Table S1. Crystal data and structure refinement for Ho(OAc2)Cl_x_3H2O.

Identification code	Ha2019_86_0m_a
Empirical formula	C4 H12 Cl Ho O7
Formula weight	372.52
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.7993(3) A b = 7.8345(3) A ß = 97.881(2) deg. c = 17.2564(7) A
Volume	1044.47(7) A^3
Z, Calculated density	4, 2.369 Mg/m^3
Absorption coefficient	7.835 mm^-1
F(000)	704
Crystal size	0.381 x 0.090 x 0.078 mm
Theta range for data collection	2.740 to 27.997 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -22<=l<=22
Reflections collected / unique	133421 / 2528 [R(int) = 0.0358]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.746 and 0.398
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2528 / 0 / 126
Goodness-of-fit on F^2	1.176
Final R indices [I>2sigma(I)]	R1 = 0.0103, wR2 = 0.0234
R indices (all data)	R1 = 0.0106, wR2 = 0.0235
Extinction coefficient	0.00185(8)
Largest diff. peak and hole	0.364 and -0.436 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Ho(OAc2)Cl_x_3H2O. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ho(1)	2715(1)	4521(1)	5400(1)	9(1)
Cl(1)	3787(1)	9611(1)	6861(1)	16(1)
O(11)	115(2)	3276(2)	5406(1)	19(1)
O(12)	-2673(2)	2810(2)	5260(1)	14(1)
C(11)	-1149(2)	2340(2)	5506(1)	11(1)
C(12)	-874(3)	658(3)	5911(1)	22(1)
O(21)	5440(2)	5624(2)	5741(1)	12(1)
O(22)	8171(2)	6299(2)	5935(1)	14(1)
C(21)	6791(2)	5992(2)	6214(1)	11(1)
C(22)	6740(2)	6046(3)	7073(1)	18(1)
O(1W)	4051(2)	1812(2)	5376(1)	14(1)
O(2W)	1656(2)	6467(2)	6251(1)	14(1)
O(3W)	3132(2)	3472(2)	6707(1)	17(1)

Table S3. Bond lengths [A] and angles [deg] for Ho(OAc2)Cl_x_3H2O.

Ho(1)-O(11)	2.252(1)
Ho(1)-O(21)	2.295(1)
Ho(1)-O(2W)	2.345(1)
Ho(1)-O(1W)	2.367(1)
Ho(1)-O(12)#1	2.378(1)
Ho(1)-O(3W)	2.381(1)
Ho(1)-O(22)#2	2.400(1)
Ho(1)-O(21)#2	2.596(1)
Ho(1)-O(11)#1	2.991(1)
Ho(1)-Ho(1)#2	4.0640(2)
Ho(1)-Ho(1)#1	4.3361(2)
O(11)-C(11)	1.259(2)
O(12)-C(11)	1.262(2)
C(11)-C(12)	1.493(2)
O(21)-C(21)	1.274(2)
O(22)-C(21)	1.261(2)
C(21)-C(22)	1.488(2)
O(11)-Ho(1)-O(21)	164.74(5)
O(11)-Ho(1)-O(2W)	83.34(4)
O(21)-Ho(1)-O(2W)	89.29(4)
O(11)-Ho(1)-O(1W)	90.59(5)
O(21)-Ho(1)-O(1W)	87.01(4)
O(2W)-Ho(1)-O(1W)	141.98(4)
O(11)-Ho(1)-O(12)#1	115.46(5)
O(21)-Ho(1)-O(12)#1	75.13(4)
O(2W)-Ho(1)-O(12)#1	75.23(4)
O(1W)-Ho(1)-O(12)#1	139.20(4)
O(11)-Ho(1)-O(3W)	81.49(5)
O(21)-Ho(1)-O(3W)	83.41(4)
O(2W)-Ho(1)-O(3W)	69.20(4)
O(1W)-Ho(1)-O(3W)	72.78(4)
O(12)#1-Ho(1)-O(3W)	138.40(4)
O(11)-Ho(1)-O(22)#2	75.38(4)
O(21)-Ho(1)-O(22)#2	118.81(4)
O(2W)-Ho(1)-O(22)#2	134.06(4)
O(1W)-Ho(1)-O(22)#2	79.21(4)
O(12)#1-Ho(1)-O(22)#2	78.04(4)
O(3W)-Ho(1)-O(22)#2	143.23(5)
O(11)-Ho(1)-O(21)#2	125.30(4)
O(21)-Ho(1)-O(21)#2	67.75(5)
O(2W)-Ho(1)-O(21)#2	141.55(4)
O(1W)-Ho(1)-O(21)#2	69.91(4)
O(12)#1-Ho(1)-O(21)#2	69.40(4)
O(3W)-Ho(1)-O(21)#2	133.30(4)
O(22)#2-Ho(1)-O(21)#2	51.44(4)
O(11)-Ho(1)-O(11)#1	69.17(5)
O(21)-Ho(1)-O(11)#1	120.04(4)
O(2W)-Ho(1)-O(11)#1	67.33(4)
O(1W)-Ho(1)-O(11)#1	143.90(4)
O(12)#1-Ho(1)-O(11)#1	46.33(4)
O(3W)-Ho(1)-O(11)#1	129.46(4)
O(22)#2-Ho(1)-O(11)#1	67.14(4)
O(21)#2-Ho(1)-O(11)#1	97.09(4)
Ho(1)#2-Ho(1)-Ho(1)#1	136.374(4)

C(11)-O(11)-Ho(1)	167.3(1)
C(11)-O(12)-Ho(1)#1	111.6(1)
O(11)-C(11)-O(12)	120.2(2)
O(11)-C(11)-C(12)	120.9(2)
O(12)-C(11)-C(12)	118.9(2)
C(21)-O(21)-Ho(1)	154.8(1)
C(21)-O(21)-Ho(1)#2	90.0(1)
Ho(1)-O(21)-Ho(1)#2	112.3(1)
C(21)-O(22)-Ho(1)#2	99.6(1)
O(22)-C(21)-O(21)	118.2(2)
O(22)-C(21)-C(22)	121.0(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 Ho(OAc2)Cl_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
Ho(1)	7(1)	10(1)	11(1)	0(1)	2(1)	-2(1)
Cl(1)	18(1)	12(1)	17(1)	1(1)	2(1)	-1(1)
O(11)	14(1)	23(1)	22(1)	-7(1)	8(1)	-9(1)
O(12)	9(1)	16(1)	18(1)	3(1)	2(1)	1(1)
C(11)	11(1)	12(1)	12(1)	-2(1)	3(1)	-1(1)
C(12)	26(1)	18(1)	22(1)	6(1)	2(1)	6(1)
O(21)	9(1)	13(1)	14(1)	0(1)	1(1)	-1(1)
O(22)	9(1)	16(1)	15(1)	-2(1)	2(1)	-2(1)
C(21)	11(1)	8(1)	14(1)	0(1)	1(1)	1(1)
C(22)	15(1)	26(1)	12(1)	-1(1)	1(1)	2(1)
O(1W)	12(1)	14(1)	16(1)	2(1)	5(1)	1(1)
O(2W)	10(1)	13(1)	17(1)	-3(1)	1(1)	0(1)
O(3W)	24(1)	14(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 Ho(OAc2)Cl_x_3H2O.

	x	y	z	U(eq)
H(12A)	-1098	-264	5526	69(6)
H(12B)	-1666	551	6302	69(6)
H(12C)	324	581	6169	69(6)
H(22A)	7913	5901	7351	50(5)
H(22B)	5998	5125	7220	50(5)
H(22C)	6275	7149	7214	50(5)
H(11W)	3999	939	5762	43(6)
H(12W)	5257	1910	5323	43(6)
H(21W)	436	6638	6247	48(6)
H(22W)	2176	7541	6415	48(6)
H(31W)	2534	3979	7100	44(6)
H(32W)	3278	2295	6857	44(6)

Table S6. Hydrogen bonds for Ho(OAc2)Cl_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	3.119(1)	162.9
O(1W)-H(12W)...O(12)#4	0.96	1.78	2.705(2)	161.2
O(2W)-H(21W)...O(22)#5	0.96	1.79	2.701(2)	156.3
O(2W)-H(22W)...Cl(1)	0.96	2.13	3.075(1)	168.2
O(3W)-H(31W)...Cl(1)#6	0.96	2.24	3.187(1)	167.7
O(3W)-H(32W)...Cl(1)#3	0.96	2.14	3.073(1)	163.7

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