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

Identification code	Ha2019_69_0m_a
Empirical formula	C4 H12 Br Lu O7
Formula weight	427.02
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.7611(3) A b = 8.0702(3) A ß = 96.098(2) deg. c = 17.2952(6) A
Volume	1077.13(7) A^3
Z, Calculated density	4, 2.633 Mg/m^3
Absorption coefficient	12.879 mm^-1
F(000)	792
Crystal size	0.408 x 0.071 x 0.054 mm
Theta range for data collection	2.776 to 27.998 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -22<=l<=22
Reflections collected / unique	103545 / 2596 [R(int) = 0.0735]
Completeness to theta = 25.242	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.741 and 0.326
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2596 / 0 / 125
Goodness-of-fit on F^2	1.055
Final R indices [I>2sigma(I)]	R1 = 0.0184, wR2 = 0.0417
R indices (all data)	R1 = 0.0233, wR2 = 0.0438
Extinction coefficient	n/a
Largest diff. peak and hole	1.131 and -1.209 e.A^-3

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

	x	y	z	U(eq)
Lu(1)	2764(1)	4435(1)	5406(1)	10(1)
Br(1)	3805(1)	9462(1)	6781(1)	17(1)
O(11)	256(3)	3207(3)	5430(1)	18(1)
O(12)	-2583(3)	3012(3)	5218(1)	13(1)
C(11)	-1123(4)	2425(4)	5479(2)	13(1)
C(12)	-1081(5)	743(5)	5846(2)	21(1)
O(21)	5375(3)	5552(3)	5742(1)	13(1)
O(22)	8096(3)	6249(3)	5899(1)	14(1)
C(21)	6732(4)	5909(4)	6197(2)	12(1)
C(22)	6700(5)	5868(5)	7059(2)	20(1)
O(1W)	4158(3)	1928(3)	5326(1)	15(1)
O(2W)	1567(3)	6209(3)	6247(1)	14(1)
O(3W)	3181(3)	3398(3)	6674(1)	17(1)

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

Lu(1)-O(11)	2.188(2)
Lu(1)-O(21)	2.238(2)
Lu(1)-O(2W)	2.305(2)
Lu(1)-O(1W)	2.306(2)
Lu(1)-O(12)#1	2.323(2)
Lu(1)-O(3W)	2.338(2)
Lu(1)-O(22)#2	2.350(2)
Lu(1)-O(21)#2	2.577(2)
Lu(1)-O(11)#1	3.238(3)
Lu(1)-Lu(1)#2	3.9862(3)
Lu(1)-Lu(1)#1	4.4638(3)
O(11)-C(11)	1.253(4)
O(12)-C(11)	1.266(4)
C(11)-C(12)	1.498(5)
O(21)-C(21)	1.278(4)
O(22)-C(21)	1.255(4)
C(21)-C(22)	1.495(5)
O(11)-Lu(1)-O(21)	163.82(9)
O(11)-Lu(1)-O(2W)	81.43(9)
O(21)-Lu(1)-O(2W)	90.02(9)
O(11)-Lu(1)-O(1W)	91.57(9)
O(21)-Lu(1)-O(1W)	87.21(9)
O(2W)-Lu(1)-O(1W)	143.68(8)
O(11)-Lu(1)-O(12)#1	113.61(9)
O(21)-Lu(1)-O(12)#1	76.80(8)
O(2W)-Lu(1)-O(12)#1	74.57(8)
O(1W)-Lu(1)-O(12)#1	139.13(8)
O(11)-Lu(1)-O(3W)	81.67(9)
O(21)-Lu(1)-O(3W)	82.49(8)
O(2W)-Lu(1)-O(3W)	69.84(9)
O(1W)-Lu(1)-O(3W)	73.90(9)
O(12)#1-Lu(1)-O(3W)	138.50(9)
O(11)-Lu(1)-O(22)#2	75.48(9)
O(21)-Lu(1)-O(22)#2	120.05(8)
O(2W)-Lu(1)-O(22)#2	131.26(8)
O(1W)-Lu(1)-O(22)#2	79.85(8)
O(12)#1-Lu(1)-O(22)#2	76.41(8)
O(3W)-Lu(1)-O(22)#2	144.47(9)
O(11)-Lu(1)-O(21)#2	126.06(8)
O(21)-Lu(1)-O(21)#2	68.41(9)
O(2W)-Lu(1)-O(21)#2	141.28(8)
O(1W)-Lu(1)-O(21)#2	69.66(8)
O(12)#1-Lu(1)-O(21)#2	69.49(8)
O(3W)-Lu(1)-O(21)#2	133.73(8)
O(22)#2-Lu(1)-O(21)#2	52.12(7)
O(11)-Lu(1)-O(11)#1	70.82(10)
O(21)-Lu(1)-O(11)#1	118.16(8)
O(2W)-Lu(1)-O(11)#1	66.15(7)
O(1W)-Lu(1)-O(11)#1	144.21(7)
O(12)#1-Lu(1)-O(11)#1	42.81(7)
O(3W)-Lu(1)-O(11)#1	130.60(7)
O(22)#2-Lu(1)-O(11)#1	65.87(7)
O(21)#2-Lu(1)-O(11)#1	95.29(7)
Lu(1)#2-Lu(1)-Lu(1)#1	133.329(7)

C(11)-O(11)-Lu(1)	175.6(3)
C(11)-O(12)-Lu(1)#1	120.3(2)
O(11)-C(11)-O(12)	121.7(3)
O(11)-C(11)-C(12)	120.3(3)
O(12)-C(11)-C(12)	117.9(3)
C(21)-O(21)-Lu(1)	156.2(2)
C(21)-O(21)-Lu(1)#2	88.9(2)
Lu(1)-O(21)-Lu(1)#2	111.6(1)
C(21)-O(22)-Lu(1)#2	100.2(2)
O(22)-C(21)-O(21)	118.2(3)
O(22)-C(21)-C(22)	121.2(3)
O(21)-C(21)-C(22)	120.6(3)

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 Lu(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
Lu(1)	8(1)	13(1)	10(1)	0(1)	1(1)	-1(1)
Br(1)	22(1)	14(1)	16(1)	1(1)	2(1)	-3(1)
O(11)	14(1)	20(1)	20(1)	-3(1)	6(1)	-6(1)
O(12)	10(1)	13(1)	16(1)	2(1)	3(1)	0(1)
C(11)	12(1)	14(2)	12(2)	-1(1)	3(1)	-2(1)
C(12)	17(2)	20(2)	25(2)	6(2)	2(1)	1(2)
O(21)	9(1)	17(1)	12(1)	0(1)	0(1)	-1(1)
O(22)	10(1)	19(1)	13(1)	1(1)	-1(1)	-1(1)
C(21)	13(2)	10(2)	14(2)	0(1)	1(1)	2(1)
C(22)	20(2)	30(2)	9(2)	0(1)	-1(1)	2(2)
O(1W)	13(1)	17(1)	15(1)	4(1)	3(1)	1(1)
O(2W)	12(1)	15(1)	15(1)	-2(1)	0(1)	0(1)
O(3W)	21(1)	19(1)	13(1)	2(1)	5(1)	2(1)

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

	x	y	z	U(eq)
H(12A)	-1873	720	6251	55(10)
H(12B)	99	498	6078	55(10)
H(12C)	-1443	-91	5450	55(10)
H(22A)	7883	5735	7312	91(15)
H(22B)	5986	4936	7199	91(15)
H(22C)	6211	6907	7232	91(15)
H(11W)	4113	1088	5717	55(12)
H(12W)	5338	1932	5208	55(12)
H(21W)	361	6435	6274	46(11)
H(22W)	2157	7204	6428	46(11)
H(31W)	2672	3875	7105	55(12)
H(32W)	3485	2288	6835	55(12)

Table S6. Hydrogen bonds for Lu(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	2.29	3.242(2)	169.4
O(1W)-H(12W)...O(12)#4	0.96	1.83	2.702(3)	149.2
O(2W)-H(21W)...O(22)#5	0.96	1.81	2.698(3)	151.6
O(2W)-H(22W)...Br(1)	0.96	2.27	3.228(2)	173.4
O(3W)-H(31W)...Br(1)#6	0.96	2.39	3.336(2)	167.6
O(3W)-H(32W)...Br(1)#3	0.96	2.30	3.216(3)	159.9

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