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

Identification code	Ha2019_59_0m_a
Empirical formula	C4 H12 Cl O7 Pr
Formula weight	348.50
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.9333(3) A b = 7.9139(3) A ß = 98.947(2) deg. c = 17.6327(6) A
Volume	1093.57(7) A^3
Z, Calculated density	4, 2.117 Mg/m^3
Absorption coefficient	4.703 mm^-1
F(000)	672
Crystal size	0.450 x 0.107 x 0.071 mm
Theta range for data collection	2.679 to 28.000 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -23<=l<=23
Reflections collected / unique	125986 / 2645 [R(int) = 0.0398]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.784 and 0.482
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2645 / 0 / 125
Goodness-of-fit on F^2	1.101
Final R indices [I>2sigma(I)]	R1 = 0.0125, wR2 = 0.0280
R indices (all data)	R1 = 0.0134, wR2 = 0.0283
Extinction coefficient	n/a
Largest diff. peak and hole	0.457 and -0.609 e.A^-3

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

	x	y	z	U(eq)
Pr(1)	2642(1)	4608(1)	5383(1)	9(1)
Cl(1)	3844(1)	9706(1)	6918(1)	16(1)
O(11)	-132(2)	3364(2)	5355(1)	15(1)
O(12)	-2793(2)	2568(2)	5258(1)	17(1)
C(11)	-1241(2)	2286(2)	5490(1)	12(1)
C(12)	-699(3)	703(2)	5923(1)	21(1)
O(21)	5534(2)	5625(2)	5749(1)	13(1)
O(22)	8226(2)	6332(2)	5993(1)	15(1)
C(21)	6850(2)	6017(2)	6232(1)	12(1)
C(22)	6732(2)	6094(3)	7070(1)	19(1)
O(1W)	3954(2)	1725(2)	5397(1)	14(1)
O(2W)	1687(2)	6651(2)	6285(1)	16(1)
O(3W)	3003(2)	3488(2)	6713(1)	18(1)

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

Pr(1)-O(11)	2.404(1)
Pr(1)-O(21)	2.422(1)
Pr(1)-O(2W)	2.468(1)
Pr(1)-O(3W)	2.482(1)
Pr(1)-O(1W)	2.506(1)
Pr(1)-O(12)#1	2.516(1)
Pr(1)-O(22)#2	2.529(1)
Pr(1)-O(21)#2	2.648(1)
Pr(1)-O(11)#1	2.725(1)
Pr(1)-Pr(1)#2	4.2173(2)
Pr(1)-Pr(1)#1	4.2451(2)
O(11)-C(11)	1.274(2)
O(12)-C(11)	1.256(2)
C(11)-C(12)	1.495(2)
O(21)-C(21)	1.280(2)
O(22)-C(21)	1.255(2)
C(21)-C(22)	1.495(2)
O(11)-Pr(1)-O(21)	165.41(4)
O(11)-Pr(1)-O(2W)	84.84(4)
O(21)-Pr(1)-O(2W)	89.08(4)
O(11)-Pr(1)-O(3W)	81.06(4)
O(21)-Pr(1)-O(3W)	84.37(4)
O(2W)-Pr(1)-O(3W)	68.12(4)
O(11)-Pr(1)-O(1W)	90.29(4)
O(21)-Pr(1)-O(1W)	85.70(4)
O(2W)-Pr(1)-O(1W)	139.36(4)
O(3W)-Pr(1)-O(1W)	71.26(4)
O(11)-Pr(1)-O(12)#1	117.49(4)
O(21)-Pr(1)-O(12)#1	73.44(4)
O(2W)-Pr(1)-O(12)#1	75.43(4)
O(3W)-Pr(1)-O(12)#1	137.36(4)
O(1W)-Pr(1)-O(12)#1	139.83(4)
O(11)-Pr(1)-O(22)#2	75.38(4)
O(21)-Pr(1)-O(22)#2	117.27(4)
O(2W)-Pr(1)-O(22)#2	138.23(4)
O(3W)-Pr(1)-O(22)#2	140.87(4)
O(1W)-Pr(1)-O(22)#2	78.01(4)
O(12)#1-Pr(1)-O(22)#2	81.66(4)
O(11)-Pr(1)-O(21)#2	124.16(4)
O(21)-Pr(1)-O(21)#2	67.51(4)
O(2W)-Pr(1)-O(21)#2	142.16(4)
O(3W)-Pr(1)-O(21)#2	133.71(4)
O(1W)-Pr(1)-O(21)#2	70.68(4)
O(12)#1-Pr(1)-O(21)#2	69.70(4)
O(22)#2-Pr(1)-O(21)#2	49.87(4)
O(11)-Pr(1)-O(11)#1	68.45(5)
O(21)-Pr(1)-O(11)#1	121.52(4)
O(2W)-Pr(1)-O(11)#1	69.33(4)
O(3W)-Pr(1)-O(11)#1	129.05(4)
O(1W)-Pr(1)-O(11)#1	144.32(4)
O(12)#1-Pr(1)-O(11)#1	49.06(4)
O(22)#2-Pr(1)-O(11)#1	69.24(4)
O(21)#2-Pr(1)-O(11)#1	97.21(4)
Pr(1)#2-Pr(1)-Pr(1)#1	139.267(5)

C(11)-O(11)-Pr(1)	157.9(1)
C(11)-O(11)-Pr(1)#1	90.6(1)
Pr(1)-O(11)-Pr(1)#1	111.6(1)
C(11)-O(12)-Pr(1)#1	101.0(1)
O(12)-C(11)-O(11)	119.4(2)
O(12)-C(11)-C(12)	120.3(2)
O(11)-C(11)-C(12)	120.3(2)
C(21)-O(21)-Pr(1)	154.0(1)
C(21)-O(21)-Pr(1)#2	92.0(1)
Pr(1)-O(21)-Pr(1)#2	112.5(1)
C(21)-O(22)-Pr(1)#2	98.2(1)
O(22)-C(21)-O(21)	119.1(2)
O(22)-C(21)-C(22)	121.1(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 Pr(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
Pr(1)	6(1)	10(1)	12(1)	1(1)	2(1)	-1(1)
Cl(1)	17(1)	13(1)	17(1)	2(1)	2(1)	-2(1)
O(11)	9(1)	16(1)	19(1)	2(1)	3(1)	-3(1)
O(12)	8(1)	17(1)	26(1)	7(1)	3(1)	-1(1)
C(11)	11(1)	14(1)	14(1)	0(1)	4(1)	0(1)
C(12)	20(1)	16(1)	27(1)	9(1)	1(1)	2(1)
O(21)	9(1)	16(1)	14(1)	0(1)	1(1)	-2(1)
O(22)	9(1)	21(1)	16(1)	-2(1)	1(1)	-3(1)
C(21)	10(1)	11(1)	15(1)	1(1)	0(1)	1(1)
C(22)	14(1)	31(1)	13(1)	-2(1)	1(1)	2(1)
O(1W)	11(1)	14(1)	18(1)	3(1)	5(1)	1(1)
O(2W)	11(1)	14(1)	21(1)	-4(1)	2(1)	0(1)
O(3W)	25(1)	14(1)	16(1)	2(1)	7(1)	5(1)

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

	x	y	z	U(eq)
H(12A)	-601	919	6475	28(5)
H(12B)	409	336	5802	28(5)
H(12C)	-1549	-184	5776	28(5)
H(12D)	412	753	6254	28(5)
H(12E)	-1590	451	6234	28(5)
H(12F)	-680	-183	5536	28(5)
H(22A)	7867	5921	7369	46(5)
H(22B)	5958	5208	7196	46(5)
H(22C)	6294	7202	7193	46(5)
H(11W)	3943	935	5810	50(6)
H(12W)	5126	1782	5322	50(6)
H(21W)	507	6782	6336	53(6)
H(22W)	2223	7683	6481	53(6)
H(31W)	2483	3970	7120	53(6)
H(32W)	3182	2320	6850	53(6)

Table S6. Hydrogen bonds for Pr(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)	165.6
O(1W)-H(12W)...O(12)#4	0.96	1.78	2.713(2)	161.9
O(2W)-H(21W)...O(22)#5	0.96	1.85	2.725(2)	150.1
O(2W)-H(22W)...Cl(1)	0.96	2.12	3.070(1)	169.2
O(3W)-H(31W)...Cl(1)#6	0.96	2.21	3.163(1)	171.7
O(3W)-H(32W)...Cl(1)#3	0.96	2.13	3.075(1)	166.6

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