Table S1. Crystal data and structure refinement for Yb(OAc)2Br_x_3H2O.

Identification code	Ha2019_99j_0m_a
Empirical formula	C4 H12 Br O7 Yb
Formula weight	425.09
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.7854(3) A b = 8.0625(3) A ß = 96.142(2) deg. c = 17.3573(7) A
Volume	1083.26(7) A^3
Z, Calculated density	4, 2.606 Mg/m^3
Absorption coefficient	12.326 mm^-1
F(000)	788
Crystal size	0.487 x 0.172 x 0.070 mm
Theta range for data collection	2.766 to 27.999 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -22<=l<=22
Reflections collected / unique	120213 / 2616 [R(int) = 0.0460]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.742 and 0.349
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2616 / 0 / 125
Goodness-of-fit on F^2	1.073
Final R indices [I>2sigma(I)]	R1 = 0.0121, wR2 = 0.0261
R indices (all data)	R1 = 0.0141, wR2 = 0.0266
Extinction coefficient	n/a
Largest diff. peak and hole	0.460 and -0.581 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Yb(OAc)2Br_x_3H2O. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Yb(1)	2751(1)	4444(1)	5404(1)	9(1)
Br(1)	3809(1)	9470(1)	6790(1)	16(1)
O(11)	235(2)	3208(2)	5419(1)	17(1)
O(12)	-2594(2)	2990(2)	5220(1)	13(1)
C(11)	-1131(3)	2413(3)	5479(1)	11(1)
C(12)	-1066(3)	741(3)	5858(2)	20(1)
O(21)	5375(2)	5557(2)	5745(1)	12(1)
O(22)	8088(2)	6241(2)	5902(1)	14(1)
C(21)	6724(3)	5899(3)	6199(1)	11(1)
C(22)	6699(3)	5864(3)	7058(1)	19(1)
O(1W)	4144(2)	1913(2)	5325(1)	14(1)
O(2W)	1554(2)	6228(2)	6246(1)	13(1)
O(3W)	3160(2)	3401(2)	6671(1)	16(1)

Table S3. Bond lengths [A] and angles [deg] for Yb(OAc)2Br_x_3H2O.

Yb(1)-O(11)	2.201(2)
Yb(1)-O(21)	2.251(1)
Yb(1)-O(2W)	2.316(2)
Yb(1)-O(1W)	2.322(2)
Yb(1)-O(12)#1	2.333(2)
Yb(1)-O(3W)	2.344(2)
Yb(1)-O(22)#2	2.358(2)
Yb(1)-O(21)#2	2.594(2)
Yb(1)-O(11)#1	3.213(2)
Yb(1)-Yb(1)#2	4.0107(2)
Yb(1)-Yb(1)#1	4.4540(2)
O(11)-C(11)	1.255(3)
O(12)-C(11)	1.267(2)
C(11)-C(12)	1.498(3)
O(21)-C(21)	1.275(2)
O(22)-C(21)	1.259(3)
C(21)-C(22)	1.493(3)
O(11)-Yb(1)-O(21)	164.01(6)
O(11)-Yb(1)-O(2W)	81.67(6)
O(21)-Yb(1)-O(2W)	90.11(5)
O(11)-Yb(1)-O(1W)	91.40(6)
O(21)-Yb(1)-O(1W)	87.11(5)
O(2W)-Yb(1)-O(1W)	143.63(5)
O(11)-Yb(1)-O(12)#1	113.88(6)
O(21)-Yb(1)-O(12)#1	76.66(5)
O(2W)-Yb(1)-O(12)#1	74.81(5)
O(1W)-Yb(1)-O(12)#1	138.88(5)
O(11)-Yb(1)-O(3W)	81.84(6)
O(21)-Yb(1)-O(3W)	82.45(5)
O(2W)-Yb(1)-O(3W)	69.77(6)
O(1W)-Yb(1)-O(3W)	73.91(6)
O(12)#1-Yb(1)-O(3W)	138.54(6)
O(11)-Yb(1)-O(22)#2	75.51(6)
O(21)-Yb(1)-O(22)#2	119.74(5)
O(2W)-Yb(1)-O(22)#2	131.58(5)
O(1W)-Yb(1)-O(22)#2	79.64(5)
O(12)#1-Yb(1)-O(22)#2	76.42(5)
O(3W)-Yb(1)-O(22)#2	144.51(6)
O(11)-Yb(1)-O(21)#2	125.69(5)
O(21)-Yb(1)-O(21)#2	68.46(6)
O(2W)-Yb(1)-O(21)#2	141.52(5)
O(1W)-Yb(1)-O(21)#2	69.46(5)
O(12)#1-Yb(1)-O(21)#2	69.44(5)
O(3W)-Yb(1)-O(21)#2	133.63(5)
O(22)#2-Yb(1)-O(21)#2	51.76(5)
O(11)-Yb(1)-O(11)#1	70.70(6)
O(21)-Yb(1)-O(11)#1	118.35(5)
O(2W)-Yb(1)-O(11)#1	66.04(5)
O(1W)-Yb(1)-O(11)#1	144.28(5)
O(12)#1-Yb(1)-O(11)#1	43.22(4)
O(3W)-Yb(1)-O(11)#1	130.39(5)
O(22)#2-Yb(1)-O(11)#1	66.25(5)
O(21)#2-Yb(1)-O(11)#1	95.63(4)
Yb(1)#2-Yb(1)-Yb(1)#1	133.712(5)

C(11)-O(11)-Yb(1)	174.4(2)
C(11)-O(12)-Yb(1)#1	119.4(1)
O(11)-C(11)-O(12)	121.4(2)
O(11)-C(11)-C(12)	120.4(2)
O(12)-C(11)-C(12)	118.2(2)
C(21)-O(21)-Yb(1)	156.0(1)
C(21)-O(21)-Yb(1)#2	88.9(1)
Yb(1)-O(21)-Yb(1)#2	111.5(1)
C(21)-O(22)-Yb(1)#2	100.5(1)
O(22)-C(21)-O(21)	118.0(2)
O(22)-C(21)-C(22)	120.9(2)
O(21)-C(21)-C(22)	121.0(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 Yb(OAc)2Br_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)	11(1)	11(1)	0(1)	0(1)	-1(1)
Br(1)	20(1)	12(1)	16(1)	1(1)	2(1)	-2(1)
O(11)	10(1)	20(1)	21(1)	-4(1)	5(1)	-6(1)
O(12)	8(1)	15(1)	17(1)	2(1)	2(1)	1(1)
C(11)	11(1)	13(1)	10(1)	-2(1)	2(1)	-1(1)
C(12)	17(1)	18(1)	26(1)	7(1)	1(1)	2(1)
O(21)	7(1)	14(1)	13(1)	0(1)	-1(1)	-1(1)
O(22)	8(1)	18(1)	15(1)	0(1)	-1(1)	-1(1)
C(21)	11(1)	10(1)	12(1)	-1(1)	0(1)	2(1)
C(22)	16(1)	29(1)	12(1)	0(1)	0(1)	1(1)
O(1W)	11(1)	14(1)	16(1)	2(1)	3(1)	1(1)
O(2W)	10(1)	13(1)	16(1)	-2(1)	1(1)	0(1)
O(3W)	21(1)	14(1)	16(1)	1(1)	5(1)	3(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Yb(OAc)2Br_x_3H2O.

	x	y	z	U(eq)
H(12A)	105	532	6105	57(7)
H(12B)	-1380	-113	5466	57(7)
H(12C)	-1882	712	6250	57(7)
H(22A)	7865	5635	7307	88(9)
H(22B)	5909	4993	7196	88(9)
H(22C)	6307	6940	7234	88(9)
H(11W)	4117	1011	5684	51(8)
H(12W)	5342	2044	5252	51(8)
H(21W)	331	6379	6246	50(7)
H(22W)	2045	7306	6354	50(7)
H(31W)	2554	3871	7072	49(7)
H(32W)	3360	2265	6820	49(7)

Table S6. Hydrogen bonds for Yb(OAc)2Br_x_3H2O [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(11W)...Br(1)#3	0.96	2.32	3.249(2)	162.7
O(1W)-H(12W)...O(12)#4	0.96	1.78	2.708(2)	160.2
O(2W)-H(21W)...O(22)#5	0.96	1.79	2.701(2)	157.8
O(2W)-H(22W)...Br(1)	0.96	2.30	3.233(2)	164.4
O(3W)-H(31W)...Br(1)#6	0.96	2.39	3.333(2)	167.3
O(3W)-H(32W)...Br(1)#3	0.96	2.28	3.213(2)	163.0

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