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

Identification code	Ha2019_80_0m_a
Empirical formula	C4 H12 Br O7 Sm
Formula weight	402.40
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.8473(3) A b = 8.0230(3) A ß = 95.987(2) deg. c = 17.8722(7) A
Volume	1119.08(7) A^3
Z, Calculated density	4, 2.388 Mg/m^3
Absorption coefficient	8.822 mm^-1
F(000)	756
Crystal size	0.210 x 0.050 x 0.045 mm
Theta range for data collection	2.739 to 27.986 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -23<=l<=23
Reflections collected / unique	113760 / 2708 [R(int) = 0.0701]
Completeness to theta = 25.242	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.746 and 0.471
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2708 / 0 / 125
Goodness-of-fit on F^2	1.084
Final R indices [I>2sigma(I)]	R1 = 0.0150, wR2 = 0.0305
R indices (all data)	R1 = 0.0201, wR2 = 0.0321
Extinction coefficient	n/a
Largest diff. peak and hole	0.442 and -0.443 e.A^-3

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

	x	y	z	U(eq)
Sm(1)	2598(1)	4602(1)	5355(1)	11(1)
Br(1)	3946(1)	9623(1)	6868(1)	18(1)
O(11)	-124(2)	3373(2)	5330(1)	16(1)
O(12)	-2815(2)	2629(2)	5227(1)	17(1)
C(11)	-1277(3)	2327(3)	5457(1)	13(1)
C(12)	-826(3)	762(3)	5885(2)	23(1)
O(21)	5418(2)	5541(2)	5737(1)	14(1)
O(22)	8119(2)	6189(2)	5977(1)	17(1)
C(21)	6706(3)	5853(3)	6214(1)	14(1)
C(22)	6543(3)	5773(4)	7036(1)	22(1)
O(1W)	3866(2)	1805(2)	5316(1)	15(1)
O(2W)	1570(2)	6525(2)	6254(1)	17(1)
O(3W)	2826(2)	3444(2)	6618(1)	19(1)

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

Sm(1)-O(11)	2.349(2)
Sm(1)-O(21)	2.370(2)
Sm(1)-O(2W)	2.425(2)
Sm(1)-O(3W)	2.431(2)
Sm(1)-O(1W)	2.459(2)
Sm(1)-O(12)#1	2.466(2)
Sm(1)-O(22)#2	2.471(2)
Sm(1)-O(21)#2	2.623(2)
Sm(1)-O(11)#1	2.722(2)
Sm(1)-Sm(1)#2	4.1510(3)
Sm(1)-Sm(1)#1	4.1911(3)
O(11)-C(11)	1.272(3)
O(12)-C(11)	1.258(3)
C(11)-C(12)	1.494(3)
O(21)-C(21)	1.277(3)
O(22)-C(21)	1.257(3)
C(21)-C(22)	1.491(3)
O(11)-Sm(1)-O(21)	163.58(6)
O(11)-Sm(1)-O(2W)	85.13(6)
O(21)-Sm(1)-O(2W)	88.45(6)
O(11)-Sm(1)-O(3W)	80.58(6)
O(21)-Sm(1)-O(3W)	83.00(6)
O(2W)-Sm(1)-O(3W)	68.00(6)
O(11)-Sm(1)-O(1W)	89.20(6)
O(21)-Sm(1)-O(1W)	85.96(6)
O(2W)-Sm(1)-O(1W)	139.73(6)
O(3W)-Sm(1)-O(1W)	71.74(6)
O(11)-Sm(1)-O(12)#1	118.21(6)
O(21)-Sm(1)-O(12)#1	74.44(6)
O(2W)-Sm(1)-O(12)#1	75.48(6)
O(3W)-Sm(1)-O(12)#1	137.28(6)
O(1W)-Sm(1)-O(12)#1	139.81(6)
O(11)-Sm(1)-O(22)#2	76.00(6)
O(21)-Sm(1)-O(22)#2	118.08(5)
O(2W)-Sm(1)-O(22)#2	138.02(6)
O(3W)-Sm(1)-O(22)#2	141.60(6)
O(1W)-Sm(1)-O(22)#2	77.88(6)
O(12)#1-Sm(1)-O(22)#2	81.01(6)
O(11)-Sm(1)-O(21)#2	125.19(6)
O(21)-Sm(1)-O(21)#2	67.60(6)
O(2W)-Sm(1)-O(21)#2	141.73(6)
O(3W)-Sm(1)-O(21)#2	133.03(5)
O(1W)-Sm(1)-O(21)#2	70.46(5)
O(12)#1-Sm(1)-O(21)#2	69.68(6)
O(22)#2-Sm(1)-O(21)#2	50.59(5)
O(11)-Sm(1)-O(11)#1	68.74(6)
O(21)-Sm(1)-O(11)#1	122.74(5)
O(2W)-Sm(1)-O(11)#1	69.36(5)
O(3W)-Sm(1)-O(11)#1	128.76(5)
O(1W)-Sm(1)-O(11)#1	143.45(5)
O(12)#1-Sm(1)-O(11)#1	49.49(5)
O(22)#2-Sm(1)-O(11)#1	68.90(6)
O(21)#2-Sm(1)-O(11)#1	98.17(5)
Sm(1)#2-Sm(1)-Sm(1)#1	140.334(7)

C(11)-O(11)-Sm(1)	159.4(2)
C(11)-O(11)-Sm(1)#1	89.3(1)
Sm(1)-O(11)-Sm(1)#1	111.3(1)
C(11)-O(12)-Sm(1)#1	101.9(1)
O(12)-C(11)-O(11)	119.4(2)
O(12)-C(11)-C(12)	119.8(2)
O(11)-C(11)-C(12)	120.8(2)
C(21)-O(21)-Sm(1)	154.8(2)
C(21)-O(21)-Sm(1)#2	90.9(1)
Sm(1)-O(21)-Sm(1)#2	112.4(1)
C(21)-O(22)-Sm(1)#2	98.6(1)
O(22)-C(21)-O(21)	118.8(2)
O(22)-C(21)-C(22)	120.8(2)
O(21)-C(21)-C(22)	120.4(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 Sm(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
Sm(1)	7(1)	13(1)	12(1)	1(1)	1(1)	-1(1)
Br(1)	21(1)	15(1)	18(1)	2(1)	1(1)	-3(1)
O(11)	11(1)	19(1)	19(1)	2(1)	3(1)	-3(1)
O(12)	9(1)	19(1)	23(1)	5(1)	2(1)	-1(1)
C(11)	12(1)	14(1)	13(1)	0(1)	3(1)	0(1)
C(12)	22(1)	20(1)	26(1)	8(1)	0(1)	0(1)
O(21)	9(1)	18(1)	14(1)	0(1)	0(1)	-2(1)
O(22)	9(1)	25(1)	16(1)	-2(1)	1(1)	-3(1)
C(21)	12(1)	13(1)	15(1)	-2(1)	1(1)	2(1)
C(22)	18(1)	33(2)	14(1)	1(1)	2(1)	3(1)
O(1W)	13(1)	16(1)	18(1)	3(1)	4(1)	0(1)
O(2W)	13(1)	16(1)	21(1)	-4(1)	2(1)	0(1)
O(3W)	26(1)	16(1)	16(1)	1(1)	6(1)	5(1)

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

	x	y	z	U(eq)
H(12A)	-949	941	6420	82(9)
H(12B)	360	454	5826	82(9)
H(12C)	-1595	-137	5691	82(9)
H(22A)	7684	5686	7314	31(8)
H(22B)	5860	4796	7144	31(8)
H(22C)	5976	6785	7192	31(8)
H(22D)	5313	5833	7087	31(8)
H(22E)	7112	6770	7259	31(8)
H(22F)	7028	4778	7296	31(8)
H(11W)	3868	1026	5724	58(8)
H(12W)	5036	1859	5206	58(8)
H(21W)	358	6638	6277	61(9)
H(22W)	2053	7554	6450	61(9)
H(31W)	2291	3903	7031	64(9)
H(32W)	3090	2312	6761	64(9)

Table S6. Hydrogen bonds for Sm(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	3.276(2)	168.2
O(1W)-H(12W)...O(12)#4	0.96	1.79	2.708(2)	158.3
O(2W)-H(21W)...O(22)#5	0.96	1.82	2.715(2)	154.0
O(2W)-H(22W)...Br(1)	0.96	2.30	3.230(2)	163.2
O(3W)-H(31W)...Br(1)#6	0.96	2.35	3.306(2)	171.1
O(3W)-H(32W)...Br(1)#3	0.96	2.26	3.207(2)	168.2

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