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

Identification code	Ha2019_99o_0m_a
Empirical formula	C4 H12 Br O7 Tb
Formula weight	410.97
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.7972(3) A b = 8.0263(3) A ß = 95.862(2) deg. c = 17.7443(8) A
Volume	1104.68(8) A^3
Z, Calculated density	4, 2.471 Mg/m^3
Absorption coefficient	10.023 mm^-1
F(000)	768
Crystal size	0.487 x 0.172 x 0.070 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	124829 / 2683 [R(int) = 0.0459]
Completeness to theta = 25.242	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.746 and 0.421
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2683 / 0 / 125
Goodness-of-fit on F^2	1.124
Final R indices [I>2sigma(I)]	R1 = 0.0133, wR2 = 0.0300
R indices (all data)	R1 = 0.0151, wR2 = 0.0305
Extinction coefficient	n/a
Largest diff. peak and hole	0.554 and -0.406 e.A^-3

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

	x	y	z	U(eq)
Tb(1)	2623(1)	4573(1)	5362(1)	11(1)
Br(1)	3919(1)	9592(1)	6848(1)	18(1)
O(11)	-40(2)	3350(2)	5343(1)	17(1)
O(12)	-2776(2)	2724(2)	5228(1)	16(1)
C(11)	-1245(3)	2355(3)	5462(1)	13(1)
C(12)	-877(3)	761(3)	5884(2)	23(1)
O(21)	5384(2)	5546(2)	5734(1)	13(1)
O(22)	8107(2)	6176(2)	5958(1)	16(1)
C(21)	6695(3)	5850(3)	6210(1)	13(1)
C(22)	6557(3)	5779(3)	7043(1)	20(1)
O(1W)	3900(2)	1853(2)	5312(1)	15(1)
O(2W)	1568(2)	6456(2)	6244(1)	15(1)
O(3W)	2880(2)	3441(2)	6619(1)	19(1)

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

Tb(1)-O(11)	2.294(2)
Tb(1)-O(21)	2.322(1)
Tb(1)-O(2W)	2.381(2)
Tb(1)-O(3W)	2.398(2)
Tb(1)-O(1W)	2.405(2)
Tb(1)-O(12)#1	2.417(2)
Tb(1)-O(22)#2	2.429(2)
Tb(1)-O(21)#2	2.612(2)
Tb(1)-O(11)#1	2.808(2)
Tb(1)-Tb(1)#2	4.1036(2)
Tb(1)-Tb(1)#1	4.2158(2)
O(11)-C(11)	1.266(3)
O(12)-C(11)	1.258(3)
C(11)-C(12)	1.496(3)
O(21)-C(21)	1.281(3)
O(22)-C(21)	1.258(3)
C(21)-C(22)	1.494(3)
O(11)-Tb(1)-O(21)	163.70(5)
O(11)-Tb(1)-O(2W)	84.74(5)
O(21)-Tb(1)-O(2W)	88.43(5)
O(11)-Tb(1)-O(3W)	80.85(6)
O(21)-Tb(1)-O(3W)	82.88(5)
O(2W)-Tb(1)-O(3W)	68.37(5)
O(11)-Tb(1)-O(1W)	89.34(5)
O(21)-Tb(1)-O(1W)	86.58(5)
O(2W)-Tb(1)-O(1W)	140.60(5)
O(3W)-Tb(1)-O(1W)	72.23(5)
O(11)-Tb(1)-O(12)#1	117.56(5)
O(21)-Tb(1)-O(12)#1	74.69(5)
O(2W)-Tb(1)-O(12)#1	75.56(5)
O(3W)-Tb(1)-O(12)#1	137.74(5)
O(1W)-Tb(1)-O(12)#1	139.43(5)
O(11)-Tb(1)-O(22)#2	75.96(5)
O(21)-Tb(1)-O(22)#2	118.45(5)
O(2W)-Tb(1)-O(22)#2	136.72(5)
O(3W)-Tb(1)-O(22)#2	142.39(6)
O(1W)-Tb(1)-O(22)#2	78.25(5)
O(12)#1-Tb(1)-O(22)#2	79.72(5)
O(11)-Tb(1)-O(21)#2	125.44(5)
O(21)-Tb(1)-O(21)#2	67.60(6)
O(2W)-Tb(1)-O(21)#2	141.63(5)
O(3W)-Tb(1)-O(21)#2	132.76(5)
O(1W)-Tb(1)-O(21)#2	70.06(5)
O(12)#1-Tb(1)-O(21)#2	69.56(5)
O(22)#2-Tb(1)-O(21)#2	51.06(5)
O(11)-Tb(1)-O(11)#1	68.96(6)
O(21)-Tb(1)-O(11)#1	121.93(5)
O(2W)-Tb(1)-O(11)#1	68.65(5)
O(3W)-Tb(1)-O(11)#1	128.90(5)
O(1W)-Tb(1)-O(11)#1	143.43(5)
O(12)#1-Tb(1)-O(11)#1	48.62(5)
O(22)#2-Tb(1)-O(11)#1	68.32(5)
O(21)#2-Tb(1)-O(11)#1	98.27(5)
Tb(1)#2-Tb(1)-Tb(1)#1	139.179(6)

C(11)-O(11)-Tb(1)	162.4(2)
C(11)-O(11)-Tb(1)#1	86.4(1)
Tb(1)-O(11)-Tb(1)#1	111.0(1)
C(11)-O(12)-Tb(1)#1	105.5(1)
O(12)-C(11)-O(11)	119.5(2)
O(12)-C(11)-C(12)	119.6(2)
O(11)-C(11)-C(12)	121.0(2)
C(21)-O(21)-Tb(1)	154.9(1)
C(21)-O(21)-Tb(1)#2	90.2(1)
Tb(1)-O(21)-Tb(1)#2	112.4(1)
C(21)-O(22)-Tb(1)#2	99.5(1)
O(22)-C(21)-O(21)	118.3(2)
O(22)-C(21)-C(22)	120.9(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 Tb(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
Tb(1)	7(1)	13(1)	12(1)	0(1)	1(1)	-2(1)
Br(1)	21(1)	15(1)	17(1)	2(1)	1(1)	-2(1)
O(11)	11(1)	21(1)	19(1)	-1(1)	4(1)	-6(1)
O(12)	9(1)	19(1)	20(1)	4(1)	2(1)	0(1)
C(11)	12(1)	16(1)	12(1)	0(1)	4(1)	-1(1)
C(12)	24(1)	20(1)	25(1)	7(1)	0(1)	3(1)
O(21)	9(1)	17(1)	14(1)	0(1)	1(1)	-1(1)
O(22)	9(1)	20(1)	18(1)	-1(1)	1(1)	-2(1)
C(21)	11(1)	13(1)	15(1)	-2(1)	0(1)	2(1)
C(22)	16(1)	32(1)	12(1)	-1(1)	0(1)	4(1)
O(1W)	12(1)	16(1)	18(1)	1(1)	4(1)	0(1)
O(2W)	10(1)	17(1)	18(1)	-4(1)	1(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 Tb(OAc)2Br_x_3H2O.

	x	y	z	U(eq)
H(12A)	364	533	5924	96(10)
H(12B)	-1501	-153	5612	96(10)
H(12C)	-1253	857	6393	96(10)
H(22A)	7726	5718	7306	23(6)
H(22B)	5904	4795	7172	23(6)
H(22C)	5987	6784	7206	23(6)
H(22D)	5334	5779	7127	23(6)
H(22E)	7122	6762	7284	23(6)
H(22F)	7109	4767	7261	23(6)
H(11W)	3827	1073	5718	52(7)
H(12W)	5101	1892	5237	52(7)
H(21W)	356	6585	6283	40(6)
H(22W)	2081	7475	6440	40(6)
H(31W)	2411	3945	7043	48(7)
H(32W)	3117	2308	6770	48(7)

Table S6. Hydrogen bonds for Tb(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	2.33	3.274(2)	168.8
O(1W)-H(12W)...O(12)#4	0.96	1.79	2.703(2)	158.7
O(2W)-H(21W)...O(22)#5	0.96	1.82	2.703(2)	151.8
O(2W)-H(22W)...Br(1)	0.96	2.29	3.232(2)	166.0
O(3W)-H(31W)...Br(1)#6	0.96	2.37	3.317(2)	167.6
O(3W)-H(32W)...Br(1)#3	0.96	2.27	3.208(2)	166.1

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