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

Identification code	Ha2019_72_0m_a
Empirical formula	C4 H12 Ce Cl O7
Formula weight	347.71
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.9625(3) A b = 7.9276(3) A ß = 99.122(2) deg. c = 17.6973(6) A
Volume	1102.99(7) A^3
Z, Calculated density	4, 2.094 Mg/m^3
Absorption coefficient	4.373 mm^-1
F(000)	668
Crystal size	0.250 x 0.139 x 0.040 mm
Theta range for data collection	2.667 to 27.994 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -23<=l<=23
Reflections collected / unique	101277 / 2664 [R(int) = 0.0460]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.762 and 0.518
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2664 / 0 / 125
Goodness-of-fit on F^2	1.225
Final R indices [I>2sigma(I)]	R1 = 0.0177, wR2 = 0.0355
R indices (all data)	R1 = 0.0186, wR2 = 0.0357
Extinction coefficient	n/a
Largest diff. peak and hole	0.532 and -0.811 e.A^-3

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

	x	y	z	U(eq)
Ce(1)	2645(1)	4603(1)	5388(1)	10(1)
Cl(1)	3847(1)	9700(1)	6921(1)	17(1)
O(11)	-141(2)	3353(2)	5355(1)	15(1)
O(12)	-2794(2)	2554(2)	5256(1)	18(1)
C(11)	-1244(3)	2276(3)	5488(1)	13(1)
C(12)	-707(3)	701(3)	5922(2)	22(1)
O(21)	5547(2)	5633(2)	5753(1)	14(1)
O(22)	8230(2)	6344(2)	5994(1)	16(1)
C(21)	6866(3)	6022(3)	6235(1)	13(1)
C(22)	6751(3)	6099(4)	7068(1)	21(1)
O(1W)	3973(2)	1709(2)	5408(1)	15(1)
O(2W)	1686(2)	6655(2)	6293(1)	16(1)
O(3W)	3005(2)	3476(2)	6722(1)	19(1)

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

Ce(1)-O(11)	2.422(2)
Ce(1)-O(21)	2.440(2)
Ce(1)-O(2W)	2.486(2)
Ce(1)-O(3W)	2.499(2)
Ce(1)-O(1W)	2.524(2)
Ce(1)-O(12)#1	2.536(2)
Ce(1)-O(22)#2	2.548(2)
Ce(1)-O(21)#2	2.665(2)
Ce(1)-O(11)#1	2.738(2)
Ce(1)-Ce(1)#2	4.2401(3)
Ce(1)-Ce(1)#1	4.2648(3)
O(11)-C(11)	1.273(3)
O(12)-C(11)	1.257(3)
C(11)-C(12)	1.493(3)
O(21)-C(21)	1.282(3)
O(22)-C(21)	1.254(3)
C(21)-C(22)	1.493(3)
O(11)-Ce(1)-O(21)	165.68(5)
O(11)-Ce(1)-O(2W)	84.80(5)
O(21)-Ce(1)-O(2W)	89.17(5)
O(11)-Ce(1)-O(3W)	81.00(6)
O(21)-Ce(1)-O(3W)	84.70(5)
O(2W)-Ce(1)-O(3W)	68.05(5)
O(11)-Ce(1)-O(1W)	90.47(5)
O(21)-Ce(1)-O(1W)	85.60(5)
O(2W)-Ce(1)-O(1W)	139.16(5)
O(3W)-Ce(1)-O(1W)	71.13(5)
O(11)-Ce(1)-O(12)#1	117.45(5)
O(21)-Ce(1)-O(12)#1	73.24(5)
O(2W)-Ce(1)-O(12)#1	75.46(5)
O(3W)-Ce(1)-O(12)#1	137.37(6)
O(1W)-Ce(1)-O(12)#1	139.87(5)
O(11)-Ce(1)-O(22)#2	75.31(5)
O(21)-Ce(1)-O(22)#2	117.14(5)
O(2W)-Ce(1)-O(22)#2	138.23(5)
O(3W)-Ce(1)-O(22)#2	140.80(6)
O(1W)-Ce(1)-O(22)#2	78.22(5)
O(12)#1-Ce(1)-O(22)#2	81.70(6)
O(11)-Ce(1)-O(21)#2	123.77(5)
O(21)-Ce(1)-O(21)#2	67.74(6)
O(2W)-Ce(1)-O(21)#2	142.35(5)
O(3W)-Ce(1)-O(21)#2	134.10(5)
O(1W)-Ce(1)-O(21)#2	70.82(5)
O(12)#1-Ce(1)-O(21)#2	69.69(5)
O(22)#2-Ce(1)-O(21)#2	49.50(5)
O(11)-Ce(1)-O(11)#1	68.68(6)
O(21)-Ce(1)-O(11)#1	121.08(5)
O(2W)-Ce(1)-O(11)#1	69.37(5)
O(3W)-Ce(1)-O(11)#1	129.15(5)
O(1W)-Ce(1)-O(11)#1	144.68(5)
O(12)#1-Ce(1)-O(11)#1	48.77(5)
O(22)#2-Ce(1)-O(11)#1	69.24(5)
O(21)#2-Ce(1)-O(11)#1	96.73(5)
Ce(1)#2-Ce(1)-Ce(1)#1	138.852(7)

C(11)-O(11)-Ce(1)	157.8(2)
C(11)-O(11)-Ce(1)#1	90.8(1)
Ce(1)-O(11)-Ce(1)#1	111.3(1)
C(11)-O(12)-Ce(1)#1	100.9(1)
O(12)-C(11)-O(11)	119.5(2)
O(12)-C(11)-C(12)	120.1(2)
O(11)-C(11)-C(12)	120.4(2)
C(21)-O(21)-Ce(1)	154.0(1)
C(21)-O(21)-Ce(1)#2	92.2(1)
Ce(1)-O(21)-Ce(1)#2	112.3(1)
C(21)-O(22)-Ce(1)#2	98.4(1)
O(22)-C(21)-O(21)	119.0(2)
O(22)-C(21)-C(22)	121.3(2)
O(21)-C(21)-C(22)	119.7(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 Ce(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
Ce(1)	6(1)	11(1)	13(1)	1(1)	2(1)	-1(1)
Cl(1)	18(1)	14(1)	18(1)	1(1)	3(1)	-2(1)
O(11)	10(1)	16(1)	20(1)	2(1)	4(1)	-3(1)
O(12)	9(1)	17(1)	27(1)	6(1)	4(1)	-1(1)
C(11)	11(1)	13(1)	16(1)	0(1)	5(1)	-1(1)
C(12)	21(1)	16(1)	30(1)	8(1)	1(1)	2(1)
O(21)	10(1)	16(1)	14(1)	0(1)	1(1)	-2(1)
O(22)	9(1)	21(1)	18(1)	-2(1)	2(1)	-2(1)
C(21)	12(1)	12(1)	15(1)	0(1)	1(1)	1(1)
C(22)	16(1)	32(1)	14(1)	-2(1)	2(1)	2(1)
O(1W)	13(1)	13(1)	20(1)	3(1)	7(1)	1(1)
O(2W)	13(1)	14(1)	22(1)	-4(1)	3(1)	-1(1)
O(3W)	26(1)	14(1)	17(1)	2(1)	8(1)	5(1)

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

	x	y	z	U(eq)
H(12A)	-1527	-200	5757	35(7)
H(12B)	-665	906	6471	35(7)
H(12C)	422	361	5824	35(7)
H(12D)	-378	-240	5618	35(7)
H(12E)	-1773	426	6105	35(7)
H(12F)	189	901	6361	35(7)
H(22A)	7887	5950	7368	57(7)
H(22B)	5999	5201	7196	57(7)
H(22C)	6293	7197	7188	57(7)
H(11W)	3928	915	5814	45(7)
H(12W)	5142	1723	5336	45(7)
H(21W)	504	6796	6329	43(7)
H(22W)	2217	7692	6482	43(7)
H(31W)	2482	3962	7124	66(9)
H(32W)	3186	2313	6863	66(9)

Table S6. Hydrogen bonds for Ce(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	3.130(2)	165.0
O(1W)-H(12W)...O(12)#4	0.96	1.80	2.715(2)	159.0
O(2W)-H(21W)...O(22)#5	0.96	1.85	2.729(2)	151.2
O(2W)-H(22W)...Cl(1)	0.96	2.12	3.069(2)	168.5
O(3W)-H(31W)...Cl(1)#6	0.96	2.21	3.163(2)	171.6
O(3W)-H(32W)...Cl(1)#3	0.96	2.14	3.075(2)	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