

Table S1. Crystal data and structure refinement for Eu(OAc)2Br·x·3H2O.

Identification code	Ha2019_96_0m_a
Empirical formula	C4 H12 Br Eu O7
Formula weight	404.01
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.8318(3) Å b = 8.0121(3) Å β = 95.972(2) deg. c = 17.8214(7) Å
Volume	1112.21(7) Å ³
Z, Calculated density	4, 2.413 Mg/m ³
Absorption coefficient	9.236 mm ⁻¹
F(000)	760
Crystal size	0.243 x 0.067 x 0.050 mm
Theta range for data collection	2.745 to 27.993 deg.
Limiting indices	-10 ≤ h ≤ 10, -10 ≤ k ≤ 10, -23 ≤ l ≤ 23
Reflections collected / unique	118192 / 2696 [R(int) = 0.0516]
Completeness to theta = 25.242	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.792 and 0.484
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2696 / 0 / 125
Goodness-of-fit on F ²	1.100
Final R indices [I > 2σ(I)]	R1 = 0.0131, wR2 = 0.0300
R indices (all data)	R1 = 0.0157, wR2 = 0.0309
Extinction coefficient	n/a
Largest diff. peak and hole	0.408 and -0.408 e.Å ⁻³

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

	x	y	z	U (eq)
Eu (1)	2599 (1)	4601 (1)	5354 (1)	10 (1)
Br (1)	3944 (1)	9617 (1)	6863 (1)	17 (1)
O (11)	-116 (2)	3379 (2)	5331 (1)	16 (1)
O (12)	-2809 (2)	2643 (2)	5225 (1)	16 (1)
C (11)	-1272 (3)	2335 (3)	5459 (1)	13 (1)
C (12)	-822 (3)	760 (3)	5886 (1)	22 (1)
O (21)	5408 (2)	5535 (2)	5734 (1)	13 (1)
O (22)	8113 (2)	6185 (2)	5976 (1)	16 (1)
C (21)	6703 (3)	5846 (3)	6216 (1)	13 (1)
C (22)	6531 (3)	5762 (3)	7040 (1)	21 (1)
O (1W)	3863 (2)	1820 (2)	5312 (1)	15 (1)
O (2W)	1567 (2)	6507 (2)	6250 (1)	16 (1)
O (3W)	2829 (2)	3441 (2)	6615 (1)	19 (1)

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

Eu(1)-O(11)	2.338(1)
Eu(1)-O(21)	2.356(1)
Eu(1)-O(2W)	2.409(2)
Eu(1)-O(3W)	2.420(2)
Eu(1)-O(1W)	2.442(2)
Eu(1)-O(12)#1	2.450(2)
Eu(1)-O(22)#2	2.459(2)
Eu(1)-O(21)#2	2.615(1)
Eu(1)-O(11)#1	2.720(2)
Eu(1)-Eu(1)#2	4.1387(2)
Eu(1)-Eu(1)#1	4.1847(2)
O(11)-C(11)	1.270(2)
O(12)-C(11)	1.257(2)
C(11)-C(12)	1.497(3)
O(21)-C(21)	1.283(2)
O(22)-C(21)	1.256(3)
C(21)-C(22)	1.489(3)
O(11)-Eu(1)-O(21)	163.49(5)
O(11)-Eu(1)-O(2W)	84.81(5)
O(21)-Eu(1)-O(2W)	88.60(5)
O(11)-Eu(1)-O(3W)	80.50(5)
O(21)-Eu(1)-O(3W)	83.00(5)
O(2W)-Eu(1)-O(3W)	68.04(5)
O(11)-Eu(1)-O(1W)	89.33(5)
O(21)-Eu(1)-O(1W)	85.96(5)
O(2W)-Eu(1)-O(1W)	139.79(5)
O(3W)-Eu(1)-O(1W)	71.75(5)
O(11)-Eu(1)-O(12)#1	118.08(5)
O(21)-Eu(1)-O(12)#1	74.53(5)
O(2W)-Eu(1)-O(12)#1	75.48(5)
O(3W)-Eu(1)-O(12)#1	137.31(5)
O(1W)-Eu(1)-O(12)#1	139.85(5)
O(11)-Eu(1)-O(22)#2	76.19(5)
O(21)-Eu(1)-O(22)#2	118.04(5)
O(2W)-Eu(1)-O(22)#2	137.95(5)
O(3W)-Eu(1)-O(22)#2	141.58(6)
O(1W)-Eu(1)-O(22)#2	77.83(5)
O(12)#1-Eu(1)-O(22)#2	81.00(5)
O(11)-Eu(1)-O(21)#2	125.57(5)
O(21)-Eu(1)-O(21)#2	67.37(6)
O(2W)-Eu(1)-O(21)#2	141.73(5)
O(3W)-Eu(1)-O(21)#2	132.85(5)
O(1W)-Eu(1)-O(21)#2	70.40(5)
O(12)#1-Eu(1)-O(21)#2	69.76(5)
O(22)#2-Eu(1)-O(21)#2	50.78(4)
O(11)-Eu(1)-O(11)#1	68.57(6)
O(21)-Eu(1)-O(11)#1	122.87(5)
O(2W)-Eu(1)-O(11)#1	69.31(5)
O(3W)-Eu(1)-O(11)#1	128.74(5)
O(1W)-Eu(1)-O(11)#1	143.34(5)
O(12)#1-Eu(1)-O(11)#1	49.51(4)
O(22)#2-Eu(1)-O(11)#1	68.88(5)
O(21)#2-Eu(1)-O(11)#1	98.37(5)
Eu(1)#2-Eu(1)-Eu(1)#1	140.418(5)

C (11)-O (11)-Eu (1)	159.5 (1)
C (11)-O (11)-Eu (1) #1	89.0 (1)
Eu (1)-O (11)-Eu (1) #1	111.4 (1)
C (11)-O (12)-Eu (1) #1	102.3 (1)
O (12)-C (11)-O (11)	119.2 (2)
O (12)-C (11)-C (12)	120.1 (2)
O (11)-C (11)-C (12)	120.8 (2)
C (21)-O (21)-Eu (1)	154.6 (1)
C (21)-O (21)-Eu (1) #2	90.8 (1)
Eu (1)-O (21)-Eu (1) #2	112.6 (1)
C (21)-O (22)-Eu (1) #2	98.9 (1)
O (22)-C (21)-O (21)	118.3 (2)
O (22)-C (21)-C (22)	121.3 (2)
O (21)-C (21)-C (22)	120.3 (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
Eu(OAc)₂Br·x·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
Eu(1)	7(1)	13(1)	12(1)	0(1)	1(1)	-1(1)
Br(1)	20(1)	15(1)	17(1)	2(1)	0(1)	-2(1)
O(11)	11(1)	18(1)	19(1)	2(1)	3(1)	-3(1)
O(12)	9(1)	18(1)	23(1)	5(1)	2(1)	0(1)
C(11)	12(1)	14(1)	14(1)	-2(1)	4(1)	-1(1)
C(12)	22(1)	20(1)	25(1)	7(1)	0(1)	0(1)
O(21)	9(1)	16(1)	14(1)	0(1)	0(1)	-1(1)
O(22)	10(1)	23(1)	16(1)	-1(1)	0(1)	-2(1)
C(21)	11(1)	14(1)	14(1)	-1(1)	-1(1)	2(1)
C(22)	16(1)	33(1)	13(1)	0(1)	1(1)	3(1)
O(1W)	11(1)	15(1)	18(1)	2(1)	4(1)	0(1)
O(2W)	12(1)	17(1)	19(1)	-3(1)	1(1)	0(1)
O(3W)	26(1)	17(1)	16(1)	2(1)	7(1)	4(1)

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

	x	y	z	U (eq)
H(12A)	-870	956	6426	87 (9)
H(12B)	340	410	5799	87 (9)
H(12C)	-1641	-118	5713	87 (9)
H(22A)	7661	5565	7316	45 (7)
H(22B)	5755	4847	7139	45 (7)
H(22C)	6063	6819	7206	45 (7)
H(22D)	7548	6191	7347	45 (7)
H(22E)	5501	6312	7190	45 (7)
H(22F)	6442	4555	7115	45 (7)
H(11W)	3826	1002	5704	50 (7)
H(12W)	5039	1842	5206	50 (7)
H(21W)	373	6689	6300	47 (7)
H(22W)	2135	7499	6448	47 (7)
H(31W)	2338	3927	7035	44 (6)
H(32W)	3158	2333	6776	44 (6)

Table S6. Hydrogen bonds for Eu(OAc)₂Br·x₃H₂O [Å 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	3.274(2)	164.7
O(1W)-H(12W)...O(12)#4	0.96	1.80	2.709(2)	156.7
O(2W)-H(21W)...O(22)#5	0.96	1.85	2.711(2)	148.0
O(2W)-H(22W)...Br(1)	0.96	2.28	3.231(2)	169.2
O(3W)-H(31W)...Br(1)#6	0.96	2.36	3.310(2)	169.6
O(3W)-H(32W)...Br(1)#3	0.96	2.26	3.204(2)	166.5

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