Table S1. Crystal data and structure refinement for Nd(OAc)2Cl)_x_3H2O.

Identification code	Ha2019_58_0m_a
Empirical formula	C4 H12 Cl Nd O7
Formula weight	351.83
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.9059(3) A b = 7.9008(3) A ß = 98.856(2) deg. c = 17.5852(7) A
Volume	1085.33(7) A^3
Z, Calculated density	4, 2.153 Mg/m^3
Absorption coefficient	5.034 mm^-1
F(000)	676
Crystal size	0.151 x 0.144 x 0.063 mm
Theta range for data collection	2.689 to 27.999 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -23<=l<=23
Reflections collected / unique	122829 / 2621 [R(int) = 0.0566]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.762 and 0.489
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2621 / 0 / 125
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0122, wR2 = 0.0270
R indices (all data)	R1 = 0.0142, wR2 = 0.0275
Extinction coefficient	n/a
Largest diff. peak and hole	0.387 and -0.358 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Nd(OAc)2Cl)_x_3H2O. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Nd(1)	2639(1)	4614(1)	5378(1)	9(1)
Cl(1)	3846(1)	9715(1)	6915(1)	16(1)
O(11)	-128(2)	3379(2)	5353(1)	14(1)
O(12)	-2798(2)	2575(2)	5257(1)	17(1)
C(11)	-1237(2)	2291(2)	5490(1)	13(1)
C(12)	-698(3)	710(2)	5920(1)	21(1)
O(21)	5521(2)	5619(2)	5745(1)	13(1)
O(22)	8223(2)	6325(2)	5990(1)	15(1)
C(21)	6840(2)	6014(2)	6231(1)	12(1)
C(22)	6715(2)	6089(3)	7069(1)	20(1)
O(1W)	3932(2)	1743(2)	5390(1)	14(1)
O(2W)	1697(2)	6648(2)	6279(1)	15(1)
O(3W)	2994(2)	3497(2)	6703(1)	18(1)

Table S3. Bond lengths [A] and angles [deg] for Nd(OAc)2Cl)_x_3H2O.

Nd(1)-O(11)	2.390(1)
Nd(1)-O(21)	2.406(1)
Nd(1)-O(2W)	2.452(1)
Nd(1)-O(3W)	2.467(1)
Nd(1)-O(1W)	2.487(1)
Nd(1)-O(12)#1	2.498(1)
Nd(1)-O(22)#2	2.510(1)
Nd(1)-O(21)#2	2.633(1)
Nd(1)-O(11)#1	2.706(1)
Nd(1)-Nd(1)#2	4.1963(2)
Nd(1)-Nd(1)#1	4.2234(2)
O(11)-C(11)	1.276(2)
O(12)-C(11)	1.259(2)
C(11)-C(12)	1.489(3)
O(21)-C(21)	1.281(2)
O(22)-C(21)	1.256(2)
C(21)-C(22)	1.493(2)
O(11)-Nd(1)-O(21)	165.12(4)
O(11)-Nd(1)-O(2W)	84.92(4)
O(21)-Nd(1)-O(2W)	88.84(4)
O(11)-Nd(1)-O(3W)	80.91(4)
O(21)-Nd(1)-O(3W)	84.23(4)
O(2W)-Nd(1)-O(3W)	68.00(4)
O(11)-Nd(1)-O(1W)	90.09(4)
O(21)-Nd(1)-O(1W)	85.84(4)
O(2W)-Nd(1)-O(1W)	139.23(4)
O(3W)-Nd(1)-O(1W)	71.25(4)
O(11)-Nd(1)-O(12)#1	117.66(4)
O(21)-Nd(1)-O(12)#1	73.46(4)
O(2W)-Nd(1)-O(12)#1	75.39(4)
O(3W)-Nd(1)-O(12)#1	137.23(4)
O(1W)-Nd(1)-O(12)#1	139.99(4)
O(11)-Nd(1)-O(22)#2	75.47(4)
O(21)-Nd(1)-O(22)#2	117.42(4)
O(2W)-Nd(1)-O(22)#2	138.50(4)
O(3W)-Nd(1)-O(22)#2	140.75(4)
O(1W)-Nd(1)-O(22)#2	77.84(4)
O(12)#1-Nd(1)-O(22)#2	81.90(4)
O(11)-Nd(1)-O(21)#2	124.57(4)
O(21)-Nd(1)-O(21)#2	67.30(5)
O(2W)-Nd(1)-O(21)#2	142.05(4)
O(3W)-Nd(1)-O(21)#2	133.43(4)
O(1W)-Nd(1)-O(21)#2	70.66(4)
O(12)#1-Nd(1)-O(21)#2	69.84(4)
O(22)#2-Nd(1)-O(21)#2	50.22(4)
O(11)-Nd(1)-O(11)#1	68.17(5)
O(21)-Nd(1)-O(11)#1	121.95(4)
O(2W)-Nd(1)-O(11)#1	69.49(4)
O(3W)-Nd(1)-O(11)#1	128.82(4)
O(1W)-Nd(1)-O(11)#1	144.03(4)
O(12)#1-Nd(1)-O(11)#1	49.49(4)
O(22)#2-Nd(1)-O(11)#1	69.32(4)
O(21)#2-Nd(1)-O(11)#1	97.73(4)
Nd(1)#2-Nd(1)-Nd(1)#1	139.761(5)

C(11)-O(11)-Nd(1)	157.6(1)
C(11)-O(11)-Nd(1)#1	90.5(1)
Nd(1)-O(11)-Nd(1)#1	111.8(1)
C(11)-O(12)-Nd(1)#1	100.9(1)
O(12)-C(11)-O(11)	119.1(2)
O(12)-C(11)-C(12)	120.3(2)
O(11)-C(11)-C(12)	120.6(2)
C(21)-O(21)-Nd(1)	154.1(1)
C(21)-O(21)-Nd(1)#2	91.8(1)
Nd(1)-O(21)-Nd(1)#2	112.7(1)
C(21)-O(22)-Nd(1)#2	98.3(1)
O(22)-C(21)-O(21)	118.9(2)
O(22)-C(21)-C(22)	121.2(2)
O(21)-C(21)-C(22)	119.9(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 Nd(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
Nd(1)	6(1)	10(1)	11(1)	1(1)	2(1)	-1(1)
Cl(1)	17(1)	13(1)	17(1)	2(1)	2(1)	-2(1)
O(11)	10(1)	15(1)	18(1)	2(1)	3(1)	-2(1)
O(12)	8(1)	16(1)	25(1)	5(1)	3(1)	-1(1)
C(11)	12(1)	14(1)	13(1)	0(1)	4(1)	0(1)
C(12)	19(1)	17(1)	27(1)	8(1)	1(1)	1(1)
O(21)	9(1)	16(1)	12(1)	0(1)	0(1)	-2(1)
O(22)	9(1)	21(1)	16(1)	-2(1)	2(1)	-3(1)
C(21)	11(1)	9(1)	15(1)	0(1)	0(1)	2(1)
C(22)	16(1)	30(1)	13(1)	0(1)	1(1)	2(1)
O(1W)	12(1)	13(1)	18(1)	2(1)	5(1)	1(1)
O(2W)	11(1)	14(1)	21(1)	-4(1)	2(1)	0(1)
O(3W)	25(1)	15(1)	15(1)	3(1)	7(1)	5(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Nd(OAc)2Cl)_x_3H2O.

	x	y	z	U(eq)
H(12A)	-599	924	6474	27(5)
H(12B)	412	341	5798	27(5)
H(12C)	-1553	-176	5772	27(5)
H(12D)	417	813	6249	27(5)
H(12E)	-1570	403	6236	27(5)
H(12F)	-639	-167	5531	27(5)
H(22A)	7855	5933	7370	49(5)
H(22B)	5951	5190	7196	49(5)
H(22C)	6257	7192	7191	49(5)
H(11W)	3920	933	5796	44(5)
H(12W)	5098	1769	5299	44(5)
H(21W)	521	6768	6347	51(6)
H(22W)	2246	7664	6490	51(6)
H(31W)	2446	3990	7100	51(6)
H(32W)	3159	2329	6845	51(6)

Table S6. Hydrogen bonds for Nd(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	2.20	3.134(1)	164.1
O(1W)-H(12W)...O(12)#4	0.96	1.79	2.712(2)	159.3
O(2W)-H(21W)...O(22)#5	0.96	1.86	2.727(2)	148.6
O(2W)-H(22W)...Cl(1)	0.96	2.12	3.070(1)	170.3
O(3W)-H(31W)...Cl(1)#6	0.96	2.22	3.168(1)	171.0
O(3W)-H(32W)...Cl(1)#3	0.96	2.13	3.074(1)	165.6

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