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

Identification code	HR2021_51_0m_a
Empirical formula	C4 H12 Br Ce O7
Formula weight	392.17
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.9597(3) A b = 8.0442(3) A ß = 96.732(2) deg. c = 18.0642(8) A
Volume	1148.67(8) A^3
Z, Calculated density	4, 2.268 Mg/m^3
Absorption coefficient	7.446 mm^-1
F(000)	740
Crystal size	0.465 x 0.120 x 0.074 mm
Theta range for data collection	2.691 to 27.995 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -23<=l<=23
Reflections collected / unique	113305 / 2770 [R(int) = 0.0572]
Completeness to theta = 25.242	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.748 and 0.505
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2770 / 0 / 125
Goodness-of-fit on F^2	1.071
Final R indices [I>2sigma(I)]	R1 = 0.0142, wR2 = 0.0310
R indices (all data)	R1 = 0.0173, wR2 = 0.0320
Extinction coefficient	n/a
Largest diff. peak and hole	0.603 and -0.312 e.A^-3

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

	x	y	z	U(eq)
Ce(1)	2604(1)	4591(1)	5369(1)	11(1)
Br(1)	3952(1)	9590(1)	6884(1)	19(1)
O(11)	-168(2)	3346(2)	5332(1)	17(1)
O(12)	-2815(2)	2563(2)	5218(1)	19(1)
C(11)	-1289(2)	2286(2)	5456(1)	15(1)
C(12)	-813(3)	744(3)	5888(1)	26(1)
O(21)	5477(2)	5544(2)	5744(1)	15(1)
O(22)	8132(2)	6245(2)	5986(1)	18(1)
C(21)	6756(2)	5875(2)	6218(1)	14(1)
C(22)	6608(3)	5784(3)	7031(1)	23(1)
O(1W)	3925(2)	1740(2)	5347(1)	17(1)
O(2W)	1544(2)	6544(2)	6277(1)	18(1)
O(3W)	2850(2)	3408(2)	6651(1)	22(1)

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

Ce(1)-O(11)	2.417(1)
Ce(1)-O(21)	2.431(1)
Ce(1)-O(2W)	2.489(1)
Ce(1)-O(3W)	2.490(2)
Ce(1)-O(1W)	2.526(1)
Ce(1)-O(12)#1	2.536(1)
Ce(1)-O(22)#2	2.539(1)
Ce(1)-O(21)#2	2.666(1)
Ce(1)-O(11)#1	2.746(1)
Ce(1)-Ce(1)#2	4.2361(3)
Ce(1)-Ce(1)#1	4.2549(3)
O(11)-C(11)	1.273(2)
O(12)-C(11)	1.260(2)
C(11)-C(12)	1.491(3)
O(21)-C(21)	1.280(2)
O(22)-C(21)	1.254(2)
C(21)-C(22)	1.488(3)
O(11)-Ce(1)-O(21)	164.58(5)
O(11)-Ce(1)-O(2W)	84.29(5)
O(21)-Ce(1)-O(2W)	89.88(5)
O(11)-Ce(1)-O(3W)	80.74(5)
O(21)-Ce(1)-O(3W)	83.84(5)
O(2W)-Ce(1)-O(3W)	67.90(5)
O(11)-Ce(1)-O(1W)	90.21(5)
O(21)-Ce(1)-O(1W)	84.91(5)
O(2W)-Ce(1)-O(1W)	139.24(5)
O(3W)-Ce(1)-O(1W)	71.36(5)
O(11)-Ce(1)-O(12)#1	117.86(5)
O(21)-Ce(1)-O(12)#1	74.09(5)
O(2W)-Ce(1)-O(12)#1	75.53(5)
O(3W)-Ce(1)-O(12)#1	137.03(5)
O(1W)-Ce(1)-O(12)#1	139.92(4)
O(11)-Ce(1)-O(22)#2	75.93(5)
O(21)-Ce(1)-O(22)#2	117.09(4)
O(2W)-Ce(1)-O(22)#2	138.13(5)
O(3W)-Ce(1)-O(22)#2	141.17(5)
O(1W)-Ce(1)-O(22)#2	78.07(5)
O(12)#1-Ce(1)-O(22)#2	81.70(5)
O(11)-Ce(1)-O(21)#2	124.35(4)
O(21)-Ce(1)-O(21)#2	67.65(5)
O(2W)-Ce(1)-O(21)#2	142.33(5)
O(3W)-Ce(1)-O(21)#2	134.13(5)
O(1W)-Ce(1)-O(21)#2	71.00(4)
O(12)#1-Ce(1)-O(21)#2	69.53(5)
O(22)#2-Ce(1)-O(21)#2	49.48(4)
O(11)-Ce(1)-O(11)#1	69.18(5)
O(21)-Ce(1)-O(11)#1	121.88(4)
O(2W)-Ce(1)-O(11)#1	69.35(4)
O(3W)-Ce(1)-O(11)#1	129.35(4)
O(1W)-Ce(1)-O(11)#1	144.49(4)
O(12)#1-Ce(1)-O(11)#1	48.68(4)
O(22)#2-Ce(1)-O(11)#1	69.19(4)
O(21)#2-Ce(1)-O(11)#1	96.48(4)
Ce(1)#2-Ce(1)-Ce(1)#1	139.248(6)

C(11)-O(11)-Ce(1)	158.3(1)
C(11)-O(11)-Ce(1)#1	90.8(1)
Ce(1)-O(11)-Ce(1)#1	110.8(1)
C(11)-O(12)-Ce(1)#1	101.2(1)
O(12)-C(11)-O(11)	119.3(2)
O(12)-C(11)-C(12)	120.1(2)
O(11)-C(11)-C(12)	120.6(2)
C(21)-O(21)-Ce(1)	154.2(1)
C(21)-O(21)-Ce(1)#2	91.9(1)
Ce(1)-O(21)-Ce(1)#2	112.4(1)
C(21)-O(22)-Ce(1)#2	98.5(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)	120.1(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 Ce(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
Ce(1)	7(1)	13(1)	14(1)	1(1)	2(1)	-1(1)
Br(1)	21(1)	16(1)	19(1)	2(1)	1(1)	-3(1)
O(11)	11(1)	17(1)	22(1)	3(1)	2(1)	-4(1)
O(12)	9(1)	19(1)	29(1)	6(1)	3(1)	-2(1)
C(11)	12(1)	15(1)	17(1)	1(1)	3(1)	-1(1)
C(12)	23(1)	21(1)	33(1)	11(1)	-1(1)	-1(1)
O(21)	11(1)	20(1)	14(1)	0(1)	0(1)	-2(1)
O(22)	10(1)	26(1)	19(1)	-2(1)	1(1)	-3(1)
C(21)	12(1)	14(1)	16(1)	-2(1)	0(1)	2(1)
C(22)	17(1)	37(1)	16(1)	0(1)	0(1)	3(1)
O(1W)	13(1)	16(1)	21(1)	3(1)	5(1)	-1(1)
O(2W)	13(1)	17(1)	23(1)	-4(1)	1(1)	0(1)
O(3W)	29(1)	19(1)	18(1)	3(1)	7(1)	6(1)

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

	x	y	z	U(eq)
H(12A)	-780	976	6422	82(7)
H(12B)	304	369	5781	82(7)
H(12C)	-1651	-126	5746	82(7)
H(22A)	7726	5580	7305	37(6)
H(22B)	5842	4875	7126	37(6)
H(22C)	6157	6836	7197	37(6)
H(22D)	5395	5859	7076	37(6)
H(22E)	7182	6777	7249	37(6)
H(22F)	7078	4792	7294	37(6)
H(11W)	3920	958	5748	51(6)
H(12W)	5091	1829	5263	51(6)
H(21W)	362	6689	6320	59(7)
H(22W)	2067	7563	6459	59(7)
H(31W)	2304	3869	7051	61(7)
H(32W)	3168	2302	6810	61(7)

Table S6. Hydrogen bonds for Ce(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	3.269(1)	167.3
O(1W)-H(12W)...O(12)#4	0.96	1.78	2.714(2)	163.7
O(2W)-H(21W)...O(22)#5	0.96	1.84	2.716(2)	150.0
O(2W)-H(22W)...Br(1)	0.96	2.29	3.222(1)	164.8
O(3W)-H(31W)...Br(1)#6	0.96	2.34	3.295(2)	171.1
O(3W)-H(32W)...Br(1)#3	0.96	2.27	3.209(2)	165.9

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