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[*N*,*N*-Diisopropyl-2,2′-(2,3-naphthalenedioxy)diacetamide]trinitratoneodymium(III) acetone solvate

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Key indicators

Single-crystal X-ray study
T = 287 K
Mean σ(C–C) = 0.004 Å
R factor = 0.025
wR factor = 0.056
Data-to-parameter ratio = 14.9

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

In the title compound, $[Nd(NO_3)_3(C_{26}H_{38}N_2O_4)]\cdot C_3H_6O$, the Nd^{III} atom is coordinated by ten O atoms in a a distorted bicapped dodecahedral geometry. The Nd—O(carbonyl) bond distances [average 2.3817 (18) Å] are significantly shorter than other Nd—O bonds in the Nd^{III} complex.

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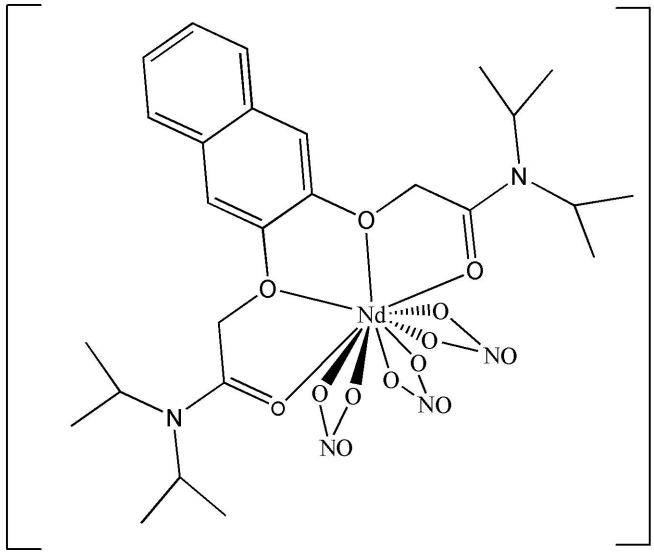
Comment

The luminescence of lanthanide complexes incorporating an open-chain crown ether has attracted our attention. As *N*,*N*-diisopropyl-2,2′-(2,3-naphthalenedioxy)diacetamide (*L*) has the proper conjugate absorption group, it has been used as a chelating ligand to prepare the title Nd^{III} complex, (I).



· CH_3COCH_3

(I)

The molecular structure of (I) is illustrated in Fig. 1. The Nd^{III} atom is coordinated by ten O atoms, four from the tetradentate *L* ligand and six from chelating nitrate anions, in a distorted bicapped dodecahedral geometry. *L* chelates to the Nd^{III} atom by four O atoms, of which atoms O1, O3 and O4 of *L* are coplanar with the Nd^{III} atom, but atom O2 deviates from the mean plane formed by O1/O3/O4/Nd by 1.108 (3) Å. The bond distances between Nd and carbonyl atoms O2 and O4 are significantly shorter than other Nd—O bond distances (Table 1).

Experimental

Ligand *L* was prepared according to the literature method of Zhang & Liu (2003). An ethyl acetate solution of $Nd(NO_3)_3\cdot 6H_2O$ (0.1 mmol) was added dropwise to an ethyl acetate solution (20 ml) of

L (0.1 mmol). The mixture was stirred for 4 h and a pale-purple precipitate appeared. The precipitate was separated and washed three times with ethyl acetate. Single crystals of (I) were obtained by recrystallization from acetone solution. Analysis calculated for $C_{29}H_{44}N_5NdO_{14}$: C 42.11, H 5.22, N 8.30%; found: C 41.88, H 5.30, N 8.42%.

Crystal data

$[Nd(NO_3)_3(C_{26}H_{38}N_2O_4)]\cdot C_3H_6O$	D_x = 1.482 Mg m^{-3}
M_r = 830.93	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 30 reflections
a = 13.457 (3) Å	θ = 4.7–12.2°
b = 19.807 (3) Å	μ = 1.46 mm^{-1}
c = 14.080 (3) Å	T = 287 (2) K
β = 97.15 (2)°	Block, pale purple
V = 3723.7 (12) Å^3	0.58 × 0.46 × 0.42 mm
Z = 4	

Data collection

Siemens P4 diffractometer	R_{int} = 0.016
ω scans	θ_{max} = 25.3°
Absorption correction: ψ scan (*SADABS*; Sheldrick, 1996)	$h = 0 \rightarrow 16$
	$k = 0 \rightarrow 23$
T_{min} = 0.435, T_{max} = 0.540	$l = -16 \rightarrow 16$
7518 measured reflections	3 standard reflections
6734 independent reflections	every 97 reflections
5404 reflections with $I > 2\sigma(I)$	intensity decay: 2.8%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0294P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.025	$(\Delta/\sigma)_{max}$ = 0.002
$wR(F^2)$ = 0.056	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
S = 0.97	$\Delta\rho_{min}$ = −0.32 e Å^{-3}
6734 reflections	Extinction correction: *SHELXL97*
453 parameters	Extinction coefficient: 0.00345 (11)
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

Nd—O1	2.5890 (18)	Nd—O6	2.514 (2)
Nd—O2	2.3946 (18)	Nd—O8	2.532 (2)
Nd—O3	2.6908 (17)	Nd—O9	2.517 (2)
Nd—O4	2.3687 (18)	Nd—O11	2.537 (2)
Nd—O5	2.555 (2)	Nd—O12	2.5340 (19)

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and torsion angles refined to fit the electron density. Other H atoms were placed in calculated positions, with C—H = 0.93 (aromatic), 0.97 (methylene) and 0.98 Å (methine), and were included in the final cycles of refinement using a riding model, with $U_{iso}(H) = 1.2U_{eq}$ of the carrier atom.

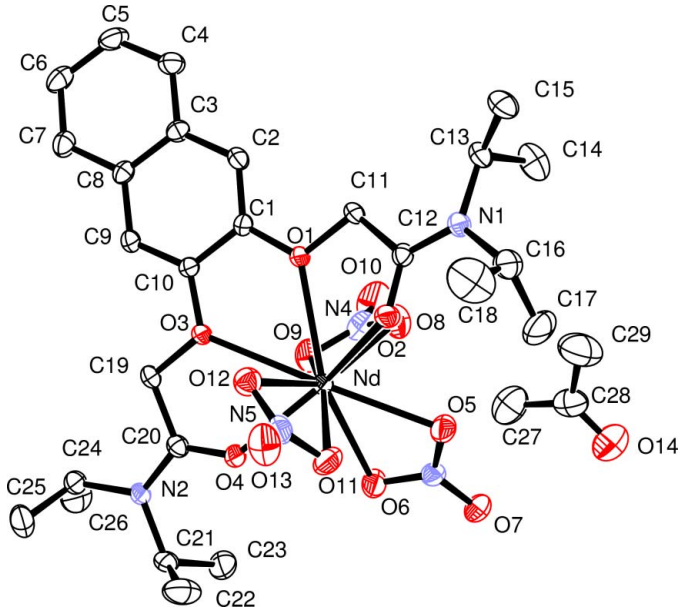


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids. H atoms have been omitted.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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