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

Identification code	Ha2019_99h_0m_a
Empirical formula	C4 H12 Cl Gd O7
Formula weight	364.84
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.8219(4) A b = 7.8592(4) A ß = 98.265(2) deg. c = 17.4434(8) A
Volume	1061.18(9) A^3
Z, Calculated density	4, 2.284 Mg/m^3
Absorption coefficient	6.506 mm^-1
F(000)	692
Crystal size	0.368 x 0.096 x 0.041 mm
Theta range for data collection	2.725 to 27.998 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -23<=l<=23
Reflections collected / unique	122742 / 2569 [R(int) = 0.0358]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.746 and 0.443
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2569 / 0 / 126
Goodness-of-fit on F^2	1.090
Final R indices [I>2sigma(I)]	R1 = 0.0094, wR2 = 0.0206
R indices (all data)	R1 = 0.0100, wR2 = 0.0208
Extinction coefficient	0.00122(7)
Largest diff. peak and hole	0.348 and -0.474 e.A^-3

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

	x	y	z	U(eq)
Gd(1)	2645(1)	4604(1)	5374(1)	9(1)
Cl(1)	3828(1)	9701(1)	6896(1)	16(1)
O(11)	-62(1)	3374(1)	5361(1)	15(1)
O(12)	-2775(1)	2649(1)	5262(1)	15(1)
C(11)	-1212(2)	2317(2)	5493(1)	12(1)
C(12)	-731(2)	702(2)	5920(1)	21(1)
O(21)	5469(1)	5608(1)	5739(1)	12(1)
O(22)	8200(1)	6283(1)	5972(1)	14(1)
C(21)	6800(2)	5984(2)	6225(1)	12(1)
C(22)	6691(2)	6059(2)	7070(1)	19(1)
O(1W)	3921(1)	1792(1)	5373(1)	14(1)
O(2W)	1687(1)	6600(1)	6257(1)	14(1)
O(3W)	3002(1)	3508(1)	6683(1)	17(1)

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

Gd(1)-O(11)	2.325(1)
Gd(1)-O(21)	2.346(1)
Gd(1)-O(2W)	2.393(1)
Gd(1)-O(3W)	2.418(1)
Gd(1)-O(1W)	2.425(1)
Gd(1)-O(12)#1	2.436(1)
Gd(1)-O(22)#2	2.449(1)
Gd(1)-O(21)#2	2.607(1)
Gd(1)-O(11)#1	2.740(1)
Gd(1)-Gd(1)#2	4.1291(2)
Gd(1)-Gd(1)#1	4.2028(2)
O(11)-C(11)	1.270(2)
O(12)-C(11)	1.258(2)
C(11)-C(12)	1.492(2)
O(21)-C(21)	1.279(2)
O(22)-C(21)	1.260(2)
C(21)-C(22)	1.491(2)
O(11)-Gd(1)-O(21)	164.48(4)
O(11)-Gd(1)-O(2W)	84.84(4)
O(21)-Gd(1)-O(2W)	88.58(4)
O(11)-Gd(1)-O(3W)	80.96(4)
O(21)-Gd(1)-O(3W)	83.56(4)
O(2W)-Gd(1)-O(3W)	68.30(4)
O(11)-Gd(1)-O(1W)	89.72(4)
O(21)-Gd(1)-O(1W)	86.29(4)
O(2W)-Gd(1)-O(1W)	139.92(4)
O(3W)-Gd(1)-O(1W)	71.63(4)
O(11)-Gd(1)-O(12)#1	117.48(4)
O(21)-Gd(1)-O(12)#1	74.10(4)
O(2W)-Gd(1)-O(12)#1	75.51(4)
O(3W)-Gd(1)-O(12)#1	137.65(4)
O(1W)-Gd(1)-O(12)#1	139.73(3)
O(11)-Gd(1)-O(22)#2	75.64(4)
O(21)-Gd(1)-O(22)#2	118.00(3)
O(2W)-Gd(1)-O(22)#2	137.53(4)
O(3W)-Gd(1)-O(22)#2	141.53(4)
O(1W)-Gd(1)-O(22)#2	78.10(4)
O(12)#1-Gd(1)-O(22)#2	80.69(4)
O(11)-Gd(1)-O(21)#2	125.29(4)
O(21)-Gd(1)-O(21)#2	67.16(4)
O(2W)-Gd(1)-O(21)#2	141.66(3)
O(3W)-Gd(1)-O(21)#2	132.80(3)
O(1W)-Gd(1)-O(21)#2	70.37(3)
O(12)#1-Gd(1)-O(21)#2	69.65(3)
O(22)#2-Gd(1)-O(21)#2	51.01(3)
O(11)-Gd(1)-O(11)#1	68.11(4)
O(21)-Gd(1)-O(11)#1	122.28(3)
O(2W)-Gd(1)-O(11)#1	69.08(3)
O(3W)-Gd(1)-O(11)#1	128.74(3)
O(1W)-Gd(1)-O(11)#1	143.50(3)
O(12)#1-Gd(1)-O(11)#1	49.39(3)
O(22)#2-Gd(1)-O(11)#1	68.70(3)
O(21)#2-Gd(1)-O(11)#1	98.42(3)
Gd(1)#2-Gd(1)-Gd(1)#1	139.698(4)

C(11)-O(11)-Gd(1)	159.8(1)
C(11)-O(11)-Gd(1)#1	88.3(1)
Gd(1)-O(11)-Gd(1)#1	111.9(1)
C(11)-O(12)-Gd(1)#1	103.2(1)
O(12)-C(11)-O(11)	119.2(1)
O(12)-C(11)-C(12)	120.0(1)
O(11)-C(11)-C(12)	120.8(1)
C(21)-O(21)-Gd(1)	154.4(1)
C(21)-O(21)-Gd(1)#2	90.9(1)
Gd(1)-O(21)-Gd(1)#2	112.8(1)
C(21)-O(22)-Gd(1)#2	98.8(1)
O(22)-C(21)-O(21)	118.5(1)
O(22)-C(21)-C(22)	121.0(1)
O(21)-C(21)-C(22)	120.6(1)

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)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
Gd(1)	6(1)	10(1)	11(1)	0(1)	2(1)	-1(1)
Cl(1)	17(1)	13(1)	17(1)	1(1)	2(1)	-1(1)
O(11)	11(1)	17(1)	18(1)	0(1)	4(1)	-4(1)
O(12)	9(1)	17(1)	21(1)	5(1)	3(1)	0(1)
C(11)	11(1)	14(1)	12(1)	-1(1)	3(1)	0(1)
C(12)	23(1)	17(1)	23(1)	7(1)	1(1)	2(1)
O(21)	9(1)	15(1)	13(1)	0(1)	1(1)	-1(1)
O(22)	9(1)	19(1)	15(1)	-1(1)	2(1)	-2(1)
C(21)	11(1)	11(1)	14(1)	0(1)	1(1)	1(1)
C(22)	15(1)	29(1)	12(1)	-1(1)	1(1)	2(1)
O(1W)	12(1)	14(1)	16(1)	2(1)	5(1)	0(1)
O(2W)	11(1)	14(1)	18(1)	-4(1)	2(1)	0(1)
O(3W)	24(1)	14(1)	15(1)	2(1)	7(1)	4(1)

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

	x	y	z	U(eq)
H(12A)	-1517	-208	5708	33(5)
H(12B)	-817	858	6470	33(5)
H(12C)	457	394	5861	33(5)
H(12D)	288	812	6315	33(5)
H(12E)	-489	-115	5525	33(5)
H(12F)	-1711	297	6162	33(5)
H(22A)	7843	5888	7364	52(4)
H(22B)	5912	5165	7204	52(4)
H(22C)	6247	7174	7198	52(4)
H(11W)	3898	994	5788	49(5)
H(12W)	5112	1853	5298	49(5)
H(21W)	491	6726	6316	44(5)
H(22W)	2230	7631	6463	44(5)
H(31W)	2462	4009	7089	54(5)
H(32W)	3197	2342	6834	54(5)

Table S6. Hydrogen bonds for Gd(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	2.19	3.134(1)	166.8
O(1W)-H(12W)...O(12)#4	0.96	1.78	2.705(1)	161.5
O(2W)-H(21W)...O(22)#5	0.96	1.84	2.712(1)	149.7
O(2W)-H(22W)...Cl(1)	0.96	2.12	3.074(1)	170.3
O(3W)-H(31W)...Cl(1)#6	0.96	2.23	3.176(1)	169.9
O(3W)-H(32W)...Cl(1)#3	0.96	2.13	3.072(1)	165.9

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