Table S1. Crystal data and structure refinement for Tb(OAc)2Cl_x_3H2O.

Identification code	Ha2019_98_0m_a
Empirical formula	C4 H12 Cl O7 Tb
Formula weight	366.51
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.8003(2) A b = 7.8539(2) A ß = 98.075(2) deg. c = 17.3942(5) A
Volume	1055.05(5) A^3
Z, Calculated density	4, 2.307 Mg/m^3
Absorption coefficient	6.960 mm^-1
F(000)	696
Crystal size	0.325 x 0.102 x 0.050 mm
Theta range for data collection	2.735 to 27.995 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -22<=l<=22
Reflections collected / unique	126109 / 2551 [R(int) = 0.0517]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.761 and 0.486
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2551 / 0 / 125
Goodness-of-fit on F^2	1.054
Final R indices [I>2sigma(I)]	R1 = 0.0108, wR2 = 0.0245
R indices (all data)	R1 = 0.0131, wR2 = 0.0253
Extinction coefficient	n/a
Largest diff. peak and hole	0.486 and -0.392 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Tb(OAc)2Cl_x_3H2O. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Tb(1)	2663(1)	4580(1)	5383(1)	9(1)
Cl(1)	3814(1)	9679(1)	6885(1)	16(1)
O(11)	-1(2)	3336(2)	5373(1)	17(1)
O(12)	-2748(2)	2708(2)	5262(1)	15(1)
C(11)	-1197(2)	2325(2)	5497(1)	12(1)
C(12)	-792(3)	684(3)	5917(1)	22(1)
O(21)	5449(2)	5618(2)	5741(1)	12(1)
O(22)	8186(2)	6281(2)	5957(1)	14(1)
C(21)	6792(2)	5989(2)	6222(1)	12(1)
C(22)	6700(2)	6059(3)	7071(1)	18(1)
O(1W)	3948(2)	1799(2)	5372(1)	14(1)
O(2W)	1680(2)	6561(2)	6252(1)	14(1)
O(3W)	3036(2)	3500(2)	6688(1)	18(1)

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

Tb(1)-O(11)	2.294(1)
Tb(1)-O(21)	2.323(1)
Tb(1)-O(2W)	2.371(1)
Tb(1)-O(3W)	2.403(1)
Tb(1)-O(1W)	2.404(1)
Tb(1)-O(12)#1	2.413(1)
Tb(1)-O(22)#2	2.428(1)
Tb(1)-O(21)#2	2.612(1)
Tb(1)-O(11)#1	2.820(1)
Tb(1)-Tb(1)#2	4.1064(2)
Tb(1)-Tb(1)#1	4.2324(2)
O(11)-C(11)	1.267(2)
O(12)-C(11)	1.258(2)
C(11)-C(12)	1.493(3)
O(21)-C(21)	1.278(2)
O(22)-C(21)	1.259(2)
C(21)-C(22)	1.490(2)
O(11)-Tb(1)-O(21)	164.52(5)
O(11)-Tb(1)-O(2W)	84.87(4)
O(21)-Tb(1)-O(2W)	88.40(4)
O(11)-Tb(1)-O(3W)	81.14(5)
O(21)-Tb(1)-O(3W)	83.43(4)
O(2W)-Tb(1)-O(3W)	68.66(4)
O(11)-Tb(1)-O(1W)	89.51(4)
O(21)-Tb(1)-O(1W)	86.88(4)
O(2W)-Tb(1)-O(1W)	140.68(4)
O(3W)-Tb(1)-O(1W)	72.02(4)
O(11)-Tb(1)-O(12)#1	117.17(4)
O(21)-Tb(1)-O(12)#1	74.27(4)
O(2W)-Tb(1)-O(12)#1	75.49(4)
O(3W)-Tb(1)-O(12)#1	138.01(5)
O(1W)-Tb(1)-O(12)#1	139.44(4)
O(11)-Tb(1)-O(22)#2	75.51(4)
O(21)-Tb(1)-O(22)#2	118.32(4)
O(2W)-Tb(1)-O(22)#2	136.56(4)
O(3W)-Tb(1)-O(22)#2	142.13(5)
O(1W)-Tb(1)-O(22)#2	78.32(4)
O(12)#1-Tb(1)-O(22)#2	79.71(5)
O(11)-Tb(1)-O(21)#2	125.07(4)
O(21)-Tb(1)-O(21)#2	67.51(5)
O(2W)-Tb(1)-O(21)#2	141.54(4)
O(3W)-Tb(1)-O(21)#2	132.84(4)
O(1W)-Tb(1)-O(21)#2	70.16(4)
O(12)#1-Tb(1)-O(21)#2	69.48(4)
O(22)#2-Tb(1)-O(21)#2	51.05(4)
O(11)-Tb(1)-O(11)#1	68.70(5)
O(21)-Tb(1)-O(11)#1	121.41(4)
O(2W)-Tb(1)-O(11)#1	68.50(4)
O(3W)-Tb(1)-O(11)#1	128.96(4)
O(1W)-Tb(1)-O(11)#1	143.54(4)
O(12)#1-Tb(1)-O(11)#1	48.51(4)
O(22)#2-Tb(1)-O(11)#1	68.32(4)
O(21)#2-Tb(1)-O(11)#1	98.13(4)
Tb(1)#2-Tb(1)-Tb(1)#1	138.586(5)

C(11)-O(11)-Tb(1)	162.5(1)
C(11)-O(11)-Tb(1)#1	86.1(1)
Tb(1)-O(11)-Tb(1)#1	111.3(1)
C(11)-O(12)-Tb(1)#1	105.9(1)
O(12)-C(11)-O(11)	119.5(2)
O(12)-C(11)-C(12)	119.6(2)
O(11)-C(11)-C(12)	120.9(2)
C(21)-O(21)-Tb(1)	154.9(1)
C(21)-O(21)-Tb(1)#2	90.4(1)
Tb(1)-O(21)-Tb(1)#2	112.5(1)
C(21)-O(22)-Tb(1)#2	99.6(1)
O(22)-C(21)-O(21)	118.3(2)
O(22)-C(21)-C(22)	121.3(2)
O(21)-C(21)-C(22)	120.5(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 (A^2 x 10^3) for Tb(OAc)2Cl_x_3H2O.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Tb(1)	7(1)	10(1)	12(1)	0(1)	2(1)	-2(1)
Cl(1)	18(1)	12(1)	17(1)	1(1)	2(1)	-1(1)
O(11)	12(1)	18(1)	21(1)	-3(1)	5(1)	-5(1)
O(12)	9(1)	16(1)	22(1)	4(1)	3(1)	1(1)
C(11)	11(1)	12(1)	13(1)	-1(1)	3(1)	-1(1)
C(12)	25(1)	17(1)	22(1)	5(1)	0(1)	4(1)
O(21)	9(1)	14(1)	13(1)	0(1)	0(1)	-1(1)
O(22)	9(1)	17(1)	17(1)	-2(1)	2(1)	-2(1)
C(21)	11(1)	9(1)	15(1)	-1(1)	1(1)	2(1)
C(22)	16(1)	27(1)	12(1)	-1(1)	1(1)	2(1)
O(1W)	12(1)	12(1)	17(1)	2(1)	5(1)	0(1)
O(2W)	11(1)	13(1)	19(1)	-4(1)	2(1)	0(1)
O(3W)	24(1)	13(1)	16(1)	2(1)	8(1)	4(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Tb(OAc)2Cl_x_3H2O.

	x	y	z	U(eq)
H(12A)	-1340	-257	5603	33(6)
H(12B)	-1236	717	6417	33(6)
H(12C)	464	514	6006	33(6)
H(12D)	-1832	126	6055	33(6)
H(12E)	-6	955	6392	33(6)
H(12F)	-210	-83	5592	33(6)
H(22A)	7858	5884	7359	45(5)
H(22B)	5920	5166	7208	45(5)
H(22C)	6260	7175	7203	45(5)
H(11W)	3912	999	5787	49(6)
H(12W)	5147	1865	5305	49(6)
H(21W)	474	6696	6293	39(5)
H(22W)	2216	7596	6459	39(5)
H(31W)	2484	3990	7095	50(6)
H(32W)	3245	2334	6838	50(6)

Table S6. Hydrogen bonds for Tb(OAc)2Cl_x_3H2O [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(11W)...Cl(1)#3	0.96	2.18	3.129(1)	167.4
O(1W)-H(12W)...O(12)#4	0.96	1.78	2.706(2)	160.8
O(2W)-H(21W)...O(22)#5	0.96	1.83	2.711(2)	151.7
O(2W)-H(22W)...Cl(1)	0.96	2.13	3.076(1)	170.0
O(3W)-H(31W)...Cl(1)#6	0.96	2.23	3.179(1)	170.3
O(3W)-H(32W)...Cl(1)#3	0.96	2.13	3.072(1)	166.1

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