

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

Identification code	Ha2019_77_0m_a
Empirical formula	C4 H12 Cl Dy O7
Formula weight	370.09
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.8106(4) Å b = 7.8433(4) Å β = 97.978(3) deg. c = 17.3400(8) Å
Volume	1051.98(9) Å ³
Z, Calculated density	4, 2.337 Mg/m ³
Absorption coefficient	7.361 mm ⁻¹
F(000)	700
Crystal size	0.448 x 0.112 x 0.076 mm
Theta range for data collection	2.734 to 27.996 deg.
Limiting indices	-10 ≤ h ≤ 10, -10 ≤ k ≤ 10, -22 ≤ l ≤ 22
Reflections collected / unique	49237 / 2547 [R(int) = 0.0328]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.783 and 0.625
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2547 / 0 / 126
Goodness-of-fit on F ²	1.187
Final R indices [I > 2σ(I)]	R1 = 0.0127, wR2 = 0.0265
R indices (all data)	R1 = 0.0131, wR2 = 0.0267
Extinction coefficient	0.00450(11)
Largest diff. peak and hole	0.489 and -0.652 e.Å ⁻³

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

	x	y	z	U (eq)
Dy (1)	2689 (1)	4549 (1)	5391 (1)	9 (1)
Cl (1)	3800 (1)	9642 (1)	6875 (1)	15 (1)
O (11)	56 (2)	3309 (2)	5388 (1)	18 (1)
O (12)	-2709 (2)	2760 (2)	5262 (1)	15 (1)
C (11)	-1172 (3)	2331 (3)	5504 (1)	11 (1)
C (12)	-829 (3)	670 (3)	5915 (1)	22 (1)
O (21)	5445 (2)	5622 (2)	5740 (1)	11 (1)
O (22)	8178 (2)	6288 (2)	5947 (1)	13 (1)
C (21)	6794 (3)	5989 (3)	6217 (1)	11 (1)
C (22)	6723 (3)	6048 (3)	7073 (1)	17 (1)
O (1W)	4006 (2)	1804 (2)	5374 (1)	14 (1)
O (2W)	1663 (2)	6516 (2)	6251 (1)	14 (1)
O (3W)	3086 (2)	3485 (2)	6696 (1)	17 (1)

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

Dy(1)-O(11)	2.274(1)
Dy(1)-O(21)	2.312(1)
Dy(1)-O(2W)	2.361(2)
Dy(1)-O(1W)	2.388(1)
Dy(1)-O(3W)	2.392(2)
Dy(1)-O(12)#1	2.396(2)
Dy(1)-O(22)#2	2.416(1)
Dy(1)-O(21)#2	2.604(1)
Dy(1)-O(11)#1	2.905(2)
Dy(1)-Dy(1)#2	4.0899(3)
Dy(1)-Dy(1)#1	4.2898(3)
O(11)-C(11)	1.265(2)
O(12)-C(11)	1.261(2)
C(11)-C(12)	1.492(3)
O(21)-C(21)	1.279(2)
O(22)-C(21)	1.258(2)
C(21)-C(22)	1.494(3)
O(11)-Dy(1)-O(21)	164.76(5)
O(11)-Dy(1)-O(2W)	83.96(5)
O(21)-Dy(1)-O(2W)	88.99(5)
O(11)-Dy(1)-O(1W)	90.29(5)
O(21)-Dy(1)-O(1W)	86.80(5)
O(2W)-Dy(1)-O(1W)	141.35(5)
O(11)-Dy(1)-O(3W)	81.44(6)
O(21)-Dy(1)-O(3W)	83.43(5)
O(2W)-Dy(1)-O(3W)	68.96(5)
O(1W)-Dy(1)-O(3W)	72.39(5)
O(11)-Dy(1)-O(12)#1	116.16(5)
O(21)-Dy(1)-O(12)#1	74.72(5)
O(2W)-Dy(1)-O(12)#1	75.43(5)
O(1W)-Dy(1)-O(12)#1	139.22(5)
O(3W)-Dy(1)-O(12)#1	138.26(5)
O(11)-Dy(1)-O(22)#2	75.45(5)
O(21)-Dy(1)-O(22)#2	118.49(5)
O(2W)-Dy(1)-O(22)#2	135.20(5)
O(1W)-Dy(1)-O(22)#2	78.87(5)
O(3W)-Dy(1)-O(22)#2	142.76(5)
O(12)#1-Dy(1)-O(22)#2	78.74(5)
O(11)-Dy(1)-O(21)#2	125.22(5)
O(21)-Dy(1)-O(21)#2	67.53(5)
O(2W)-Dy(1)-O(21)#2	141.59(5)
O(1W)-Dy(1)-O(21)#2	69.97(5)
O(3W)-Dy(1)-O(21)#2	133.01(5)
O(12)#1-Dy(1)-O(21)#2	69.41(5)
O(22)#2-Dy(1)-O(21)#2	51.27(4)
O(11)-Dy(1)-O(11)#1	68.75(6)
O(21)-Dy(1)-O(11)#1	120.77(5)
O(2W)-Dy(1)-O(11)#1	67.83(5)
O(1W)-Dy(1)-O(11)#1	143.81(5)
O(3W)-Dy(1)-O(11)#1	129.20(5)
O(12)#1-Dy(1)-O(11)#1	47.45(4)
O(22)#2-Dy(1)-O(11)#1	67.69(5)
O(21)#2-Dy(1)-O(11)#1	97.68(4)
Dy(1)#2-Dy(1)-Dy(1)#1	137.511(5)

C (11)-O (11)-Dy (1)	164.6 (2)
C (11)-O (11)-Dy (1) #1	84.1 (1)
Dy (1)-O (11)-Dy (1) #1	111.3 (1)
C (11)-O (12)-Dy (1) #1	108.9 (1)
O (12)-C (11)-O (11)	119.6 (2)
O (12)-C (11)-C (12)	119.4 (2)
O (11)-C (11)-C (12)	121.0 (2)
C (21)-O (21)-Dy (1)	154.8 (1)
C (21)-O (21)-Dy (1) #2	90.1 (1)
Dy (1)-O (21)-Dy (1) #2	112.5 (1)
C (21)-O (22)-Dy (1) #2	99.5 (1)
O (22)-C (21)-O (21)	118.3 (2)
O (22)-C (21)-C (22)	121.1 (2)
O (21)-C (21)-C (22)	120.6 (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 ($\text{\AA}^2 \times 10^3$) for Dy(OAc)₂Cl₂·3H₂O.

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 ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Dy(1)	7(1)	10(1)	10(1)	0(1)	2(1)	-2(1)
Cl(1)	18(1)	12(1)	16(1)	1(1)	2(1)	-1(1)
O(11)	13(1)	22(1)	20(1)	-5(1)	7(1)	-8(1)
O(12)	9(1)	17(1)	18(1)	3(1)	2(1)	1(1)
C(11)	11(1)	12(1)	12(1)	-2(1)	4(1)	0(1)
C(12)	26(1)	17(1)	23(1)	6(1)	1(1)	5(1)
O(21)	8(1)	13(1)	12(1)	-1(1)	0(1)	-2(1)
O(22)	9(1)	17(1)	15(1)	-1(1)	2(1)	-1(1)
C(21)	11(1)	8(1)	14(1)	0(1)	0(1)	1(1)
C(22)	14(1)	27(1)	10(1)	-2(1)	1(1)	2(1)
O(1W)	12(1)	13(1)	17(1)	2(1)	5(1)	0(1)
O(2W)	11(1)	14(1)	17(1)	-3(1)	1(1)	-1(1)
O(3W)	24(1)	13(1)	16(1)	2(1)	8(1)	4(1)

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

	x	y	z	U (eq)
H(12A)	-1030	-266	5539	81 (8)
H(12B)	-1606	545	6310	81 (8)
H(12C)	373	637	6168	81 (8)
H(22A)	7896	5951	7356	48 (6)
H(22B)	6016	5100	7219	48 (6)
H(22C)	6211	7131	7206	48 (6)
H(11W)	3938	955	5768	50 (7)
H(12W)	5216	1905	5336	50 (7)
H(21W)	452	6720	6253	50 (7)
H(22W)	2221	7559	6433	50 (7)
H(31W)	2562	4024	7102	52 (7)
H(32W)	3238	2316	6855	52 (7)

Table S6. Hydrogen bonds for Dy(OAc)₂Cl_x·3H₂O [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	2.19	3.128(2)	164.0
O(1W)-H(12W)...O(12)#4	0.96	1.77	2.706(2)	162.5
O(2W)-H(21W)...O(22)#5	0.96	1.81	2.706(2)	153.3
O(2W)-H(22W)...Cl(1)	0.96	2.12	3.077(2)	171.3
O(3W)-H(31W)...Cl(1)#6	0.96	2.24	3.186(2)	166.3
O(3W)-H(32W)...Cl(1)#3	0.96	2.14	3.073(2)	163.1

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