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Tetraaquatrinitratoeuropium(III) dihydrate

Thorsten Stumpf[a] and Michael Bolte[b]*

[a]Forschungszentrum Rossendorf, Institut für Radiochemie, PO Box 510119, 01324 Dresden, Germany, and [b]Institut für Organische Chemie, J. W. Goethe-Universität Frankfurt, Marie-Curie-Strasse 11, 60439 Frankfurt/Main, Germany

Correspondence e-mail: bolte@chemie.uni-frankfurt.de

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(O–N) = 0.003 Å
R factor = 0.016
wR factor = 0.039
Data-to-parameter ratio = 15.6

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

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In the title compound, $[Eu(NO_3)_3(H_2O)_4]\cdot 2H_2O$, the Eu atom is ten-coordinated by three bidentate nitrates and four water molecules. Furthermore, two water molecules are included in the crystal structure forming a complicated network of hydrogen bonds. $[Eu(NO_3)_3(H_2O)_4]\cdot 2H_2O$ is isostructural with other lanthanide analogues.

Comment

In the series of tetraaquatrinitratolanthanide dihydrates, the structures from cerium to terbium with the exception of the Pm and Eu compounds are known. Whereas this fact is not astonishing in the case of promethium, which is radioactive, it is surprising that the europium structure has not been determined yet. In order to fill this gap, we present in this article the structure of $[Eu(NO_3)_3(H_2O)_4]\cdot 2H_2O$.

Three bidentate nitrates and four coordinated water molecules produce a ten-coordinated europium with six different Eu—O bonds between 2.511 (2) and 2.741 (2) Å to the nitrate groups and four slightly shorter bonds to water molecules between 2.379 (2) and 2.412 (2) Å. One nitrate ion is asymmetrically bonded and the Eu—O21 distance is about 0.2 Å longer than the other Eu—O distances. Two further H_2O molecules in the second coordination sphere of the europium are included as crystal water. The three nitrate groups are located on the same side of the Eu ion, while the water molecules are located on the other side. The crystal packing is stabilized by a complicated network of hydrogen bonds.

The structure of the title compound is isostructural with the already known $[Ln(NO_3)_3(H_2O)_4]\cdot 2H_2O$ structures [Ln = Pr (Fuller & Jacobsen, 1976; Volodina *et al.*, 1961; Rumanova *et al.*, 1964), Nd (Rogers *et al.*, 1983; Shi & Wang, 1991), Sm (Shi & Wang, 1990), Gd (Ma *et al.*, 1991) and Tb (Moret *et al.*, 1990)]. It fits well into and completes this series.

Experimental

At 373 K, 0.352 g (1 mmol) Eu_2O_3 (99.99%; Across) was dissolved in 10 ml 1.0 mol l^{-1} HNO_3. From the light yellow solution, crystals appeared at room temperature within 5 d.

Crystal data

$[Eu(NO_3)_3(H_2O)_4]\cdot 2H_2O$
M_r = 446.09
Triclinic, $P\overline{1}$
a = 6.705 (1) Å
b = 9.140 (1) Å
c = 11.647 (1) Å
α = 69.71 (1)°
β = 88.94 (1)°
γ = 69.29 (1)°
V = 621.79 (13) Å^3
Z = 2
D_x = 2.383 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5718 reflections
θ = 1–25°
μ = 5.13 mm^{-1}
T = 173 (2) K
Block, colourless
0.41 × 0.39 × 0.28 mm

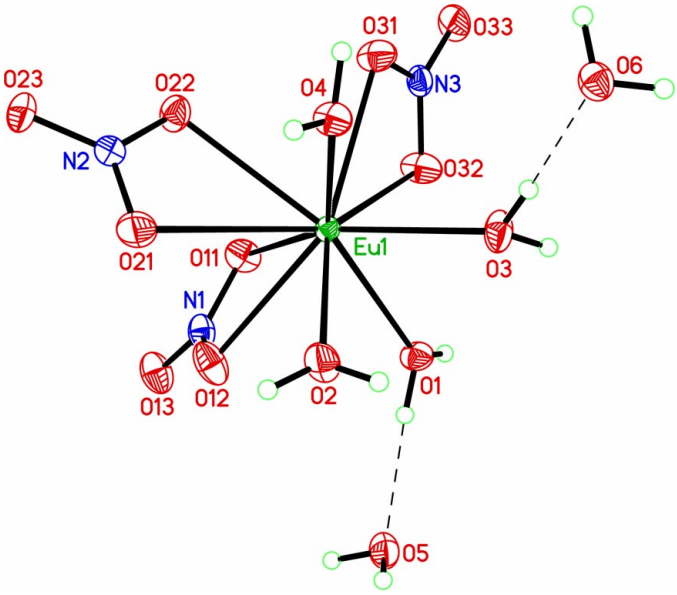

Figure 1
A perspective view of the title compound with the atom-numbering scheme. Displacement ellipsoids are at the 50% probability level.

Data collection

Siemens CCD three-circle diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
T_{min} = 0.148, T_{max} = 0.238
12 544 measured reflections
3448 independent reflections
3284 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 30.9°
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 13$
$l = -15 \rightarrow 15$
255 standard reflections
frequency: 1200 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.039
S = 1.13
3448 reflections
221 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0218P)^2 + 0.0630P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0410 (9)

Table 1
Selected geometric parameters (Å).

Eu1—O3	2.3787 (16)	Eu1—O32	2.5364 (17)
Eu1—O4	2.4029 (15)	Eu1—O12	2.5396 (18)
Eu1—O2	2.4063 (16)	Eu1—O22	2.5671 (16)
Eu1—O1	2.4118 (15)	Eu1—O11	2.5891 (16)
Eu1—O31	2.5105 (16)	Eu1—O21	2.7407 (19)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*A*···O5	0.837 (10)	1.889 (11)	2.723 (2)	175 (3)
O1—H1*B*···O11^{i}	0.835 (10)	2.117 (11)	2.951 (2)	176 (3)
O2—H2*A*···O11^{ii}	0.833 (10)	2.48 (3)	3.180 (2)	143 (4)
O2—H2*A*···O22^{ii}	0.833 (10)	2.49 (3)	3.149 (2)	137 (4)
O2—H2*B*···O21^{iii}	0.834 (10)	2.260 (12)	3.081 (2)	168 (3)
O2—H2*B*···O23^{iii}	0.834 (10)	2.40 (2)	3.058 (2)	136 (3)
O3—H3*A*···O5^{iv}	0.831 (10)	1.906 (12)	2.731 (2)	171 (4)
O3—H3*B*···O6	0.829 (10)	1.904 (10)	2.733 (2)	177 (3)
O4—H4*A*···O6^{v}	0.837 (10)	1.857 (13)	2.675 (2)	165 (3)
O4—H4*B*···O22^{vi}	0.836 (10)	2.141 (13)	2.962 (2)	167 (3)
O5—H5*A*···O13^{ii}	0.837 (10)	1.993 (13)	2.821 (3)	170 (4)
O5—H5*B*···O33^{vii}	0.827 (10)	2.26 (3)	2.906 (2)	135 (4)
O5—H5*B*···O33^{i}	0.827 (10)	2.55 (4)	3.085 (3)	124 (4)
O6—H6*A*···O23^{vi}	0.842 (10)	2.013 (14)	2.829 (2)	163 (3)
O6—H6*B*···O12^{viii}	0.835 (10)	2.23 (3)	2.885 (2)	136 (3)
O6—H6*B*···O33^{ii}	0.835 (10)	2.42 (3)	3.005 (2)	128 (3)

Symmetry codes: (i) $-x, 1-y, -z$; (ii) $1+x, y, z$; (iii) $1-x, -y, 1-z$; (iv) $1-x, 1-y, -z$; (v) $1-x, 1-y, 1-z$; (vi) $-x, 1-y, 1-z$; (vii) $1+x, y-1, z$; (viii) $x, 1+y, z$.

All H atoms were located by difference Fourier synthesis and refined isotropically applying a restraint of 0.84 (1) Å to the O—H distances.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97.

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