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

Identification code	Ha2019_54_0m_a
Empirical formula	C4 H12 Cl Er O7
Formula weight	374.85
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.7927(3) A b = 7.8301(3) A ß = 97.695(2) deg. c = 17.1904(7) A
Volume	1039.47(7) A^3
Z, Calculated density	4, 2.395 Mg/m^3
Absorption coefficient	8.335 mm^-1
F(000)	708
Crystal size	0.486 x 0.220 x 0.162 mm
Theta range for data collection	2.746 to 27.996 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -22<=l<=22
Reflections collected / unique	93617 / 2514 [R(int) = 0.0305]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.738 and 0.256
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2514 / 0 / 126
Goodness-of-fit on F^2	1.415
Final R indices [I>2sigma(I)]	R1 = 0.0135, wR2 = 0.0292
R indices (all data)	R1 = 0.0135, wR2 = 0.0292
Extinction coefficient	0.00115(9)
Largest diff. peak and hole	0.524 and -0.603 e.A^-3

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

	x	y	z	U(eq)
Er(1)	2742(1)	4493(1)	5409(1)	8(1)
Cl(1)	3771(1)	9583(1)	6847(1)	15(1)
O(11)	175(2)	3237(2)	5424(1)	18(1)
O(12)	-2635(2)	2865(2)	5257(1)	12(1)
C(11)	-1129(3)	2347(3)	5509(1)	10(1)
C(12)	-925(3)	644(3)	5905(2)	20(1)
O(21)	5435(2)	5627(2)	5742(1)	10(1)
O(22)	8164(2)	6312(2)	5922(1)	12(1)
C(21)	6795(3)	6002(3)	6212(1)	10(1)
C(22)	6760(3)	6053(4)	7075(1)	16(1)
O(1W)	4100(2)	1823(2)	5378(1)	12(1)
O(2W)	1648(2)	6420(2)	6251(1)	13(1)
O(3W)	3179(2)	3459(2)	6717(1)	16(1)

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

Er(1)-O(11)	2.232(2)
Er(1)-O(21)	2.280(2)
Er(1)-O(2W)	2.331(2)
Er(1)-O(1W)	2.346(2)
Er(1)-O(12)#1	2.362(2)
Er(1)-O(3W)	2.372(2)
Er(1)-O(22)#2	2.386(2)
Er(1)-O(21)#2	2.588(2)
Er(1)-O(11)#1	3.083(2)
Er(1)-Er(1)#2	4.0390(2)
Er(1)-Er(1)#1	4.3894(2)
O(11)-C(11)	1.257(3)
O(12)-C(11)	1.262(3)
C(11)-C(12)	1.495(3)
O(21)-C(21)	1.278(3)
O(22)-C(21)	1.260(3)
C(21)-C(22)	1.487(3)
O(11)-Er(1)-O(21)	164.74(6)
O(11)-Er(1)-O(2W)	82.83(6)
O(21)-Er(1)-O(2W)	89.57(6)
O(11)-Er(1)-O(1W)	90.89(6)
O(21)-Er(1)-O(1W)	87.15(6)
O(2W)-Er(1)-O(1W)	142.62(6)
O(11)-Er(1)-O(12)#1	114.71(6)
O(21)-Er(1)-O(12)#1	75.64(6)
O(2W)-Er(1)-O(12)#1	75.01(6)
O(1W)-Er(1)-O(12)#1	139.16(6)
O(11)-Er(1)-O(3W)	81.61(6)
O(21)-Er(1)-O(3W)	83.35(6)
O(2W)-Er(1)-O(3W)	69.52(6)
O(1W)-Er(1)-O(3W)	73.12(6)
O(12)#1-Er(1)-O(3W)	138.61(6)
O(11)-Er(1)-O(22)#2	75.17(6)
O(21)-Er(1)-O(22)#2	119.22(6)
O(2W)-Er(1)-O(22)#2	132.87(6)
O(1W)-Er(1)-O(22)#2	79.60(6)
O(12)#1-Er(1)-O(22)#2	77.29(6)
O(3W)-Er(1)-O(22)#2	143.64(6)
O(11)-Er(1)-O(21)#2	125.25(6)
O(21)-Er(1)-O(21)#2	68.02(6)
O(2W)-Er(1)-O(21)#2	141.50(6)
O(1W)-Er(1)-O(21)#2	69.81(5)
O(12)#1-Er(1)-O(21)#2	69.42(5)
O(3W)-Er(1)-O(21)#2	133.56(5)
O(22)#2-Er(1)-O(21)#2	51.65(5)
O(11)-Er(1)-O(11)#1	69.69(7)
O(21)-Er(1)-O(11)#1	119.25(5)
O(2W)-Er(1)-O(11)#1	66.82(5)
O(1W)-Er(1)-O(11)#1	144.07(5)
O(12)#1-Er(1)-O(11)#1	45.05(5)
O(3W)-Er(1)-O(11)#1	129.82(5)
O(22)#2-Er(1)-O(11)#1	66.56(5)
O(21)#2-Er(1)-O(11)#1	96.43(5)
Er(1)#2-Er(1)-Er(1)#1	135.170(5)

C(11)-O(11)-Er(1)	170.2(2)
C(11)-O(12)-Er(1)#1	114.8(1)
O(11)-C(11)-O(12)	120.7(2)
O(11)-C(11)-C(12)	120.6(2)
O(12)-C(11)-C(12)	118.7(2)
C(21)-O(21)-Er(1)	155.0(2)
C(21)-O(21)-Er(1)#2	89.9(1)
Er(1)-O(21)-Er(1)#2	112.0(1)
C(21)-O(22)-Er(1)#2	99.9(1)
O(22)-C(21)-O(21)	117.9(2)
O(22)-C(21)-C(22)	121.3(2)
O(21)-C(21)-C(22)	120.8(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 Er(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
Er(1)	6(1)	8(1)	10(1)	0(1)	2(1)	-2(1)
Cl(1)	18(1)	11(1)	15(1)	1(1)	2(1)	-2(1)
O(11)	13(1)	20(1)	21(1)	-6(1)	7(1)	-8(1)
O(12)	7(1)	13(1)	17(1)	3(1)	2(1)	1(1)
C(11)	10(1)	10(1)	10(1)	-2(1)	3(1)	-1(1)
C(12)	23(1)	15(1)	21(1)	6(1)	1(1)	3(1)
O(21)	7(1)	12(1)	12(1)	0(1)	0(1)	-2(1)
O(22)	7(1)	14(1)	15(1)	-1(1)	2(1)	-2(1)
C(21)	10(1)	7(1)	12(1)	0(1)	1(1)	1(1)
C(22)	14(1)	26(1)	10(1)	-1(1)	1(1)	1(1)
O(1W)	12(1)	11(1)	15(1)	2(1)	5(1)	1(1)
O(2W)	10(1)	12(1)	16(1)	-3(1)	2(1)	-1(1)
O(3W)	23(1)	12(1)	13(1)	2(1)	6(1)	4(1)

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

	x	y	z	U(eq)
H(12A)	-1746	550	6287	60(8)
H(12B)	260	530	6175	60(8)
H(12C)	-1154	-262	5511	60(8)
H(22A)	7942	5939	7348	45(6)
H(22B)	6047	5111	7228	45(6)
H(22C)	6268	7143	7218	45(6)
H(11W)	4066	930	5758	47(8)
H(12W)	5302	1940	5318	47(8)
H(21W)	427	6589	6249	44(8)
H(22W)	2166	7500	6408	44(8)
H(31W)	2678	4003	7133	49(8)
H(32W)	3310	2282	6871	49(8)

Table S6. Hydrogen bonds for Er(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	2.19	3.113(2)	161.7
O(1W)-H(12W)...O(12)#4	0.96	1.78	2.706(2)	161.3
O(2W)-H(21W)...O(22)#5	0.96	1.79	2.700(2)	156.6
O(2W)-H(22W)...Cl(1)	0.96	2.13	3.077(2)	168.1
O(3W)-H(31W)...Cl(1)#6	0.96	2.26	3.192(2)	164.9
O(3W)-H(32W)...Cl(1)#3	0.96	2.15	3.073(2)	162.1

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