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

Identification code	Ha2019_64_0m_a
Empirical formula	C4 H12 Br O7 Pr
Formula weight	392.96
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.9293(3) A b = 8.0327(3) A ß = 96.533(2) deg. c = 18.0186(6) A
Volume	1140.22(7) A^3
Z, Calculated density	4, 2.289 Mg/m^3
Absorption coefficient	7.781 mm^-1
F(000)	744
Crystal size	0.465 x 0.120 x 0.074 mm
Theta range for data collection	2.275 to 27.994 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -23<=l<=23
Reflections collected / unique	92529 / 2753 [R(int) = 0.0497]
Completeness to theta = 25.242	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.813 and 0.412
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2753 / 0 / 125
Goodness-of-fit on F^2	1.080
Final R indices [I>2sigma(I)]	R1 = 0.0141, wR2 = 0.0295
R indices (all data)	R1 = 0.0175, wR2 = 0.0305
Extinction coefficient	n/a
Largest diff. peak and hole	0.441 and -0.499 e.A^-3

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

	x	y	z	U(eq)
Pr(1)	2601(1)	4596(1)	5364(1)	11(1)
Br(1)	3952(1)	9603(1)	6879(1)	18(1)
O(11)	-163(2)	3358(2)	5330(1)	16(1)
O(12)	-2817(2)	2578(2)	5220(1)	18(1)
C(11)	-1293(2)	2299(3)	5456(1)	14(1)
C(12)	-811(3)	750(3)	5884(1)	24(1)
O(21)	5462(2)	5543(2)	5740(1)	14(1)
O(22)	8132(2)	6231(2)	5987(1)	18(1)
C(21)	6742(2)	5871(3)	6219(1)	14(1)
C(22)	6580(3)	5780(3)	7036(1)	23(1)
O(1W)	3901(2)	1761(2)	5333(1)	15(1)
O(2W)	1555(2)	6539(2)	6272(1)	17(1)
O(3W)	2844(2)	3417(2)	6642(1)	20(1)

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

Pr(1)-O(11)	2.401(1)
Pr(1)-O(21)	2.416(1)
Pr(1)-O(2W)	2.471(1)
Pr(1)-O(3W)	2.476(1)
Pr(1)-O(1W)	2.504(1)
Pr(1)-O(12)#1	2.516(2)
Pr(1)-O(22)#2	2.527(1)
Pr(1)-O(21)#2	2.652(1)
Pr(1)-O(11)#1	2.730(1)
Pr(1)-Pr(1)#2	4.2146(2)
Pr(1)-Pr(1)#1	4.2332(2)
O(11)-C(11)	1.274(2)
O(12)-C(11)	1.255(2)
C(11)-C(12)	1.492(3)
O(21)-C(21)	1.282(2)
O(22)-C(21)	1.256(2)
C(21)-C(22)	1.495(3)
O(11)-Pr(1)-O(21)	164.37(5)
O(11)-Pr(1)-O(2W)	84.53(5)
O(21)-Pr(1)-O(2W)	89.47(5)
O(11)-Pr(1)-O(3W)	80.78(5)
O(21)-Pr(1)-O(3W)	83.59(5)
O(2W)-Pr(1)-O(3W)	67.87(5)
O(11)-Pr(1)-O(1W)	89.98(5)
O(21)-Pr(1)-O(1W)	85.21(5)
O(2W)-Pr(1)-O(1W)	139.43(5)
O(3W)-Pr(1)-O(1W)	71.57(5)
O(11)-Pr(1)-O(12)#1	117.94(5)
O(21)-Pr(1)-O(12)#1	74.14(5)
O(2W)-Pr(1)-O(12)#1	75.57(5)
O(3W)-Pr(1)-O(12)#1	137.07(5)
O(1W)-Pr(1)-O(12)#1	139.78(4)
O(11)-Pr(1)-O(22)#2	75.96(5)
O(21)-Pr(1)-O(22)#2	117.29(4)
O(2W)-Pr(1)-O(22)#2	138.26(5)
O(3W)-Pr(1)-O(22)#2	141.26(5)
O(1W)-Pr(1)-O(22)#2	77.83(5)
O(12)#1-Pr(1)-O(22)#2	81.58(5)
O(11)-Pr(1)-O(21)#2	124.63(4)
O(21)-Pr(1)-O(21)#2	67.54(5)
O(2W)-Pr(1)-O(21)#2	142.20(5)
O(3W)-Pr(1)-O(21)#2	133.71(5)
O(1W)-Pr(1)-O(21)#2	70.70(4)
O(12)#1-Pr(1)-O(21)#2	69.59(5)
O(22)#2-Pr(1)-O(21)#2	49.82(4)
O(11)-Pr(1)-O(11)#1	68.96(5)
O(21)-Pr(1)-O(11)#1	122.19(5)
O(2W)-Pr(1)-O(11)#1	69.50(4)
O(3W)-Pr(1)-O(11)#1	129.26(4)
O(1W)-Pr(1)-O(11)#1	144.03(4)
O(12)#1-Pr(1)-O(11)#1	48.98(4)
O(22)#2-Pr(1)-O(11)#1	69.11(5)
O(21)#2-Pr(1)-O(11)#1	96.99(4)
Pr(1)#2-Pr(1)-Pr(1)#1	139.645(6)

C(11)-O(11)-Pr(1)	158.5(1)
C(11)-O(11)-Pr(1)#1	90.4(1)
Pr(1)-O(11)-Pr(1)#1	111.0(1)
C(11)-O(12)-Pr(1)#1	101.2(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)	120.4(2)
C(21)-O(21)-Pr(1)	154.1(1)
C(21)-O(21)-Pr(1)#2	91.8(1)
Pr(1)-O(21)-Pr(1)#2	112.5(1)
C(21)-O(22)-Pr(1)#2	98.4(1)
O(22)-C(21)-O(21)	118.8(2)
O(22)-C(21)-C(22)	121.1(2)
O(21)-C(21)-C(22)	120.2(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)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
Pr(1)	7(1)	13(1)	13(1)	1(1)	2(1)	-1(1)
Br(1)	21(1)	16(1)	18(1)	2(1)	1(1)	-3(1)
O(11)	11(1)	18(1)	19(1)	3(1)	2(1)	-3(1)
O(12)	10(1)	19(1)	26(1)	6(1)	3(1)	-1(1)
C(11)	12(1)	16(1)	14(1)	-1(1)	4(1)	-1(1)
C(12)	23(1)	21(1)	28(1)	10(1)	1(1)	1(1)
O(21)	10(1)	19(1)	14(1)	0(1)	0(1)	-1(1)
O(22)	10(1)	26(1)	18(1)	-2(1)	1(1)	-2(1)
C(21)	11(1)	15(1)	16(1)	-1(1)	0(1)	2(1)
C(22)	18(1)	36(1)	14(1)	1(1)	1(1)	4(1)
O(1W)	13(1)	16(1)	18(1)	3(1)	5(1)	0(1)
O(2W)	13(1)	16(1)	22(1)	-4(1)	2(1)	0(1)
O(3W)	28(1)	18(1)	16(1)	3(1)	7(1)	6(1)

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

	x	y	z	U(eq)
H(12A)	-848	955	6418	80(7)
H(12B)	340	418	5799	80(7)
H(12C)	-1609	-142	5718	80(7)
H(22A)	7699	5572	7312	36(6)
H(22B)	5807	4872	7131	36(6)
H(22C)	6130	6836	7202	36(6)
H(22D)	5362	5855	7081	36(6)
H(22E)	7154	6777	7253	36(6)
H(22F)	7051	4790	7302	36(6)
H(11W)	3925	959	5730	54(7)
H(12W)	5058	1854	5230	54(7)
H(21W)	368	6689	6313	56(7)
H(22W)	2079	7564	6449	56(7)
H(31W)	2343	3905	7051	50(6)
H(32W)	3135	2302	6801	50(6)

Table S6. Hydrogen bonds for Pr(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	2.34	3.276(1)	165.7
O(1W)-H(12W)...O(12)#4	0.96	1.78	2.714(2)	162.2
O(2W)-H(21W)...O(22)#5	0.96	1.84	2.716(2)	150.2
O(2W)-H(22W)...Br(1)	0.96	2.29	3.223(1)	165.2
O(3W)-H(31W)...Br(1)#6	0.96	2.35	3.303(1)	169.6
O(3W)-H(32W)...Br(1)#3	0.96	2.26	3.202(2)	165.8

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