Table S1. Crystal data and structure refinement for Lu(OAc)2Cl_x_3H2O.

Identification code	Ha2019_67_0m_a
Empirical formula	C4 H12 Cl Lu O7
Formula weight	382.56
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.7668(3) A b = 7.8297(3) A ß = 97.336(2) deg. c = 17.0618(7) A
Volume	1029.06(7) A^3
Z, Calculated density	4, 2.469 Mg/m^3
Absorption coefficient	9.857 mm^-1
F(000)	720
Crystal size	0.292 x 0.065 x 0.057 mm
Theta range for data collection	2.762 to 27.999 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -22<=l<=22
Reflections collected / unique	100183 / 2490 [R(int) = 0.0653]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.749 and 0.356
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2490 / 0 / 125
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0119, wR2 = 0.0264
R indices (all data)	R1 = 0.0143, wR2 = 0.0270
Extinction coefficient	n/a
Largest diff. peak and hole	0.365 and -0.421 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Lu(OAc)2Cl_x_3H2O. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Lu(1)	2779(1)	4453(1)	5425(1)	8(1)
Cl(1)	3742(1)	9541(1)	6817(1)	15(1)
O(11)	265(2)	3197(2)	5452(1)	15(1)
O(12)	-2579(2)	2951(2)	5245(1)	12(1)
C(11)	-1099(3)	2368(3)	5511(1)	10(1)
C(12)	-1003(3)	638(3)	5891(2)	18(1)
O(21)	5409(2)	5616(2)	5745(1)	11(1)
O(22)	8135(2)	6332(2)	5897(1)	12(1)
C(21)	6780(3)	6008(3)	6207(1)	10(1)
C(22)	6780(3)	6054(3)	7077(1)	17(1)
O(1W)	4162(2)	1853(2)	5375(1)	13(1)
O(2W)	1631(2)	6337(2)	6255(1)	12(1)
O(3W)	3241(2)	3438(2)	6729(1)	15(1)

Table S3. Bond lengths [A] and angles [deg] for Lu(OAc)2Cl_x_3H2O.

Lu(1)-O(11)	2.193(1)
Lu(1)-O(21)	2.239(1)
Lu(1)-O(2W)	2.302(2)
Lu(1)-O(1W)	2.309(2)
Lu(1)-O(12)#1	2.327(2)
Lu(1)-O(3W)	2.346(2)
Lu(1)-O(22)#2	2.358(2)
Lu(1)-O(21)#2	2.585(2)
Lu(1)-O(11)#1	3.211(2)
Lu(1)-Lu(1)#2	4.0016(2)
Lu(1)-Lu(1)#1	4.4585(2)
O(11)-C(11)	1.257(2)
O(12)-C(11)	1.266(2)
C(11)-C(12)	1.500(3)
O(21)-C(21)	1.279(3)
O(22)-C(21)	1.263(3)
C(21)-C(22)	1.484(3)
O(11)-Lu(1)-O(21)	164.70(6)
O(11)-Lu(1)-O(2W)	81.86(5)
O(21)-Lu(1)-O(2W)	90.14(5)
O(11)-Lu(1)-O(1W)	91.42(5)
O(21)-Lu(1)-O(1W)	87.35(5)
O(2W)-Lu(1)-O(1W)	143.75(5)
O(11)-Lu(1)-O(12)#1	113.47(5)
O(21)-Lu(1)-O(12)#1	76.48(5)
O(2W)-Lu(1)-O(12)#1	74.67(5)
O(1W)-Lu(1)-O(12)#1	138.97(5)
O(11)-Lu(1)-O(3W)	81.76(6)
O(21)-Lu(1)-O(3W)	83.26(5)
O(2W)-Lu(1)-O(3W)	70.00(5)
O(1W)-Lu(1)-O(3W)	73.79(5)
O(12)#1-Lu(1)-O(3W)	138.93(5)
O(11)-Lu(1)-O(22)#2	75.10(5)
O(21)-Lu(1)-O(22)#2	119.55(5)
O(2W)-Lu(1)-O(22)#2	131.49(5)
O(1W)-Lu(1)-O(22)#2	79.59(5)
O(12)#1-Lu(1)-O(22)#2	76.41(5)
O(3W)-Lu(1)-O(22)#2	144.03(5)
O(11)-Lu(1)-O(21)#2	125.51(5)
O(21)-Lu(1)-O(21)#2	68.12(6)
O(2W)-Lu(1)-O(21)#2	141.29(5)
O(1W)-Lu(1)-O(21)#2	69.59(5)
O(12)#1-Lu(1)-O(21)#2	69.41(5)
O(3W)-Lu(1)-O(21)#2	133.83(5)
O(22)#2-Lu(1)-O(21)#2	51.92(5)
O(11)-Lu(1)-O(11)#1	70.26(6)
O(21)-Lu(1)-O(11)#1	118.35(5)
O(2W)-Lu(1)-O(11)#1	66.40(5)
O(1W)-Lu(1)-O(11)#1	143.74(5)
O(12)#1-Lu(1)-O(11)#1	43.25(4)
O(3W)-Lu(1)-O(11)#1	130.56(5)
O(22)#2-Lu(1)-O(11)#1	65.78(5)
O(21)#2-Lu(1)-O(11)#1	95.34(4)
Lu(1)#2-Lu(1)-Lu(1)#1	133.215(5)

C(11)-O(11)-Lu(1)	174.4(2)
C(11)-O(12)-Lu(1)#1	119.4(1)
O(11)-C(11)-O(12)	121.4(2)
O(11)-C(11)-C(12)	120.3(2)
O(12)-C(11)-C(12)	118.2(2)
C(21)-O(21)-Lu(1)	155.4(2)
C(21)-O(21)-Lu(1)#2	89.4(1)
Lu(1)-O(21)-Lu(1)#2	111.9(6)
C(21)-O(22)-Lu(1)#2	100.6(1)
O(22)-C(21)-O(21)	117.5(2)
O(22)-C(21)-C(22)	121.4(2)
O(21)-C(21)-C(22)	121.1(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 Lu(OAc)2Cl_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)	5(1)	8(1)	11(1)	0(1)	1(1)	-1(1)
Cl(1)	18(1)	11(1)	16(1)	1(1)	2(1)	-2(1)
O(11)	10(1)	16(1)	20(1)	-3(1)	5(1)	-5(1)
O(12)	7(1)	13(1)	16(1)	2(1)	1(1)	0(1)
C(11)	10(1)	12(1)	8(1)	-3(1)	3(1)	-1(1)
C(12)	16(1)	16(1)	21(1)	4(1)	2(1)	2(1)
O(21)	8(1)	12(1)	12(1)	-1(1)	0(1)	0(1)
O(22)	7(1)	13(1)	16(1)	0(1)	1(1)	-1(1)
C(21)	10(1)	5(1)	15(1)	1(1)	-1(1)	3(1)
C(22)	14(1)	26(1)	11(1)	0(1)	0(1)	1(1)
O(1W)	10(1)	12(1)	17(1)	2(1)	5(1)	1(1)
O(2W)	8(1)	12(1)	17(1)	-3(1)	1(1)	-1(1)
O(3W)	19(1)	12(1)	16(1)	2(1)	6(1)	3(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Lu(OAc)2Cl_x_3H2O.

	x	y	z	U(eq)
H(12A)	-1185	-244	5481	48(6)
H(12B)	-1904	543	6242	48(6)
H(12C)	141	485	6198	48(6)
H(22A)	7971	5927	7339	58(6)
H(22B)	6064	5118	7237	58(6)
H(22C)	6305	7147	7229	58(6)
H(11W)	4107	959	5756	45(7)
H(12W)	5364	1918	5299	45(7)
H(21W)	408	6538	6238	40(6)
H(22W)	2169	7408	6412	40(6)
H(31W)	2652	3935	7135	56(7)
H(32W)	3357	2250	6864	56(7)

Table S6. Hydrogen bonds for Lu(OAc)2Cl_x_3H2O [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(11W)...Cl(1)#3	0.96	2.17	3.105(2)	163.5
O(1W)-H(12W)...O(12)#4	0.96	1.80	2.709(2)	156.0
O(2W)-H(21W)...O(22)#5	0.96	1.79	2.706(2)	157.5
O(2W)-H(22W)...Cl(1)	0.96	2.13	3.082(2)	170.5
O(3W)-H(31W)...Cl(1)#6	0.96	2.26	3.202(2)	168.1
O(3W)-H(32W)...Cl(1)#3	0.96	2.14	3.078(2)	163.5

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