Table S1. Crystal data and structure refinement for Dy(OAc)2Br_x_3H2O.

Identification code	Ha2019_78_0m_a
Empirical formula	C4 H12 Br Dy O7
Formula weight	414.55
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.8038(3) A b = 8.0288(3) A ß = 96.034(2) deg. c = 17.6550(7) A
Volume	1100.05(7) A^3
Z, Calculated density	4, 2.503 Mg/m^3
Absorption coefficient	10.429 mm^-1
F(000)	772
Crystal size	0.484 x 0.123 x 0.077 mm
Theta range for data collection	2.790 to 27.995 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -23<=l<=23
Reflections collected / unique	101683 / 2666 [R(int) = 0.0444]
Completeness to theta = 25.242	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.734 and 0.267
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2666 / 0 / 126
Goodness-of-fit on F^2	1.118
Final R indices [I>2sigma(I)]	R1 = 0.0129, wR2 = 0.0321
R indices (all data)	R1 = 0.0140, wR2 = 0.0325
Extinction coefficient	0.00126(9)
Largest diff. peak and hole	0.779 and -0.601 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Dy(OAc)2Br_x_3H2O. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Dy(1)	2659(1)	4535(1)	5373(1)	10(1)
Br(1)	3891(1)	9551(1)	6837(1)	17(1)
O(11)	34(2)	3315(2)	5364(1)	19(1)
O(12)	-2722(2)	2796(2)	5229(1)	16(1)
C(11)	-1207(2)	2373(3)	5470(1)	13(1)
C(12)	-914(3)	749(3)	5881(1)	24(1)
O(21)	5388(2)	5548(2)	5734(1)	13(1)
O(22)	8104(2)	6194(2)	5945(1)	15(1)
C(21)	6709(3)	5861(2)	6208(1)	13(1)
C(22)	6598(3)	5792(3)	7044(1)	21(1)
O(1W)	3978(2)	1860(2)	5318(1)	15(1)
O(2W)	1557(2)	6397(2)	6240(1)	15(1)
O(3W)	2968(2)	3430(2)	6634(1)	20(1)

Table S3. Bond lengths [A] and angles [deg] for Dy(OAc)2Br_x_3H2O.

Dy(1)-O(11)	2.269(1)
Dy(1)-O(21)	2.307(1)
Dy(1)-O(2W)	2.365(1)
Dy(1)-O(3W)	2.386(2)
Dy(1)-O(1W)	2.389(1)
Dy(1)-O(12)#1	2.395(2)
Dy(1)-O(22)#2	2.412(2)
Dy(1)-O(21)#2	2.603(1)
Dy(1)-O(11)#1	2.917(2)
Dy(1)-Dy(1)#2	4.0809(2)
Dy(1)-Dy(1)#1	4.2848(2)
O(11)-C(11)	1.258(2)
O(12)-C(11)	1.260(2)
C(11)-C(12)	1.497(3)
O(21)-C(21)	1.281(2)
O(22)-C(21)	1.256(2)
C(21)-C(22)	1.490(3)
O(11)-Dy(1)-O(21)	163.91(5)
O(11)-Dy(1)-O(2W)	83.57(5)
O(21)-Dy(1)-O(2W)	89.20(5)
O(11)-Dy(1)-O(3W)	81.29(6)
O(21)-Dy(1)-O(3W)	82.70(5)
O(2W)-Dy(1)-O(3W)	68.82(5)
O(11)-Dy(1)-O(1W)	90.24(5)
O(21)-Dy(1)-O(1W)	86.49(5)
O(2W)-Dy(1)-O(1W)	141.45(5)
O(3W)-Dy(1)-O(1W)	72.64(5)
O(11)-Dy(1)-O(12)#1	116.35(5)
O(21)-Dy(1)-O(12)#1	75.28(5)
O(2W)-Dy(1)-O(12)#1	75.39(5)
O(3W)-Dy(1)-O(12)#1	137.93(5)
O(1W)-Dy(1)-O(12)#1	139.26(5)
O(11)-Dy(1)-O(22)#2	75.97(5)
O(21)-Dy(1)-O(22)#2	118.66(5)
O(2W)-Dy(1)-O(22)#2	135.09(5)
O(3W)-Dy(1)-O(22)#2	143.18(5)
O(1W)-Dy(1)-O(22)#2	78.83(5)
O(12)#1-Dy(1)-O(22)#2	78.67(5)
O(11)-Dy(1)-O(21)#2	125.67(5)
O(21)-Dy(1)-O(21)#2	67.68(6)
O(2W)-Dy(1)-O(21)#2	141.61(5)
O(3W)-Dy(1)-O(21)#2	132.98(5)
O(1W)-Dy(1)-O(21)#2	69.98(5)
O(12)#1-Dy(1)-O(21)#2	69.43(5)
O(22)#2-Dy(1)-O(21)#2	51.24(4)
O(11)-Dy(1)-O(11)#1	69.20(6)
O(21)-Dy(1)-O(11)#1	121.05(5)
O(2W)-Dy(1)-O(11)#1	67.73(5)
O(3W)-Dy(1)-O(11)#1	129.31(5)
O(1W)-Dy(1)-O(11)#1	143.84(5)
O(12)#1-Dy(1)-O(11)#1	47.18(4)
O(22)#2-Dy(1)-O(11)#1	67.70(5)
O(21)#2-Dy(1)-O(11)#1	97.56(4)
Dy(1)#2-Dy(1)-Dy(1)#1	137.751(5)

C(11)-O(11)-Dy(1)	165.2(2)
C(11)-O(12)-Dy(1)#1	109.2(1)
O(11)-C(11)-O(12)	119.8(2)
O(11)-C(11)-C(12)	121.0(2)
O(12)-C(11)-C(12)	119.2(2)
C(21)-O(21)-Dy(1)	154.9(1)
C(21)-O(21)-Dy(1)#2	90.0(1)
Dy(1)-O(21)-Dy(1)#2	112.3(1)
C(21)-O(22)-Dy(1)#2	99.7(1)
O(22)-C(21)-O(21)	118.0(2)
O(22)-C(21)-C(22)	121.1(2)
O(21)-C(21)-C(22)	120.9(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 Dy(OAc)2Br_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
Dy(1)	8(1)	13(1)	11(1)	0(1)	2(1)	-2(1)
Br(1)	21(1)	14(1)	16(1)	1(1)	1(1)	-2(1)
O(11)	14(1)	25(1)	21(1)	-5(1)	6(1)	-7(1)
O(12)	10(1)	20(1)	18(1)	3(1)	2(1)	1(1)
C(11)	12(1)	15(1)	11(1)	-1(1)	2(1)	-1(1)
C(12)	26(1)	21(1)	24(1)	8(1)	1(1)	5(1)
O(21)	10(1)	16(1)	13(1)	-1(1)	0(1)	-1(1)
O(22)	9(1)	21(1)	16(1)	-2(1)	1(1)	-2(1)
C(21)	13(1)	11(1)	14(1)	-1(1)	0(1)	2(1)
C(22)	16(1)	33(1)	12(1)	0(1)	-1(1)	3(1)
O(1W)	13(1)	16(1)	17(1)	2(1)	5(1)	0(1)
O(2W)	11(1)	16(1)	18(1)	-2(1)	1(1)	0(1)
O(3W)	27(1)	17(1)	15(1)	2(1)	8(1)	4(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Dy(OAc)2Br_x_3H2O.

	x	y	z	U(eq)
H(12A)	-1424	795	6364	92(9)
H(12B)	327	541	5981	92(9)
H(12C)	-1452	-152	5565	92(9)
H(22A)	7762	5731	7312	94(10)
H(22B)	5941	4805	7166	94(10)
H(22C)	6019	6796	7205	94(10)
H(11W)	3911	1035	5707	45(6)
H(12W)	5174	1900	5236	45(6)
H(21W)	351	6552	6283	46(7)
H(22W)	2090	7424	6415	46(7)
H(31W)	2459	3937	7049	54(7)
H(32W)	3243	2315	6801	54(7)

Table S6. Hydrogen bonds for Dy(OAc)2Br_x_3H2O [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(11W)...Br(1)#3	0.96	2.33	3.267(2)	166.8
O(1W)-H(12W)...O(12)#4	0.96	1.79	2.703(2)	156.9
O(2W)-H(21W)...O(22)#5	0.96	1.81	2.695(2)	151.0
O(2W)-H(22W)...Br(1)	0.96	2.29	3.231(1)	167.8
O(3W)-H(31W)...Br(1)#6	0.96	2.38	3.320(2)	166.9
O(3W)-H(32W)...Br(1)#3	0.96	2.28	3.209(2)	163.8

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