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

Identification code	Ha2019_79_0m_a
Empirical formula	C4 H12 Br Er O7
Formula weight	419.31
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.8069(3) A b = 8.0529(3) A ß = 96.154(2) deg. c = 17.4494(7) A
Volume	1090.69(7) A^3
Z, Calculated density	4, 2.554 Mg/m^3
Absorption coefficient	11.362 mm^-1
F(000)	780
Crystal size	0.362 x 0.162 x 0.144 mm
Theta range for data collection	2.758 to 27.998 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -23<=l<=23
Reflections collected / unique	121468 / 2636 [R(int) = 0.0413]
Completeness to theta = 25.242	99.8 %
Absorption correction	Mutli-scan
Max. and min. transmission	0.683 and 0.267
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2636 / 0 / 126
Goodness-of-fit on F^2	1.181
Final R indices [I>2sigma(I)]	R1 = 0.0114, wR2 = 0.0253
R indices (all data)	R1 = 0.0123, wR2 = 0.0255
Extinction coefficient	0.00082(5)
Largest diff. peak and hole	0.364 and -0.467 e.A^-3

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

	x	y	z	U(eq)
Er(1)	2728(1)	4468(1)	5393(1)	10(1)
Br(1)	3842(1)	9488(1)	6807(1)	16(1)
O(11)	172(2)	3238(2)	5403(1)	19(1)
O(12)	-2632(2)	2923(2)	5227(1)	14(1)
C(11)	-1153(2)	2395(3)	5479(1)	12(1)
C(12)	-1012(3)	735(3)	5867(1)	22(1)
O(21)	5396(2)	5555(2)	5738(1)	12(1)
O(22)	8106(2)	6236(2)	5919(1)	14(1)
C(21)	6731(2)	5890(2)	6202(1)	12(1)
C(22)	6677(3)	5837(3)	7054(1)	19(1)
O(1W)	4103(2)	1889(2)	5326(1)	14(1)
O(2W)	1559(2)	6284(2)	6244(1)	14(1)
O(3W)	3112(2)	3407(2)	6664(1)	18(1)

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

Er(1)-O(11)	2.229(1)
Er(1)-O(21)	2.280(1)
Er(1)-O(2W)	2.338(1)
Er(1)-O(1W)	2.347(2)
Er(1)-O(12)#1	2.360(2)
Er(1)-O(3W)	2.365(2)
Er(1)-O(22)#2	2.382(1)
Er(1)-O(21)#2	2.582(1)
Er(1)-O(11)#1	3.129(2)
Er(1)-Er(1)#2	4.0312(2)
Er(1)-Er(1)#1	4.4158(2)
O(11)-C(11)	1.256(2)
O(12)-C(11)	1.264(2)
C(11)-C(12)	1.497(3)
O(21)-C(21)	1.278(2)
O(22)-C(21)	1.259(2)
C(21)-C(22)	1.493(3)
O(11)-Er(1)-O(21)	164.05(5)
O(11)-Er(1)-O(2W)	82.09(5)
O(21)-Er(1)-O(2W)	89.99(5)
O(11)-Er(1)-O(1W)	91.24(6)
O(21)-Er(1)-O(1W)	86.73(5)
O(2W)-Er(1)-O(1W)	142.83(5)
O(11)-Er(1)-O(12)#1	114.50(5)
O(21)-Er(1)-O(12)#1	76.28(5)
O(2W)-Er(1)-O(12)#1	74.89(5)
O(1W)-Er(1)-O(12)#1	139.20(5)
O(11)-Er(1)-O(3W)	81.70(6)
O(21)-Er(1)-O(3W)	82.55(5)
O(2W)-Er(1)-O(3W)	69.47(5)
O(1W)-Er(1)-O(3W)	73.40(5)
O(12)#1-Er(1)-O(3W)	138.23(5)
O(11)-Er(1)-O(22)#2	75.49(5)
O(21)-Er(1)-O(22)#2	119.55(5)
O(2W)-Er(1)-O(22)#2	132.47(5)
O(1W)-Er(1)-O(22)#2	79.64(5)
O(12)#1-Er(1)-O(22)#2	77.25(5)
O(3W)-Er(1)-O(22)#2	144.05(5)
O(11)-Er(1)-O(21)#2	125.77(5)
O(21)-Er(1)-O(21)#2	68.14(5)
O(2W)-Er(1)-O(21)#2	141.48(5)
O(1W)-Er(1)-O(21)#2	69.83(5)
O(12)#1-Er(1)-O(21)#2	69.43(5)
O(3W)-Er(1)-O(21)#2	133.55(5)
O(22)#2-Er(1)-O(21)#2	51.80(4)
O(11)-Er(1)-O(11)#1	70.15(6)
O(21)-Er(1)-O(11)#1	119.20(5)
O(2W)-Er(1)-O(11)#1	66.44(5)
O(1W)-Er(1)-O(11)#1	144.40(5)
O(12)#1-Er(1)-O(11)#1	44.38(4)
O(3W)-Er(1)-O(11)#1	130.00(5)
O(22)#2-Er(1)-O(11)#1	66.64(4)
O(21)#2-Er(1)-O(11)#1	96.16(4)
Er(1)#2-Er(1)-Er(1)#1	135.053(5)

C(11)-O(11)-Er(1)	171.5(2)
C(11)-O(12)-Er(1)#1	116.2(1)
O(11)-C(11)-O(12)	120.9(2)
O(11)-C(11)-C(12)	120.6(2)
O(12)-C(11)-C(12)	118.5(2)
C(21)-O(21)-Er(1)	155.3(1)
C(21)-O(21)-Er(1)#2	89.7(1)
Er(1)-O(21)-Er(1)#2	111.9(1)
C(21)-O(22)-Er(1)#2	99.7(1)
O(22)-C(21)-O(21)	118.1(2)
O(22)-C(21)-C(22)	120.8(2)
O(21)-C(21)-C(22)	121.1(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)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
Er(1)	7(1)	11(1)	11(1)	0(1)	2(1)	-2(1)
Br(1)	20(1)	12(1)	16(1)	1(1)	2(1)	-2(1)
O(11)	13(1)	23(1)	22(1)	-6(1)	7(1)	-8(1)
O(12)	9(1)	16(1)	17(1)	2(1)	1(1)	1(1)
C(11)	11(1)	13(1)	11(1)	-2(1)	3(1)	0(1)
C(12)	21(1)	19(1)	24(1)	7(1)	1(1)	3(1)
O(21)	8(1)	15(1)	12(1)	0(1)	1(1)	0(1)
O(22)	9(1)	18(1)	16(1)	-1(1)	1(1)	-2(1)
C(21)	11(1)	10(1)	15(1)	-1(1)	1(1)	1(1)
C(22)	17(1)	29(1)	11(1)	0(1)	0(1)	2(1)
O(1W)	12(1)	15(1)	16(1)	2(1)	5(1)	0(1)
O(2W)	11(1)	14(1)	18(1)	-2(1)	1(1)	0(1)
O(3W)	24(1)	15(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 Er(OAc)2Br_x_3H2O.

	x	y	z	U(eq)
H(12A)	-1808	687	6264	71(7)
H(12B)	170	570	6105	71(7)
H(12C)	-1307	-139	5484	71(7)
H(22A)	7847	5688	7310	73(7)
H(22B)	5952	4908	7185	73(7)
H(22C)	6198	6880	7227	73(7)
H(11W)	4085	1049	5716	50(7)
H(12W)	5295	2005	5247	50(7)
H(21W)	343	6441	6253	58(8)
H(22W)	2060	7352	6368	58(8)
H(31W)	2514	3860	7069	48(7)
H(32W)	3316	2265	6803	48(7)

Table S6. Hydrogen bonds for Er(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	2.31	3.252(2)	167.8
O(1W)-H(12W)...O(12)#4	0.96	1.78	2.705(2)	160.0
O(2W)-H(21W)...O(22)#5	0.96	1.79	2.695(2)	156.4
O(2W)-H(22W)...Br(1)	0.96	2.29	3.229(2)	165.0
O(3W)-H(31W)...Br(1)#6	0.96	2.38	3.327(1)	169.0
O(3W)-H(32W)...Br(1)#3	0.96	2.27	3.212(2)	165.4

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