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

Identification code	Ha2019_84_0m_a
Empirical formula	C4 H12 Br Ho O7
Formula weight	416.98
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.8117(3) A b = 8.0361(4) A ß = 96.096(3) deg. c = 17.5440(9) A
Volume	1095.11(9) A^3
Z, Calculated density	4, 2.529 Mg/m^3
Absorption coefficient	10.878 mm^-1
F(000)	776
Crystal size	0.487 x 0.172 x 0.070 mm
Theta range for data collection	2.755 to 28.000 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -23<=l<=23
Reflections collected / unique	102663 / 2655 [R(int) = 0.0734]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.754 and 0.365
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2655 / 0 / 125
Goodness-of-fit on F^2	1.051
Final R indices [I>2sigma(I)]	R1 = 0.0148, wR2 = 0.0337
R indices (all data)	R1 = 0.0196, wR2 = 0.0354
Extinction coefficient	n/a
Largest diff. peak and hole	0.508 and -0.579 e.A^-3

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

	x	y	z	U(eq)
Ho(1)	2694(1)	4500(1)	5383(1)	11(1)
Br(1)	3868(1)	9517(1)	6823(1)	17(1)
O(11)	106(2)	3278(2)	5385(1)	21(1)
O(12)	-2677(2)	2860(2)	5228(1)	16(1)
C(11)	-1183(3)	2384(3)	5472(2)	13(1)
C(12)	-959(4)	739(4)	5875(2)	25(1)
O(21)	5392(2)	5551(2)	5736(1)	13(1)
O(22)	8104(2)	6221(2)	5931(1)	15(1)
C(21)	6718(3)	5872(3)	6203(2)	13(1)
C(22)	6636(3)	5812(4)	7046(2)	19(1)
O(1W)	4039(2)	1873(2)	5321(1)	15(1)
O(2W)	1557(2)	6333(2)	6241(1)	14(1)
O(3W)	3039(2)	3418(2)	6649(1)	19(1)

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

Ho(1)-O(11)	2.248(2)
Ho(1)-O(21)	2.294(2)
Ho(1)-O(2W)	2.346(2)
Ho(1)-O(1W)	2.366(2)
Ho(1)-O(3W)	2.373(2)
Ho(1)-O(12)#1	2.376(2)
Ho(1)-O(22)#2	2.395(2)
Ho(1)-O(21)#2	2.591(2)
Ho(1)-O(11)#1	3.026(2)
Ho(1)-Ho(1)#2	4.0576(3)
Ho(1)-Ho(1)#1	4.3544(3)
O(11)-C(11)	1.260(3)
O(12)-C(11)	1.260(3)
C(11)-C(12)	1.500(4)
O(21)-C(21)	1.277(3)
O(22)-C(21)	1.260(3)
C(21)-C(22)	1.489(4)
O(11)-Ho(1)-O(21)	164.01(7)
O(11)-Ho(1)-O(2W)	82.64(6)
O(21)-Ho(1)-O(2W)	89.75(6)
O(11)-Ho(1)-O(1W)	90.81(7)
O(21)-Ho(1)-O(1W)	86.61(6)
O(2W)-Ho(1)-O(1W)	142.19(6)
O(11)-Ho(1)-O(3W)	81.47(7)
O(21)-Ho(1)-O(3W)	82.69(6)
O(2W)-Ho(1)-O(3W)	69.09(6)
O(1W)-Ho(1)-O(3W)	73.11(6)
O(11)-Ho(1)-O(12)#1	115.40(7)
O(21)-Ho(1)-O(12)#1	75.75(6)
O(2W)-Ho(1)-O(12)#1	75.19(6)
O(1W)-Ho(1)-O(12)#1	139.19(6)
O(3W)-Ho(1)-O(12)#1	138.05(7)
O(11)-Ho(1)-O(22)#2	75.72(6)
O(21)-Ho(1)-O(22)#2	119.09(6)
O(2W)-Ho(1)-O(22)#2	133.78(6)
O(1W)-Ho(1)-O(22)#2	79.09(6)
O(3W)-Ho(1)-O(22)#2	143.53(7)
O(12)#1-Ho(1)-O(22)#2	78.09(6)
O(11)-Ho(1)-O(21)#2	125.84(6)
O(21)-Ho(1)-O(21)#2	67.80(7)
O(2W)-Ho(1)-O(21)#2	141.62(6)
O(1W)-Ho(1)-O(21)#2	69.86(6)
O(3W)-Ho(1)-O(21)#2	133.27(6)
O(12)#1-Ho(1)-O(21)#2	69.42(6)
O(22)#2-Ho(1)-O(21)#2	51.61(5)
O(11)-Ho(1)-O(11)#1	69.56(7)
O(21)-Ho(1)-O(11)#1	120.20(6)
O(2W)-Ho(1)-O(11)#1	67.08(6)
O(1W)-Ho(1)-O(11)#1	144.02(6)
O(3W)-Ho(1)-O(11)#1	129.61(6)
O(12)#1-Ho(1)-O(11)#1	45.86(5)
O(22)#2-Ho(1)-O(11)#1	67.19(6)
O(21)#2-Ho(1)-O(11)#1	96.90(5)
Ho(1)#2-Ho(1)-Ho(1)#1	136.417(6)

C(11)-O(11)-Ho(1)	168.5(2)
C(11)-O(12)-Ho(1)#1	112.7(2)
O(11)-C(11)-O(12)	120.6(2)
O(11)-C(11)-C(12)	120.4(2)
O(12)-C(11)-C(12)	119.0(2)
C(21)-O(21)-Ho(1)	155.1(2)
C(21)-O(21)-Ho(1)#2	89.7(2)
Ho(1)-O(21)-Ho(1)#2	112.2(1)
C(21)-O(22)-Ho(1)#2	99.4(2)
O(22)-C(21)-O(21)	118.3(2)
O(22)-C(21)-C(22)	120.8(2)
O(21)-C(21)-C(22)	120.9(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(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
Ho(1)	7(1)	13(1)	12(1)	0(1)	2(1)	-2(1)
Br(1)	21(1)	14(1)	18(1)	1(1)	2(1)	-2(1)
O(11)	14(1)	26(1)	24(1)	-5(1)	7(1)	-11(1)
O(12)	10(1)	19(1)	18(1)	2(1)	2(1)	2(1)
C(11)	13(1)	13(1)	13(1)	-2(1)	5(1)	1(1)
C(12)	26(2)	22(2)	25(2)	9(1)	1(1)	4(1)
O(21)	10(1)	14(1)	14(1)	-1(1)	1(1)	-2(1)
O(22)	8(1)	19(1)	18(1)	-3(1)	0(1)	-3(1)
C(21)	12(1)	12(1)	14(1)	-2(1)	1(1)	1(1)
C(22)	15(1)	28(2)	13(1)	1(1)	0(1)	3(1)
O(1W)	13(1)	16(1)	17(1)	1(1)	5(1)	0(1)
O(2W)	10(1)	16(1)	17(1)	-4(1)	2(1)	0(1)
O(3W)	26(1)	16(1)	17(1)	2(1)	7(1)	4(1)

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

	x	y	z	U(eq)
H(12A)	256	580	6063	86(10)
H(12B)	-1334	-157	5516	86(10)
H(12C)	-1655	719	6308	86(10)
H(22A)	7806	5751	7310	24(8)
H(22B)	5983	4829	7175	24(8)
H(22C)	6066	6817	7210	24(8)
H(22D)	5411	5872	7119	24(8)
H(22E)	7227	6804	7267	24(8)
H(22F)	7143	4815	7301	24(8)
H(11W)	4051	1048	5717	63(9)
H(12W)	5217	1969	5216	63(9)
H(21W)	351	6473	6284	47(8)
H(22W)	2078	7362	6421	47(8)
H(31W)	2494	3909	7060	50(8)
H(32W)	3320	2305	6816	50(8)

Table S6. Hydrogen bonds for Ho(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	3.260(2)	167.8
O(1W)-H(12W)...O(12)#4	0.96	1.79	2.706(2)	158.0
O(2W)-H(21W)...O(22)#5	0.96	1.81	2.696(2)	152.2
O(2W)-H(22W)...Br(1)	0.96	2.29	3.233(2)	167.5
O(3W)-H(31W)...Br(1)#6	0.96	2.38	3.322(2)	167.5
O(3W)-H(32W)...Br(1)#3	0.96	2.28	3.210(2)	162.6

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