(1)	2(1)
C(22)	15(1)	24(1)	12(1)	-1(1)	1(1)	2(1)
O(1W)	12(1)	12(1)	15(1)	2(1)	4(1)	2(1)
O(2W)	10(1)	12(1)	16(1)	-2(1)	1(1)	-1(1)
O(3W)	21(1)	13(1)	14(1)	2(1)	6(1)	3(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Tm}(\text{OAc})_2\text{Cl} \cdot 3\text{H}_2\text{O}$.

	x	y	z	U (eq)
H(12A)	201	527	6194	52 (6)
H(12B)	-1149	-250	5500	52 (6)
H(12C)	-1832	541	6262	52 (6)
H(22A)	7947	5910	7344	52 (5)
H(22B)	6018	5155	7229	52 (5)
H(22C)	6317	7174	7221	52 (5)
H(11W)	4110	990	5784	44 (6)
H(12W)	5290	1895	5275	44 (6)
H(21W)	427	6539	6263	40 (6)
H(22W)	2154	7475	6423	40 (6)
H(31W)	2623	3934	7130	46 (6)
H(32W)	3415	2289	6867	46 (6)

Table S6. Hydrogen bonds for Tm(OAc)₂Cl_x_3H₂O [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(11W)...Cl(1)#3	0.96	2.17	3.109(1)	165.9
O(1W)-H(12W)...O(12)#4	0.96	1.81	2.714(2)	155.8
O(2W)-H(21W)...O(22)#5	0.96	1.80	2.705(2)	156.1
O(2W)-H(22W)...Cl(1)	0.96	2.13	3.079(1)	168.3
O(3W)-H(31W)...Cl(1)#6	0.96	2.24	3.193(1)	170.1
O(3W)-H(32W)...Cl(1)#3	0.96	2.14	3.076(2)	163.4

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1 #2 -x+1,-y+1,-z+1 #3 x,y-1,z
#4 x+1,y,z #5 x-1,y,z #6 -x+1/2,y-1/2,-z+3/2