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

Identification code	Ha2019_57_0m_a
Empirical formula	C4 H12 Cl O7 Yb
Formula weight	380.63
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.7710(3) A b = 7.8224(3) A ß = 97.422(2) deg. c = 17.1055(8) A
Volume	1031.09(7) A^3
Z, Calculated density	4, 2.452 Mg/m^3
Absorption coefficient	9.333 mm^-1
F(000)	716
Crystal size	0.316 x 0.092 x 0.048 mm
Theta range for data collection	2.868 to 27.999 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -22<=l<=22
Reflections collected / unique	70583 / 2491 [R(int) = 0.0721]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.742 and 0.498
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2491 / 0 / 125
Goodness-of-fit on F^2	1.061
Final R indices [I>2sigma(I)]	R1 = 0.0162, wR2 = 0.0302
R indices (all data)	R1 = 0.0217, wR2 = 0.0318
Extinction coefficient	n/a
Largest diff. peak and hole	0.522 and -0.480 e.A^-3

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

	x	y	z	U(eq)
Yb(1)	2767(1)	4465(1)	5422(1)	9(1)
Cl(1)	3744(1)	9556(1)	6827(1)	16(1)
O(11)	243(2)	3202(3)	5444(1)	16(1)
O(12)	-2595(2)	2931(3)	5249(1)	12(1)
C(11)	-1107(4)	2361(4)	5512(2)	11(1)
C(12)	-986(4)	644(4)	5895(2)	19(1)
O(21)	5405(2)	5623(3)	5748(1)	12(1)
O(22)	8137(2)	6323(3)	5898(1)	13(1)
C(21)	6788(4)	6003(4)	6209(2)	11(1)
C(22)	6777(4)	6062(4)	7075(2)	18(1)
O(1W)	4141(2)	1842(3)	5375(1)	13(1)
O(2W)	1631(2)	6364(3)	6256(1)	12(1)
O(3W)	3223(3)	3449(3)	6724(1)	15(1)

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

Yb(1)-O(11)	2.201(2)
Yb(1)-O(21)	2.246(2)
Yb(1)-O(2W)	2.312(2)
Yb(1)-O(1W)	2.320(2)
Yb(1)-O(12)#1	2.334(2)
Yb(1)-O(3W)	2.347(2)
Yb(1)-O(22)#2	2.359(2)
Yb(1)-O(21)#2	2.601(2)
Yb(1)-O(11)#1	3.178(2)
Yb(1)-Yb(1)#2	4.0169(3)
Yb(1)-Yb(1)#1	4.4352(3)
O(11)-C(11)	1.256(3)
O(12)-C(11)	1.267(3)
C(11)-C(12)	1.492(4)
O(21)-C(21)	1.283(3)
O(22)-C(21)	1.260(3)
C(21)-C(22)	1.483(4)
O(11)-Yb(1)-O(21)	164.65(8)
O(11)-Yb(1)-O(2W)	82.28(7)
O(21)-Yb(1)-O(2W)	89.82(7)
O(11)-Yb(1)-O(1W)	91.10(7)
O(21)-Yb(1)-O(1W)	87.46(7)
O(2W)-Yb(1)-O(1W)	143.53(7)
O(11)-Yb(1)-O(12)#1	113.94(7)
O(21)-Yb(1)-O(12)#1	76.24(7)
O(2W)-Yb(1)-O(12)#1	74.98(7)
O(1W)-Yb(1)-O(12)#1	138.77(7)
O(11)-Yb(1)-O(3W)	81.82(8)
O(21)-Yb(1)-O(3W)	83.11(7)
O(2W)-Yb(1)-O(3W)	69.83(7)
O(1W)-Yb(1)-O(3W)	73.74(7)
O(12)#1-Yb(1)-O(3W)	138.97(7)
O(11)-Yb(1)-O(22)#2	75.15(7)
O(21)-Yb(1)-O(22)#2	119.48(7)
O(2W)-Yb(1)-O(22)#2	131.96(7)
O(1W)-Yb(1)-O(22)#2	79.44(7)
O(12)#1-Yb(1)-O(22)#2	76.45(7)
O(3W)-Yb(1)-O(22)#2	144.06(7)
O(11)-Yb(1)-O(21)#2	125.31(7)
O(21)-Yb(1)-O(21)#2	68.26(8)
O(2W)-Yb(1)-O(21)#2	141.43(7)
O(1W)-Yb(1)-O(21)#2	69.50(7)
O(12)#1-Yb(1)-O(21)#2	69.29(7)
O(3W)-Yb(1)-O(21)#2	133.66(7)
O(22)#2-Yb(1)-O(21)#2	51.72(6)
O(11)-Yb(1)-O(11)#1	70.24(8)
O(21)-Yb(1)-O(11)#1	118.51(6)
O(2W)-Yb(1)-O(11)#1	66.58(6)
O(1W)-Yb(1)-O(11)#1	143.70(6)
O(12)#1-Yb(1)-O(11)#1	43.73(6)
O(3W)-Yb(1)-O(11)#1	130.45(6)
O(22)#2-Yb(1)-O(11)#1	66.00(6)
O(21)#2-Yb(1)-O(11)#1	95.63(6)
Yb(1)#2-Yb(1)-Yb(1)#1	133.619(7)

C(11)-O(11)-Yb(1)	173.3(2)
C(11)-O(12)-Yb(1)#1	118.3(2)
O(11)-C(11)-O(12)	121.1(3)
O(11)-C(11)-C(12)	120.4(3)
O(12)-C(11)-C(12)	118.4(3)
C(21)-O(21)-Yb(1)	155.7(2)
C(21)-O(21)-Yb(1)#2	89.0(2)
Yb(1)-O(21)-Yb(1)#2	111.7(1)
C(21)-O(22)-Yb(1)#2	101.0(2)
O(22)-C(21)-O(21)	117.6(3)
O(22)-C(21)-C(22)	121.8(3)
O(21)-C(21)-C(22)	120.6(3)

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 Yb(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
Yb(1)	6(1)	8(1)	12(1)	0(1)	1(1)	-1(1)
Cl(1)	18(1)	11(1)	17(1)	1(1)	3(1)	-2(1)
O(11)	11(1)	17(1)	20(1)	-5(1)	5(1)	-6(1)
O(12)	8(1)	14(1)	14(1)	2(1)	2(1)	2(1)
C(11)	10(1)	12(2)	12(1)	-3(1)	4(1)	-2(1)
C(12)	18(2)	16(2)	23(2)	5(2)	3(1)	2(1)
O(21)	8(1)	11(1)	15(1)	-1(1)	0(1)	0(1)
O(22)	7(1)	13(1)	18(1)	1(1)	1(1)	0(1)
C(21)	10(1)	8(1)	14(2)	0(1)	-1(1)	3(1)
C(22)	15(2)	24(2)	13(2)	-1(1)	0(1)	2(1)
O(1W)	11(1)	11(1)	19(1)	2(1)	5(1)	1(1)
O(2W)	10(1)	11(1)	16(1)	-3(1)	2(1)	0(1)
O(3W)	19(1)	12(1)	15(1)	2(1)	7(1)	4(1)

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

	x	y	z	U(eq)
H(12A)	-1909	526	6232	50(8)
H(12B)	146	525	6217	50(8)
H(12C)	-1116	-246	5489	50(8)
H(22A)	7961	5903	7341	48(8)
H(22B)	6030	5149	7233	48(8)
H(22C)	6332	7172	7223	48(8)
H(11W)	4095	955	5760	51(9)
H(12W)	5343	1921	5302	51(9)
H(21W)	401	6550	6213	44(9)
H(22W)	2140	7461	6388	44(9)
H(31W)	2682	3956	7141	43(9)
H(32W)	3302	2253	6849	43(9)

Table S6. Hydrogen bonds for Yb(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	3.108(2)	163.4
O(1W)-H(12W)...O(12)#4	0.96	1.80	2.710(3)	157.3
O(2W)-H(21W)...O(22)#5	0.96	1.78	2.706(3)	160.6
O(2W)-H(22W)...Cl(1)	0.96	2.14	3.078(2)	166.7
O(3W)-H(31W)...Cl(1)#6	0.96	2.25	3.195(2)	167.5
O(3W)-H(32W)...Cl(1)#3	0.96	2.14	3.074(2)	164.4

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