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

Identification code	Ha2019_63_0m_a
Empirical formula	C4 H12 Br Nd O7
Formula weight	396.29
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.9027(3) A b = 8.0349(3) A ß = 96.414(2) deg. c = 17.9481(6) A
Volume	1132.52(7) A^3
Z, Calculated density	4, 2.324 Mg/m^3
Absorption coefficient	8.117 mm^-1
F(000)	748
Crystal size	0.314 x 0.236 x 0.176 mm
Theta range for data collection	2.715 to 27.995 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -23<=l<=23
Reflections collected / unique	132337 / 2735 [R(int) = 0.0553]
Completeness to theta = 25.242	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.746 and 0.414
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2735 / 0 / 125
Goodness-of-fit on F^2	1.055
Final R indices [I>2sigma(I)]	R1 = 0.0129, wR2 = 0.0300
R indices (all data)	R1 = 0.0154, wR2 = 0.0306
Extinction coefficient	n/a
Largest diff. peak and hole	0.402 and -0.415 e.A^-3

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

	x	y	z	U(eq)
Nd(1)	2598(1)	4603(1)	5359(1)	10(1)
Br(1)	3953(1)	9613(1)	6876(1)	18(1)
O(11)	-159(2)	3373(2)	5328(1)	15(1)
O(12)	-2818(2)	2587(2)	5220(1)	17(1)
C(11)	-1287(2)	2308(2)	5454(1)	14(1)
C(12)	-803(3)	756(3)	5886(1)	23(1)
O(21)	5453(2)	5540(2)	5736(1)	14(1)
O(22)	8129(2)	6221(2)	5984(1)	18(1)
C(21)	6732(2)	5863(2)	6217(1)	14(1)
C(22)	6564(3)	5779(3)	7036(1)	22(1)
O(1W)	3885(2)	1779(2)	5328(1)	15(1)
O(2W)	1560(2)	6537(2)	6266(1)	17(1)
O(3W)	2835(2)	3426(2)	6632(1)	20(1)

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

Nd(1)-O(11)	2.388(1)
Nd(1)-O(21)	2.403(1)
Nd(1)-O(2W)	2.457(1)
Nd(1)-O(3W)	2.461(1)
Nd(1)-O(1W)	2.490(1)
Nd(1)-O(12)#1	2.499(1)
Nd(1)-O(22)#2	2.504(1)
Nd(1)-O(21)#2	2.632(1)
Nd(1)-O(11)#1	2.711(1)
Nd(1)-Nd(1)#2	4.1920(2)
Nd(1)-Nd(1)#1	4.2124(2)
O(11)-C(11)	1.274(2)
O(12)-C(11)	1.256(2)
C(11)-C(12)	1.495(3)
O(21)-C(21)	1.280(2)
O(22)-C(21)	1.257(2)
C(21)-C(22)	1.492(3)
O(11)-Nd(1)-O(21)	164.11(5)
O(11)-Nd(1)-O(2W)	84.60(5)
O(21)-Nd(1)-O(2W)	89.27(5)
O(11)-Nd(1)-O(3W)	80.61(5)
O(21)-Nd(1)-O(3W)	83.50(5)
O(2W)-Nd(1)-O(3W)	67.92(5)
O(11)-Nd(1)-O(1W)	89.78(5)
O(21)-Nd(1)-O(1W)	85.35(4)
O(2W)-Nd(1)-O(1W)	139.36(5)
O(3W)-Nd(1)-O(1W)	71.45(5)
O(11)-Nd(1)-O(12)#1	118.05(4)
O(21)-Nd(1)-O(12)#1	74.18(4)
O(2W)-Nd(1)-O(12)#1	75.38(5)
O(3W)-Nd(1)-O(12)#1	136.99(5)
O(1W)-Nd(1)-O(12)#1	140.04(4)
O(11)-Nd(1)-O(22)#2	75.98(4)
O(21)-Nd(1)-O(22)#2	117.49(4)
O(2W)-Nd(1)-O(22)#2	138.39(5)
O(3W)-Nd(1)-O(22)#2	141.06(5)
O(1W)-Nd(1)-O(22)#2	77.74(5)
O(12)#1-Nd(1)-O(22)#2	81.85(5)
O(11)-Nd(1)-O(21)#2	124.98(4)
O(21)-Nd(1)-O(21)#2	67.36(5)
O(2W)-Nd(1)-O(21)#2	142.11(5)
O(3W)-Nd(1)-O(21)#2	133.37(4)
O(1W)-Nd(1)-O(21)#2	70.65(4)
O(12)#1-Nd(1)-O(21)#2	69.86(4)
O(22)#2-Nd(1)-O(21)#2	50.19(4)
O(11)-Nd(1)-O(11)#1	68.74(5)
O(21)-Nd(1)-O(11)#1	122.52(4)
O(2W)-Nd(1)-O(11)#1	69.46(4)
O(3W)-Nd(1)-O(11)#1	129.01(4)
O(1W)-Nd(1)-O(11)#1	143.90(4)
O(12)#1-Nd(1)-O(11)#1	49.30(4)
O(22)#2-Nd(1)-O(11)#1	69.26(4)
O(21)#2-Nd(1)-O(11)#1	97.59(4)
Nd(1)#2-Nd(1)-Nd(1)#1	140.204(6)

C(11)-O(11)-Nd(1)	158.3(1)
C(11)-O(11)-Nd(1)#1	90.4(1)
Nd(1)-O(11)-Nd(1)#1	111.3(1)
C(11)-O(12)-Nd(1)#1	101.0(1)
O(12)-C(11)-O(11)	119.2(2)
O(12)-C(11)-C(12)	120.2(2)
O(11)-C(11)-C(12)	120.6(2)
C(21)-O(21)-Nd(1)	154.1(1)
C(21)-O(21)-Nd(1)#2	91.6(1)
Nd(1)-O(21)-Nd(1)#2	112.6(1)
C(21)-O(22)-Nd(1)#2	98.3(1)
O(22)-C(21)-O(21)	118.6(2)
O(22)-C(21)-C(22)	121.1(2)
O(21)-C(21)-C(22)	120.3(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 Nd(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
Nd(1)	6(1)	13(1)	12(1)	1(1)	1(1)	-1(1)
Br(1)	20(1)	15(1)	17(1)	2(1)	1(1)	-3(1)
O(11)	10(1)	18(1)	19(1)	3(1)	2(1)	-3(1)
O(12)	9(1)	18(1)	23(1)	6(1)	2(1)	-1(1)
C(11)	12(1)	16(1)	14(1)	0(1)	3(1)	0(1)
C(12)	21(1)	20(1)	28(1)	9(1)	1(1)	-1(1)
O(21)	8(1)	19(1)	14(1)	0(1)	0(1)	-1(1)
O(22)	9(1)	25(1)	18(1)	-2(1)	1(1)	-3(1)
C(21)	12(1)	12(1)	16(1)	-1(1)	-1(1)	2(1)
C(22)	17(1)	36(1)	14(1)	1(1)	1(1)	4(1)
O(1W)	12(1)	16(1)	18(1)	2(1)	4(1)	0(1)
O(2W)	12(1)	17(1)	20(1)	-4(1)	1(1)	-1(1)
O(3W)	28(1)	17(1)	15(1)	2(1)	7(1)	5(1)

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

	x	y	z	U(eq)
H(12A)	-728	992	6424	77(7)
H(12B)	304	362	5760	77(7)
H(12C)	-1667	-102	5756	77(7)
H(22A)	7676	5528	7312	75(7)
H(22B)	5752	4902	7129	75(7)
H(22C)	6154	6851	7204	75(7)
H(11W)	3860	973	5721	49(6)
H(12W)	5053	1821	5229	49(6)
H(21W)	364	6674	6298	54(7)
H(22W)	2069	7566	6447	54(7)
H(31W)	2320	3895	7044	53(6)
H(32W)	3158	2318	6790	53(6)

Table S6. Hydrogen bonds for Nd(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	2.34	3.274(1)	165.1
O(1W)-H(12W)...O(12)#4	0.96	1.79	2.713(2)	159.4
O(2W)-H(21W)...O(22)#5	0.96	1.83	2.715(2)	151.9
O(2W)-H(22W)...Br(1)	0.96	2.29	3.227(1)	164.3
O(3W)-H(31W)...Br(1)#6	0.96	2.35	3.304(1)	171.0
O(3W)-H(32W)...Br(1)#3	0.96	2.26	3.206(2)	166.8

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