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

Identification code	Ha2020_2_0m_a
Empirical formula	C4 H12 Br Gd O7
Formula weight	409.30
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.8191(2) A b = 8.0130(2) A ß = 95.929(2) deg. c = 17.7804(6) A
Volume	1108.06(5) A^3
Z, Calculated density	4, 2.453 Mg/m^3
Absorption coefficient	9.595 mm^-1
F(000)	764
Crystal size	0.418 x 0.112 x 0.078 mm
Theta range for data collection	2.750 to 27.999 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -23<=l<=23
Reflections collected / unique	132199 / 2690 [R(int) = 0.0410]
Completeness to theta = 25.242	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.714 and 0.333
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2690 / 0 / 125
Goodness-of-fit on F^2	1.134
Final R indices [I>2sigma(I)]	R1 = 0.0155, wR2 = 0.0403
R indices (all data)	R1 = 0.0168, wR2 = 0.0410
Extinction coefficient	n/a
Largest diff. peak and hole	0.695 and -0.977 e.A^-3

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

	x	y	z	U(eq)
Gd(1)	2604(1)	4596(1)	5355(1)	10(1)
Br(1)	3937(1)	9611(1)	6858(1)	17(1)
O(11)	-98(2)	3379(2)	5333(1)	16(1)
O(12)	-2803(2)	2664(2)	5227(1)	16(1)
C(11)	-1264(3)	2345(3)	5460(1)	13(1)
C(12)	-822(3)	762(3)	5888(2)	22(1)
O(21)	5400(2)	5533(2)	5731(1)	13(1)
O(22)	8114(2)	6178(2)	5972(1)	16(1)
C(21)	6698(3)	5839(3)	6215(1)	12(1)
C(22)	6536(3)	5761(4)	7046(1)	21(1)
O(1W)	3869(2)	1838(2)	5309(1)	15(1)
O(2W)	1568(2)	6495(2)	6246(1)	16(1)
O(3W)	2836(2)	3443(2)	6614(1)	19(1)

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

Gd(1)-O(11)	2.324(2)
Gd(1)-O(21)	2.343(2)
Gd(1)-O(2W)	2.398(2)
Gd(1)-O(3W)	2.412(2)
Gd(1)-O(1W)	2.426(2)
Gd(1)-O(12)#1	2.439(2)
Gd(1)-O(22)#2	2.447(2)
Gd(1)-O(21)#2	2.608(2)
Gd(1)-O(11)#1	2.733(2)
Gd(1)-Gd(1)#2	4.1265(2)
Gd(1)-Gd(1)#1	4.1863(2)
O(11)-C(11)	1.269(3)
O(12)-C(11)	1.258(3)
C(11)-C(12)	1.501(3)
O(21)-C(21)	1.285(3)
O(22)-C(21)	1.259(3)
C(21)-C(22)	1.497(3)
O(11)-Gd(1)-O(21)	163.54(6)
O(11)-Gd(1)-O(2W)	84.75(6)
O(21)-Gd(1)-O(2W)	88.67(6)
O(11)-Gd(1)-O(3W)	80.52(6)
O(21)-Gd(1)-O(3W)	83.03(6)
O(2W)-Gd(1)-O(3W)	68.14(6)
O(11)-Gd(1)-O(1W)	89.44(6)
O(21)-Gd(1)-O(1W)	85.96(5)
O(2W)-Gd(1)-O(1W)	140.08(6)
O(3W)-Gd(1)-O(1W)	71.94(5)
O(11)-Gd(1)-O(12)#1	117.96(6)
O(21)-Gd(1)-O(12)#1	74.60(5)
O(2W)-Gd(1)-O(12)#1	75.51(6)
O(3W)-Gd(1)-O(12)#1	137.46(6)
O(1W)-Gd(1)-O(12)#1	139.62(5)
O(11)-Gd(1)-O(22)#2	76.12(5)
O(21)-Gd(1)-O(22)#2	118.12(5)
O(2W)-Gd(1)-O(22)#2	137.61(5)
O(3W)-Gd(1)-O(22)#2	141.74(6)
O(1W)-Gd(1)-O(22)#2	77.90(6)
O(12)#1-Gd(1)-O(22)#2	80.68(6)
O(11)-Gd(1)-O(21)#2	125.74(5)
O(21)-Gd(1)-O(21)#2	67.18(6)
O(2W)-Gd(1)-O(21)#2	141.60(5)
O(3W)-Gd(1)-O(21)#2	132.76(5)
O(1W)-Gd(1)-O(21)#2	70.23(5)
O(12)#1-Gd(1)-O(21)#2	69.65(5)
O(22)#2-Gd(1)-O(21)#2	51.07(5)
O(11)-Gd(1)-O(11)#1	68.49(6)
O(21)-Gd(1)-O(11)#1	122.86(5)
O(2W)-Gd(1)-O(11)#1	69.12(5)
O(3W)-Gd(1)-O(11)#1	128.65(5)
O(1W)-Gd(1)-O(11)#1	143.29(5)
O(12)#1-Gd(1)-O(11)#1	49.47(5)
O(22)#2-Gd(1)-O(11)#1	68.71(5)
O(21)#2-Gd(1)-O(11)#1	98.54(5)
Gd(1)#2-Gd(1)-Gd(1)#1	140.308(5)

C(11)-O(11)-Gd(1)	160.0(2)
C(11)-O(11)-Gd(1)#1	88.4(1)
Gd(1)-O(11)-Gd(1)#1	111.5(1)
C(11)-O(12)-Gd(1)#1	102.8(1)
O(12)-C(11)-O(11)	119.3(2)
O(12)-C(11)-C(12)	120.1(2)
O(11)-C(11)-C(12)	120.7(2)
C(21)-O(21)-Gd(1)	154.5(2)
C(21)-O(21)-Gd(1)#2	90.6(2)
Gd(1)-O(21)-Gd(1)#2	112.8(2)
C(21)-O(22)-Gd(1)#2	98.9(1)
O(22)-C(21)-O(21)	118.3(2)
O(22)-C(21)-C(22)	121.0(2)
O(21)-C(21)-C(22)	120.7(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 Gd(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
Gd(1)	6(1)	13(1)	12(1)	0(1)	1(1)	-1(1)
Br(1)	19(1)	15(1)	17(1)	2(1)	0(1)	-2(1)
O(11)	10(1)	18(1)	19(1)	1(1)	3(1)	-4(1)
O(12)	9(1)	19(1)	21(1)	4(1)	2(1)	-1(1)
C(11)	10(1)	16(1)	14(1)	-1(1)	3(1)	-1(1)
C(12)	20(1)	20(1)	25(1)	8(1)	0(1)	1(1)
O(21)	9(1)	18(1)	13(1)	0(1)	-1(1)	-1(1)
O(22)	9(1)	22(1)	16(1)	-2(1)	1(1)	-3(1)
C(21)	10(1)	12(1)	14(1)	-1(1)	0(1)	0(1)
C(22)	15(1)	33(1)	13(1)	0(1)	1(1)	4(1)
O(1W)	12(1)	15(1)	18(1)	2(1)	4(1)	0(1)
O(2W)	10(1)	17(1)	19(1)	-3(1)	1(1)	0(1)
O(3W)	25(1)	17(1)	15(1)	3(1)	6(1)	4(1)

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

	x	y	z	U(eq)
H(12A)	-608	1010	6429	37(8)
H(12B)	212	267	5712	37(8)
H(12C)	-1781	-26	5802	37(8)
H(12D)	283	727	6203	37(8)
H(12E)	-1760	603	6206	37(8)
H(12F)	-858	-126	5508	37(8)
H(22A)	7667	5549	7320	80(9)
H(22B)	5746	4859	7148	80(9)
H(22C)	6087	6826	7213	80(9)
H(11W)	3850	1063	5720	47(7)
H(12W)	5044	1859	5198	47(7)
H(21W)	366	6666	6287	30(6)
H(22W)	2119	7494	6447	30(6)
H(31W)	2378	3941	7041	40(7)
H(32W)	3143	2327	6771	40(7)

Table S6. Hydrogen bonds for Gd(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	3.278(2)	169.3
O(1W)-H(12W)...O(12)#4	0.96	1.80	2.703(2)	155.9
O(2W)-H(21W)...O(22)#5	0.96	1.83	2.706(2)	149.6
O(2W)-H(22W)...Br(1)	0.96	2.28	3.230(2)	168.1
O(3W)-H(31W)...Br(1)#6	0.96	2.36	3.311(2)	168.4
O(3W)-H(32W)...Br(1)#3	0.96	2.26	3.207(2)	166.9

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