Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diimidazolium aquapentakis(nitrato)-neodymate(III)

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Received 8 February 2006
Accepted 21 March 2006.

Key indicators

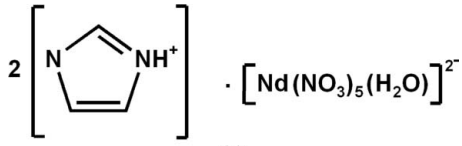
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.017
wR factor = 0.042
Data-to-parameter ratio = 15.6

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

The asymmetric unit of the title compound, $(Him)_2[Nd(NO_3)_5H_2O]$ (Him is 1*H*-imidazolium, $C_3H_5N_2$), contains one $[Nd(NO_3)_5H_2O]^{2-}$ anion and two imdidazolium cations. Nd is coordinated by 11 O atoms. N—H···O and O—H···O hydrogen-bond interactions link cations and anions, forming a three-dimensional network.

Comment

Some metal chloride complexes containing imidazolium have been investigated, such as $(EMI)_3[LaCl_6]$ (EMI is 1-ethyl-3-methylimidazolium, $C_6H_{11}N_2$) (Matsumoto *et al.*, 2002), $(EMI)_2[PdCl_4]$ (II) (Ortwerth *et al.*, 1998) and Him[TaC1$_6$] (Him is 1H-imidazolium) (Levasseur & Beauchamp, 1991). Neodymium nitrate complexes containing alkali metals that have been investigated include $Na_2[Nd(NO_3)_5H_2O]$ (Vigdorchik *et al.*, 1990), $K_2[Nd(NO_3)_5(H_2O)_2]$ (Held *et al.*, 2000) and $Cs_2[Nd(NO_3)_5(H_2O)_2]$ (Vigdorchik *et al.*, 1989), but little work has been focused on neodmium nitrates containing imidazolium. In the title compound, (I), Nd is coordinated by 11 O atoms from five nitrate ions and one water molecule; Nd is coordinated by 12 O atoms in $Na_2[Nd(NO_3)_5H_2O]$ and $K_2[Nd(NO_3)_5(H_2O)_2]$ and by 10 O atoms in $Cs_2[Nd(NO_3)_5(H_2O)_2]$.



(I)

Bond distances for Nd—O and N—O are in the range 2.4397 (18)–2.6442 (15) Å and 1.216 (2)–1.271 (2) Å, respectively. O—N—O bond angles are in the range 116.25 (14)–122.37 (15)°. These results are in agreement with those of $A_2[Nd(NO_3)_5(H_2O)_2]$ (A = Na, K, Cs) complexes. In (I), two types of donor H atoms, *viz*. the imidazole NH and the water H (H1*W* and H2*W*) atoms are engaged in hydrogen bonds with O atoms of nitrate groups. Hydrogen-bond distances for O—H···O and N—H···O are in the ranges 2.753 (2)–2.822 (2) Å and 2.915 (2)–3.274 (3) Å, respectively. These hydrogen bonds link cations and anions, forming a three-dimensional network.

Experimental

Crystals of (I) were obtained from the reaction of $Nd(NO_3)_3$ (5 mmol) and imidazole (5 mmol) in dilute HNO_3 solution (30 ml) at room temperature. After a few days, pink block crystals appeared.

Crystal data

$[(C_3H_5N_2)_2Nd(NO_3)_5(H_2O)]$
M_r = 610.49
Triclinic, $P\overline{1}$
a = 7.3817 (15) Å
b = 7.8831 (16) Å
c = 18.073 (4) Å
α = 89.37 (3)°
β = 89.49 (3)°
γ = 63.12 (3)°
V = 938.0 (4) Å^3
Z = 2
D_x = 2.162 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4652 reflections
θ = 1.1–28.3°
μ = 2.87 mm^{-1}
T = 293 (2) K
Block, pink
0.20 × 0.18 × 0.15 mm

Data collection

Bruker APEX CCD diffractometer
ω scan
Absorption correction: multi-scan (*SADABS* in *SAINT*; Bruker, 1998)
T_{min} = 0.56, T_{max} = 0.65
12985 measured reflections
4652 independent reflections
4530 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 28.3°
$h = -9 \rightarrow 9$
$k = -10 \rightarrow 10$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.042
S = 1.05
4652 reflections
298 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0177P)^2 + 0.3143P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}
Extinction correction: *SHELXL*
Extinction coefficient: 0.0174 (5)

Table 1
Selected geometric parameters (Å, °).

Nd1—O16	2.4397 (18)	O3—N2	1.268 (2)
Nd1—O8	2.5468 (16)	O4—N2	1.271 (2)
Nd1—O1	2.5560 (15)	O5—N3	1.262 (2)
Nd1—O10	2.5633 (14)	O6—N3	1.2582 (19)
Nd1—O5	2.5652 (16)	O7—N4	1.262 (2)
Nd1—O9	2.5685 (14)	O8—N4	1.262 (2)
Nd1—O3	2.5709 (16)	O9—N5	1.267 (2)
Nd1—O6	2.5839 (17)	O10—N5	1.265 (2)
Nd1—O7	2.6221 (16)	O11—N1	1.2258 (19)
Nd1—O4	2.6242 (15)	O12—N2	1.216 (2)
Nd1—O2	2.6442 (15)	O13—N3	1.227 (2)
O1—N1	1.2675 (19)	O14—N4	1.218 (2)
O2—N1	1.2515 (19)	O15—N5	1.216 (2)
O16—Nd1—O1	89.53 (6)	O12—N2—O3	122.18 (16)
O16—Nd1—O10	83.83 (5)	O12—N2—O4	121.57 (16)
O10—Nd1—O9	49.74 (5)	O3—N2—O4	116.25 (14)
O5—Nd1—O6	49.48 (5)	O13—N3—O6	121.47 (15)
O16—Nd1—O7	66.49 (6)	O13—N3—O5	120.91 (15)
O8—Nd1—O7	49.10 (5)	O6—N3—O5	117.57 (14)
O16—Nd1—O4	64.70 (6)	O14—N4—O7	121.82 (17)
O3—Nd1—O4	49.02 (5)	O14—N4—O8	121.43 (17)
O1—Nd1—O2	48.73 (4)	O7—N4—O8	116.75 (15)
O3—Nd1—O2	110.55 (5)	O15—N5—O10	121.12 (15)
O11—N1—O2	122.37 (15)	O15—N5—O9	121.96 (16)
O11—N1—O1	120.71 (15)	O10—N5—O9	116.90 (14)
O2—N1—O1	116.92 (14)		

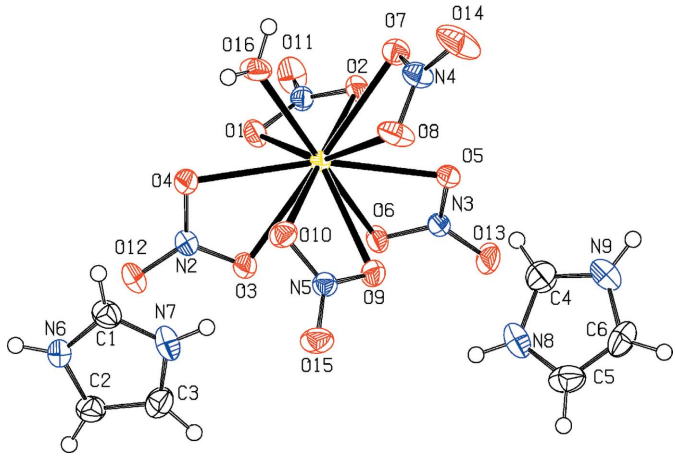


Figure 1
The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

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

D—H···A	D—H	H···A	D···A	D—H···A
O16—H2W···O11^{i}	0.79 (3)	1.96 (3)	2.753 (2)	175 (3)
O16—H1W···O13^{ii}	0.81 (3)	2.01 (3)	2.822 (2)	173 (3)
N9—H9···O14^{iii}	0.86	2.51	3.073 (3)	124
N9—H9···O7^{iii}	0.86	2.49	3.274 (3)	152
N9—H9···O13^{iv}	0.86	2.48	3.079 (3)	128
N8—H8···O2^{v}	0.86	2.21	2.919 (2)	140
N8—H8···O9	0.86	2.55	3.112 (3)	124
N7—H7···O10^{vi}	0.86	2.55	3.160 (2)	128
N7—H7···O6^{iv}	0.86	2.39	3.054 (2)	135
N7—H7···O15^{vi}	0.86	2.28	2.921 (2)	132
N6—H6···O4^{vii}	0.86	2.11	2.915 (2)	156

Symmetry codes: (i) $x-1, y, z$; (ii) $x-1, y+1, z$; (iii) $-x+1, -y+2, -z+1$; (iv) $-x+2, -y+1, -z+1$; (v) $x, y-1, z$; (vi) $-x+1, -y+1, -z+1$; (vii) $x+1, y-1, z+1$.

Imidazole H atoms were constrained to an ideal geometry with C—H and N—H distances of 0.93 and 0.86 Å, respectively. H atoms were refined with fixed isotropic displacement parameters U_{iso}(H) = 1.2U_{eq}(C,N). Aqua H1W and H2W atoms were located in a difference electronic density map, and their positions and isotropic displacement parameters were refined freely.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL* (Bruker, 1997); molecular graphics: *ORTEP*III (Farrugia, 1997) and *DIAMOND* (Brandenburg & Berndt, 1999); software used to prepare material for publication: *SHELXTL* (Bruker, 1997).

This work was financially supported by the Natural Science Foundation of China (NSFC No.50572078 and No. 20571059), ICDD Grant-in-Aid project under Grant No. 04–056 and the Opening Fund of the Key Laboratory of Nonferrous Materials and New Processing Technology, Ministry of Education of China.

References

Brandenburg, K. & Berndt, M. (1999). *DIAMOND*. Release 2.1e. Crystal Impact GbR, Bonn, Germany.

Bruker (1997). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1998). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Held, P., Hellwig, H., Ruehle, S. & Bohaty, L. (2000). *J Appl. Cryst.* **33**, 372–377.
Matsumoto, K., Tsuda, T., Nohira, T., Hagiwara, R., Ito, Y. & Tamada, O. (2002). *Acta Cryst.* C**58**, m186–m187.
Levasseur, G. & Beauchamp, A. L. (1991). *Acta Cryst.* C**47**, 547–550.
Ortwerth, M. F., Wyzlic, M. J. & Baughman, R. G. (1998). *Acta Cryst.* C**54**, 1594–1596.
Vigdorchik, A. G., Malinovskii, Y. A., Andrianov, V. I. & Dryuchko, A. G. (1990). *Izv. Akad. Nauk SSSR Neorg. Mater.* **26**, 2357–2362 (In Russian.).
Vigdorchik, A. G., Malinovskii, Y. A. & Dryuchko, A. G. (1989). *Kristallografiya*, **34**, 292–296. (In Russian.)