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Heptaaquabis(hydrogen maleato-κO)europium(III) hydrogen maleate monohydrate

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The title compound, $[Eu(C_4H_3O_4)_2(H_2O)_7](C_4H_3O_4)\cdot H_2O$, is isostructural with the Nd^{III} analogue. The Eu^{III} atom is coordinated by O atoms from two hydrogen maleate anions and by seven water molecules, forming a distorted monocapped square-antiprismatic coordination geometry.

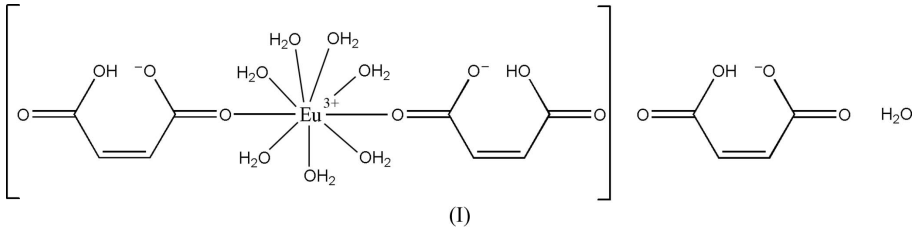
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.027
wR factor = 0.071
Data-to-parameter ratio = 14.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Complexes of lanthanide elements with maleic acid, $Ln_2L_3\cdot nH_2O$ and $Ln(HL)_3\cdot nH_2O$ (Ln = lanthanide, L = $C_4H_2O_4^{2-}$), have been studied previously (Oczko *et al.*, 2002). The title compound, $[Eu(C_4H_3O_4)_2(H_2O)_7](C_4H_3O_4)H_2O$, (I), is isostructural with its Nd^{III} analogue.



(I)

In (I), the Eu^{III} atom is coordinated by O atoms from two hydrogen maleate anions and by seven water molecules, forming a distorted monocapped square-antiprismatic coordination geometry (Fig. 1 and Table 1). The dihedral angles between the planes [C9/C10/C11/C12/O11/O10] and [C1/C2/C3/C4/O3/O2], [C9/C10/C11/C12/O11/O10] and [C5/C6/C7/C8/O7/O6], and [C1/C2/C3/C4/O3/O2] and [C5/C6/C7/C8/O7/O6] are 38.4 (19), 34.2 (18) and 5.7 (18)°, respectively.

Experimental

Europium oxide (0.01 mol) and aqueous HCl (0.06 mol) were combined to form a clear $EuCl_3$ solution, which was heated to near dryness. Aqueous NaOH (20 wt%, 0.06 mol) was added, and the deposited $Eu(OH)_3$ was filtered and washed with deionized water. Solid $Eu(OH)_3$ (0.02 mol) was then added to an aqueous solution (100 ml) of maleic acid (0.06 mol) with continous stirring at 323 K for 2 h. The solution was left to evaporate at room temperature, and colourless block-like crystals were formed over the course of 7 d.

Crystal data

$[Eu(C_4H_3O_4)_2(H_2O)_7](C_4H_3O_4)\cdot H_2O$
M_r = 641.28
Triclinic, $P\overline{1}$
a = 7.2220 (14) Å
b = 10.350 (2) Å
c = 16.672 (3) Å
α = 72.08 (3)°
β = 88.06 (3)°
γ = 70.89 (3)°
V = 1117.3 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.90 mm^{-1}
T = 293 (2) K
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.375, T_{max} = 0.568
4740 measured reflections
4370 independent reflections
4144 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.071
S = 1.09
4370 reflections
299 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −1.13 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1···O3	1.20	1.21	2.410 (4)	180
O6—H2···O7	1.20	1.20	2.405 (4)	180
O10—H3···O11	1.21	1.22	2.434 (5)	180

H atoms bound to C atoms were positioned geometrically with C—H = 0.93 Å and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C). H atoms of the water molecules were placed geometrically with O—H = 0.96 Å so as to form a reasonable hydrogen-bond network and allowed to ride with U_{iso}(H) = 1.5U_{eq}(O). H atoms of the hydrogen maleate anions were included in positions indicated by difference Fourier maps, approximately midway between O2/O3, O5/O6 and O10/O11, respectively. They were allowed to ride on the closest O atom with U_{iso}(H) = 1.5U_{eq}(O). The deepest residual electron density hole is located 0.09 Å from atom Eu.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

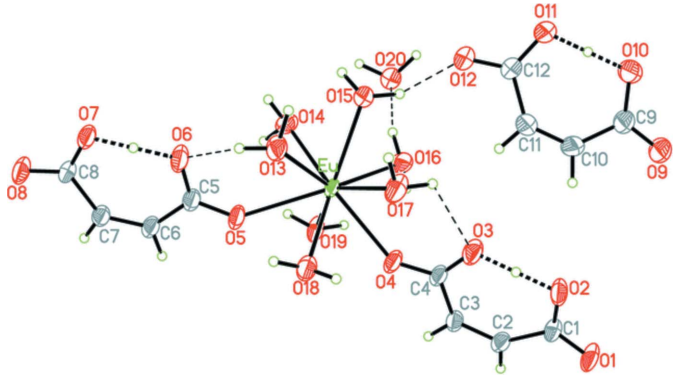


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 30% probability level for non-H atoms. Dashed lines indicate O—H···O hydrogen bonds.

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