

Hexaaquadibromidoeuropium(III) bromide, [EuBr₂(H₂O)₆]Br

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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{Eu}-\text{O}) = 0.004$ Å; R factor = 0.029; wR factor = 0.049; data-to-parameter ratio = 22.4.

The title compound crystallizes with the $\text{GdCl}_3 \cdot 6\text{H}_2\text{O}$ structure type, exhibiting discrete $[\text{EuBr}_2(\text{H}_2\text{O})_6]^+$ cations as the main building blocks, linked with isolated bromide anions via $\text{H} \cdots \text{Br}$ hydrogen bonds to form a complex framework. The Eu atom and one Br atom each lie on a twofold rotation axis.

Related literature

For related literature, see: Bärnighausen *et al.* (1965); Bell & Smith (1990); Burns & Peterson (1971); Demyanets *et al.* (1974); Duhlev *et al.* (1988); Graeber *et al.* (1966); Habenschuss & Spedding (1980); Junk *et al.* (1999); Kolitsch (2006); Marezio *et al.* (1961); Reuter *et al.* (1994); Tegenfeldt *et al.* (1979); Wickleder & Meyer (1995).

Experimental

Crystal data

[EuBr₂(H₂O)₆]Br
 $M_r = 499.79$
 Monoclinic, $P2_1/c$
 $a = 8.1672$ (7) Å
 $b = 6.7538$ (4) Å
 $c = 12.5451$ (10) Å
 $\beta = 127.077$ (5)°

$V = 552.08$ (8) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 16.52$ mm⁻¹
 $T = 293$ (2) K
 $0.25 \times 0.24 \times 0.18$ mm

Data collection

Stoe IPDSII diffractometer
 Absorption correction: numerical
 $[X\text{-RED}$ (Stoe & Cie, 2001) and
 $X\text{-SHAPE}$ (Stoe & Cie, 1999)]
 $T_{\min} = 0.065$, $T_{\max} = 0.155$

10921 measured reflections
 1613 independent reflections
 1397 reflections with $I > 2s(I)$
 $R_{\text{int}} = 0.067$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.049$
 $S = 1.11$
 1613 reflections

72 parameters
 All H-atom parameters refined
 $\Delta\rho_{\text{max}} = 1.14$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.10$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Eu1—Br1	2.9449 (5)	Eu1—O2	2.422 (3)
Eu1—O1	2.424 (3)	Eu1—O3	2.388 (3)
Br1—Eu1—O1	146.89 (8)	O2—Eu1—O2 ⁱ	146.8 (2)
Br1—Eu1—O1 ⁱ	76.21 (9)	O3—Eu1—O3 ⁱ	84.5 (2)
Br1—Eu1—O2	77.33 (8)	O1—Eu1—O2	72.6 (1)
Br1—Eu1—O2 ⁱ	78.22 (8)	O1—Eu1—O2 ⁱ	122.0 (1)
Br1—Eu1—O3	107.21 (9)	O1—Eu1—O3	75.8 (1)
Br1—Eu1—O3 ⁱ	143.18 (8)	O1—Eu1—O3 ⁱ	69.3 (1)
Br1—Eu1—Br1 ⁱ	84.41 (2)	O2—Eu1—O3	70.9 (1)
O1—Eu1—O1 ⁱ	132.3 (2)	O2—Eu1—O3 ⁱ	138.6 (1)

Symmetry code: (i) $-x + 1, y, -z + \frac{1}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

$D\text{—}H \cdots A$	$D\text{—}H$	$H \cdots A$	$D \cdots A$	$D\text{—}H \cdots A$
O1—H11 \cdots Br2 ⁱⁱ	0.83 (2)	2.53 (8)	3.343 (4)	168 (6)
O1—H12 \cdots Br1 ⁱⁱⁱ	0.83 (2)	2.52 (13)	3.333 (4)	165 (6)
O2—H21 \cdots Br1 ^{iv}	0.82 (2)	2.49 (10)	3.307 (4)	172 (6)
O2—H22 \cdots Br2 ^v	0.83 (2)	2.63 (11)	3.417 (4)	161 (6)
O3—H31 \cdots Br1 ^{vi}	0.83 (2)	2.46 (8)	3.288 (4)	173 (6)
O3—H32 \cdots Br2	0.83 (2)	2.52 (11)	3.328 (5)	163 (6)

Symmetry codes: (ii) $-x, -y + 1, -z$; (iii) $x - 1, -y, z - \frac{1}{2}$; (iv) $-x + 1, -y, -z + 1$; (v) $x, y - 1, z$; (vi) $x, y + 1, z$.

Data collection: *X-AREA* (Stoe & Cie, 2006); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DRAWXTL* (Finger *et al.*, 2007); software used to prepare material for publication: *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MG2051).

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