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

Identification code	Ha2019_99b_0m_a
Empirical formula	C4 H12 Br O7 Tm
Formula weight	420.98
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.7868(5) A b = 8.0675(5) A ß = 96.154(2) deg. c = 17.3994(7) A
Volume	1086.73(11) A^3
Z, Calculated density	4, 2.573 Mg/m^3
Absorption coefficient	11.845 mm^-1
F(000)	784
Crystal size	0.187 x 0.084 x 0.058 mm
Theta range for data collection	2.765 to 27.999 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -22<=l<=22
Reflections collected / unique	112602 / 2626 [R(int) = 0.0488]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.746 and 0.374
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2626 / 0 / 125
Goodness-of-fit on F^2	1.086
Final R indices [I>2sigma(I)]	R1 = 0.0118, wR2 = 0.0265
R indices (all data)	R1 = 0.0141, wR2 = 0.0272
Extinction coefficient	n/a
Largest diff. peak and hole	0.383 and -0.336 e.A^-3

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

	x	y	z	U(eq)
Tm(1)	2737(1)	4459(1)	5396(1)	10(1)
Br(1)	3823(1)	9489(1)	6799(1)	16(1)
O(11)	201(2)	3222(2)	5411(1)	18(1)
O(12)	-2620(2)	2963(2)	5226(1)	14(1)
C(11)	-1143(3)	2406(3)	5480(1)	12(1)
C(12)	-1044(3)	737(3)	5862(1)	21(1)
O(21)	5382(2)	5566(2)	5742(1)	12(1)
O(22)	8102(2)	6239(2)	5912(1)	14(1)
C(21)	6728(3)	5902(3)	6201(1)	12(1)
C(22)	6681(3)	5859(3)	7056(1)	20(1)
O(1W)	4107(2)	1898(2)	5322(1)	14(1)
O(2W)	1568(2)	6260(2)	6244(1)	14(1)
O(3W)	3131(2)	3411(2)	6665(1)	17(1)

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

Tm(1)-O(11)	2.216(2)
Tm(1)-O(21)	2.266(1)
Tm(1)-O(2W)	2.325(2)
Tm(1)-O(1W)	2.336(2)
Tm(1)-O(12)#1	2.342(2)
Tm(1)-O(3W)	2.353(2)
Tm(1)-O(22)#2	2.368(2)
Tm(1)-O(21)#2	2.587(2)
Tm(1)-O(11)#1	3.165(2)
Tm(1)-Tm(1)#2	4.0162(3)
Tm(1)-Tm(1)#1	4.4237(3)
O(11)-C(11)	1.253(3)
O(12)-C(11)	1.270(3)
C(11)-C(12)	1.500(3)
O(21)-C(21)	1.277(3)
O(22)-C(21)	1.260(3)
C(21)-C(22)	1.493(3)
O(11)-Tm(1)-O(21)	163.84(6)
O(11)-Tm(1)-O(2W)	82.20(6)
O(21)-Tm(1)-O(2W)	89.54(5)
O(11)-Tm(1)-O(1W)	90.85(6)
O(21)-Tm(1)-O(1W)	87.46(5)
O(2W)-Tm(1)-O(1W)	143.17(5)
O(11)-Tm(1)-O(12)#1	114.53(6)
O(21)-Tm(1)-O(12)#1	76.22(5)
O(2W)-Tm(1)-O(12)#1	74.92(5)
O(1W)-Tm(1)-O(12)#1	139.06(5)
O(11)-Tm(1)-O(3W)	81.62(6)
O(21)-Tm(1)-O(3W)	82.48(5)
O(2W)-Tm(1)-O(3W)	69.51(5)
O(1W)-Tm(1)-O(3W)	73.71(5)
O(12)#1-Tm(1)-O(3W)	138.38(6)
O(11)-Tm(1)-O(22)#2	75.49(5)
O(21)-Tm(1)-O(22)#2	119.86(5)
O(2W)-Tm(1)-O(22)#2	132.24(5)
O(1W)-Tm(1)-O(22)#2	79.46(5)
O(12)#1-Tm(1)-O(22)#2	76.92(5)
O(3W)-Tm(1)-O(22)#2	144.22(6)
O(11)-Tm(1)-O(21)#2	125.73(5)
O(21)-Tm(1)-O(21)#2	68.47(6)
O(2W)-Tm(1)-O(21)#2	141.55(5)
O(1W)-Tm(1)-O(21)#2	69.59(5)
O(12)#1-Tm(1)-O(21)#2	69.51(5)
O(3W)-Tm(1)-O(21)#2	133.45(5)
O(22)#2-Tm(1)-O(21)#2	51.87(5)
O(11)-Tm(1)-O(11)#1	70.66(6)
O(21)-Tm(1)-O(11)#1	118.55(5)
O(2W)-Tm(1)-O(11)#1	66.33(5)
O(1W)-Tm(1)-O(11)#1	144.21(5)
O(12)#1-Tm(1)-O(11)#1	43.90(4)
O(3W)-Tm(1)-O(11)#1	130.12(5)
O(22)#2-Tm(1)-O(11)#1	66.55(5)
O(21)#2-Tm(1)-O(11)#1	96.11(4)
Tm(1)#2-Tm(1)-Tm(1)#1	134.568(5)

C(11)-O(11)-Tm(1)	173.0(2)
C(11)-O(11)-Tm(1)#1	77.4(1)
Tm(1)-O(11)-Tm(1)#1	109.3(1)
C(11)-O(12)-Tm(1)#1	117.7(1)
O(11)-C(11)-O(12)	121.0(2)
O(11)-C(11)-C(12)	120.7(2)
O(12)-C(11)-C(12)	118.3(2)
C(21)-O(21)-Tm(1)	155.7(1)
C(21)-O(21)-Tm(1)#2	89.2(1)
Tm(1)-O(21)-Tm(1)#2	111.5(1)
C(21)-O(22)-Tm(1)#2	100.0(1)
O(22)-C(21)-O(21)	118.1(2)
O(22)-C(21)-C(22)	121.1(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 Tm(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
Tm(1)	6(1)	11(1)	12(1)	0(1)	1(1)	-1(1)
Br(1)	20(1)	13(1)	17(1)	1(1)	2(1)	-3(1)
O(11)	11(1)	22(1)	21(1)	-4(1)	5(1)	-6(1)
O(12)	8(1)	17(1)	16(1)	2(1)	2(1)	1(1)
C(11)	12(1)	13(1)	10(1)	-2(1)	4(1)	-1(1)
C(12)	18(1)	19(1)	25(1)	6(1)	0(1)	2(1)
O(21)	9(1)	15(1)	12(1)	-1(1)	0(1)	-1(1)
O(22)	8(1)	18(1)	16(1)	-1(1)	1(1)	-1(1)
C(21)	10(1)	11(1)	15(1)	0(1)	0(1)	2(1)
C(22)	16(1)	31(1)	12(1)	-1(1)	-1(1)	3(1)
O(1W)	13(1)	15(1)	17(1)	3(1)	5(1)	2(1)
O(2W)	10(1)	14(1)	17(1)	-2(1)	1(1)	-1(1)
O(3W)	22(1)	14(1)	17(1)	2(1)	7(1)	3(1)

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

	x	y	z	U(eq)
H(12A)	118	568	6126	60(7)
H(12B)	-1296	-128	5470	60(7)
H(12C)	-1891	679	6239	60(7)
H(22A)	7852	5684	7311	84(9)
H(22B)	5932	4950	7190	84(9)
H(22C)	6229	6913	7229	84(9)
H(11W)	4081	1037	5702	54(7)
H(12W)	5302	2008	5242	54(7)
H(21W)	344	6393	6248	56(8)
H(22W)	2046	7334	6375	56(8)
H(31W)	2520	3885	7062	48(7)
H(32W)	3302	2270	6810	48(7)

Table S6. Hydrogen bonds for Tm(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	3.249(2)	166.1
O(1W)-H(12W)...O(12)#4	0.96	1.79	2.712(2)	158.7
O(2W)-H(21W)...O(22)#5	0.96	1.78	2.699(2)	157.9
O(2W)-H(22W)...Br(1)	0.96	2.29	3.230(2)	164.8
O(3W)-H(31W)...Br(1)#6	0.96	2.39	3.329(2)	166.9
O(3W)-H(32W)...Br(1)#3	0.96	2.28	3.214(2)	164.0

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