

Table S1. Crystal data and structure refinement for Sm(OAc)2Cl\_x\_3H2O.

Identification code	Ha2019_99g_0m_a
Empirical formula	C4 H12 Cl O7 Sm
Formula weight	357.94
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.8503(3) Å b = 7.8844(3) Å    β = 98.483(2) deg. c = 17.5192(6) Å
Volume	1072.49(7) Å <sup>3</sup>
Z, Calculated density	4, 2.217 Mg/m <sup>3</sup>
Absorption coefficient	5.728 mm <sup>-1</sup>
F(000)	684
Crystal size	0.448 x 0.112 x 0.076 mm
Theta range for data collection	2.712 to 27.998 deg.
Limiting indices	-10 ≤ h ≤ 10, -10 ≤ k ≤ 10, -23 ≤ l ≤ 23
Reflections collected / unique	130814 / 2595 [R(int) = 0.0344]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	2595 / 0 / 126
Goodness-of-fit on F <sup>2</sup>	1.129
Final R indices [I > 2σ(I)]	R1 = 0.0101, wR2 = 0.0234
R indices (all data)	R1 = 0.0105, wR2 = 0.0236
Extinction coefficient	0.00104(9)
Largest diff. peak and hole	0.381 and -0.529 e.Å <sup>-3</sup>

Table S2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $\text{Sm}(\text{OAc})_2\text{Cl} \cdot 3\text{H}_2\text{O}$ .  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	U (eq)
Sm(1)	2639(1)	4612(1)	5375(1)	9(1)
Cl(1)	3835(1)	9718(1)	6908(1)	16(1)
O(11)	-90(1)	3372(1)	5356(1)	14(1)
O(12)	-2791(1)	2619(2)	5262(1)	16(1)
C(11)	-1228(2)	2305(2)	5491(1)	12(1)
C(12)	-718(2)	703(2)	5919(1)	21(1)
O(21)	5490(1)	5618(1)	5742(1)	13(1)
O(22)	8213(1)	6296(2)	5980(1)	15(1)
C(21)	6816(2)	6000(2)	6228(1)	12(1)
C(22)	6699(2)	6080(2)	7069(1)	19(1)
O(1W)	3915(1)	1766(1)	5380(1)	14(1)
O(2W)	1697(1)	6630(1)	6267(1)	15(1)
O(3W)	2992(2)	3509(2)	6689(1)	18(1)

Table S3. Bond lengths [Å] and angles [deg] for Sm(OAc)2Cl\_x\_3H2O.

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Sm(1)-O(11)	2.351(1)
Sm(1)-O(21)	2.373(1)
Sm(1)-O(2W)	2.421(1)
Sm(1)-O(3W)	2.438(1)
Sm(1)-O(1W)	2.457(1)
Sm(1)-O(12)#1	2.462(1)
Sm(1)-O(22)#2	2.475(1)
Sm(1)-O(21)#2	2.620(1)
Sm(1)-O(11)#1	2.723(1)
Sm(1)-Sm(1)#2	4.1563(2)
Sm(1)-Sm(1)#1	4.2026(2)
O(11)-C(11)	1.274(2)
O(12)-C(11)	1.258(2)
C(11)-C(12)	1.493(2)
O(21)-C(21)	1.279(2)
O(22)-C(21)	1.259(2)
C(21)-C(22)	1.492(2)
O(11)-Sm(1)-O(21)	164.62(4)
O(11)-Sm(1)-O(2W)	85.27(4)
O(21)-Sm(1)-O(2W)	88.33(4)
O(11)-Sm(1)-O(3W)	80.85(4)
O(21)-Sm(1)-O(3W)	83.79(4)
O(2W)-Sm(1)-O(3W)	68.16(4)
O(11)-Sm(1)-O(1W)	89.46(4)
O(21)-Sm(1)-O(1W)	86.36(4)
O(2W)-Sm(1)-O(1W)	139.56(4)
O(3W)-Sm(1)-O(1W)	71.42(4)
O(11)-Sm(1)-O(12)#1	117.86(4)
O(21)-Sm(1)-O(12)#1	73.72(4)
O(2W)-Sm(1)-O(12)#1	75.49(4)
O(3W)-Sm(1)-O(12)#1	137.52(4)
O(1W)-Sm(1)-O(12)#1	139.86(4)
O(11)-Sm(1)-O(22)#2	75.51(4)
O(21)-Sm(1)-O(22)#2	117.88(4)
O(2W)-Sm(1)-O(22)#2	138.07(4)
O(3W)-Sm(1)-O(22)#2	141.20(4)
O(1W)-Sm(1)-O(22)#2	77.98(4)
O(12)#1-Sm(1)-O(22)#2	81.16(4)
O(11)-Sm(1)-O(21)#2	124.82(4)
O(21)-Sm(1)-O(21)#2	67.39(4)
O(2W)-Sm(1)-O(21)#2	141.79(4)
O(3W)-Sm(1)-O(21)#2	133.03(4)
O(1W)-Sm(1)-O(21)#2	70.51(3)
O(12)#1-Sm(1)-O(21)#2	69.71(4)
O(22)#2-Sm(1)-O(21)#2	50.64(3)
O(11)-Sm(1)-O(11)#1	68.37(4)
O(21)-Sm(1)-O(11)#1	122.06(4)
O(2W)-Sm(1)-O(11)#1	69.31(4)
O(3W)-Sm(1)-O(11)#1	128.73(4)
O(1W)-Sm(1)-O(11)#1	143.68(4)
O(12)#1-Sm(1)-O(11)#1	49.51(3)
O(22)#2-Sm(1)-O(11)#1	69.01(4)
O(21)#2-Sm(1)-O(11)#1	98.22(3)
Sm(1)#2-Sm(1)-Sm(1)#1	139.819(4)

C (11)-O (11)-Sm (1)	159.1 (1)
C (11)-O (11)-Sm (1) #1	89.2 (1)
Sm (1)-O (11)-Sm (1) #1	111.6 (1)
C (11)-O (12)-Sm (1) #1	102.1 (1)
O (12)-C (11)-O (11)	119.2 (1)
O (12)-C (11)-C (12)	120.3 (1)
O (11)-C (11)-C (12)	120.5 (1)
C (21)-O (21)-Sm (1)	154.4 (1)
C (21)-O (21)-Sm (1) #2	91.3 (1)
Sm (1)-O (21)-Sm (1) #2	112.6 (1)
C (21)-O (22)-Sm (1) #2	98.7 (1)
O (22)-C (21)-O (21)	118.6 (1)
O (22)-C (21)-C (22)	121.1 (1)
O (21)-C (21)-C (22)	120.3 (1)

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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 ( $\text{\AA}^2 \times 10^3$ ) for Sm(OAc)<sub>2</sub>Cl<sub>2</sub>·3H<sub>2</sub>O.

The anisotropic displacement factor exponent takes the form:  
 $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>23</sub>	U <sub>13</sub>	U <sub>12</sub>
Sm(1)	6(1)	10(1)	11(1)	1(1)	2(1)	-1(1)
Cl(1)	17(1)	13(1)	17(1)	1(1)	2(1)	-2(1)
O(11)	10(1)	16(1)	18(1)	1(1)	4(1)	-3(1)
O(12)	9(1)	16(1)	23(1)	5(1)	4(1)	0(1)
C(11)	11(1)	13(1)	13(1)	-1(1)	3(1)	0(1)
C(12)	21(1)	17(1)	25(1)	7(1)	1(1)	2(1)
O(21)	9(1)	16(1)	13(1)	0(1)	1(1)	-1(1)
O(22)	9(1)	20(1)	15(1)	-1(1)	2(1)	-2(1)
C(21)	11(1)	10(1)	14(1)	1(1)	0(1)	2(1)
C(22)	15(1)	29(1)	12(1)	-1(1)	1(1)	3(1)
O(1W)	12(1)	13(1)	17(1)	2(1)	5(1)	0(1)
O(2W)	11(1)	14(1)	19(1)	-4(1)	2(1)	0(1)
O(3W)	25(1)	14(1)	15(1)	2(1)	7(1)	5(1)

Table S5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $\text{Sm}(\text{OAc})_2\text{Cl}\cdot 3\text{H}_2\text{O}$ .

	x	y	z	U (eq)
H(12A)	-1534	-198	5733	32 (5)
H(12B)	-726	882	6472	32 (5)
H(12C)	442	373	5832	32 (5)
H(12D)	326	880	6292	32 (5)
H(12E)	-1646	293	6189	32 (5)
H(12F)	-533	-108	5515	32 (5)
H(22A)	7846	5913	7366	48 (4)
H(22B)	5924	5187	7201	48 (4)
H(22C)	6251	7190	7193	48 (4)
H(11W)	3869	970	5791	45 (5)
H(12W)	5109	1818	5318	45 (5)
H(21W)	507	6758	6326	49 (5)
H(22W)	2242	7656	6472	49 (5)
H(31W)	2459	4013	7093	54 (6)
H(32W)	3190	2348	6842	54 (6)

Table S6. Hydrogen bonds for Sm(OAc)<sub>2</sub>Cl<sub>x</sub>·3H<sub>2</sub>O [Å 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)	165.7
O(1W)-H(12W)...O(12)#4	0.96	1.78	2.709(2)	161.4
O(2W)-H(21W)...O(22)#5	0.96	1.85	2.720(2)	149.3
O(2W)-H(22W)...Cl(1)	0.96	2.12	3.074(1)	170.5
O(3W)-H(31W)...Cl(1)#6	0.96	2.22	3.171(1)	170.1
O(3W)-H(32W)...Cl(1)#3	0.96	2.13	3.073(1)	165.7

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