Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Neodymium triiodide nonahydrate

Tudor Timofte, Arash Babai, Gerd Meyer and Anja-Verena Mudring*

Institut für Anorganische Chemie, Universität zu Köln, Greinstrasse 6, D-50939 Köln, Germany

Correspondence e-mail: a.mudring@uni-koeln.de

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(d–O) = 0.008 Å
H-atom completeness 0%
R factor = 0.048
wR factor = 0.143
Data-to-parameter ratio = 27.4

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

Received 8 April 2005
Accepted 19 April 2005
Online 27 April 2005

$NdI_3·9H_2O$ contains Nd^{3+} ions bonded to water molecules in a tricapped trigonal prismatic coordination geometry (coordination number 9).

Comment

Trivalent rare earth cations exhibit interesting optical properties, of which use is made in many everyday materials. Although favourable properties, such as long lifetimes and high quantum yields for luminescence, are usually found in solid materials, we have been able to show that thoughtfully designed ionic liquids are well suited media for liquid phosphors with excellent properties (Arenz *et al.*, 2005), as long as no water is present in these systems. In order to study quantitatively the effect of water on the luminescent properties of rare earth triiodides, we have attempted to synthesize rare earth triiodides with a defined hydration shell of the rare earth cation. According to X-ray powder diffraction studies, nonahydrates are the maximally hydrated species for triiodides of La–Ho (Kwestroo & von Hal, 1976; Heinio *et al.*, 1980). The single-crystal structure of the isotypic compounds has been unequivocally established for La, Sm, Gd, Dy and Ho (Lim *et al.*, 2000) in the space group *Pmmn* (No. 59). We are now able to add to this list the title compound, $NdI_3·9H_2O$ (Fig. 1).

As expected, the title hydrated neodymium iodide crystallizes isotypically with the known nonahydrates in the same orthorhombic centrosymmetric primitive space group. The nature of the complex is more precisely described by the formulation $[Nd(OH_2)_9]I_3$, all water molecules (four crystallographically independent O atoms) being bonded to the ninefold coordinated Nd^{3+} cation (site symmetry *mm*2)

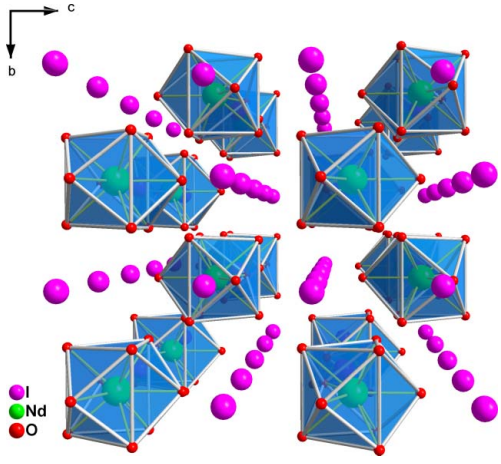

Figure 1
The unit cell of $NdI_3·9H_2O$, viewed along the *a* axis.

(Fig. 2). The I atoms are situated around these Nd—H_2O entities in rows, separating the $[Nd(OH_2)_9]^{3+}$ coordination polyhedra.

Experimental

All reactions were carried out under an argon atmosphere. Neodymium carbonate, $[Nd_2(CO_3)_3]$ (99.9%, Chempur, 2 mmol), was dissolved in multiply distilled hydroiodic acid (HI, 57%, Acros Organics, 4 ml). The solution was heated to 313 K and stirred for 30 min. The total dissolution of $Nd_2(CO_3)_3$ in the hydroiodic acid was observed under control of the pH (acidic, 0–1). The solution was slowly cooled to 298 K and allowed to stand under an argon atmosphere, and the product crystallized after 6 d. On exposure to normal atmosphere, the product decomposed and became liquid. The crystals obtained were therefore placed in glass capillaries with the mother liquor and then mounted on the diffractometer.

Crystal data

$NdI_3·9H_2O$
M_r = 687.08
Orthorhombic, *Pmmn*
a = 11.6604 (15) Å
b = 8.0103 (11) Å
c = 8.9702 (16) Å
V = 837.8 (2) Å^3
Z = 2
D_x = 2.723 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1391 reflections
θ = 1.9–28.0°
μ = 8.64 mm^{-1}
T = 278 (2) K
Prism, pale yellow
0.5 × 0.5 × 0.2 mm

Data collection

Stoe IPDS-I diffractometer
2° φ scans
Absorption correction: numerical [*X-RED* (Stoe & Cie, 2002) and *X-SHAPE* (Stoe & Cie, 1999)]
T_{min} = 0.058, T_{max} = 0.509
7674 measured reflections
1123 independent reflections
843 reflections with $I > 2\sigma(I)$
R_{int} = 0.095
θ_{max} = 28.0°
$h = -14 \rightarrow 15$
$k = -9 \rightarrow 10$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.143
S = 1.02
1123 reflections
41 parameters
H atoms not located
$w = 1/[\sigma^2(F_o^2) + (0.1174P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.22 e Å^{-3}
$\Delta\rho_{min}$ = −2.56 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.084 (7)

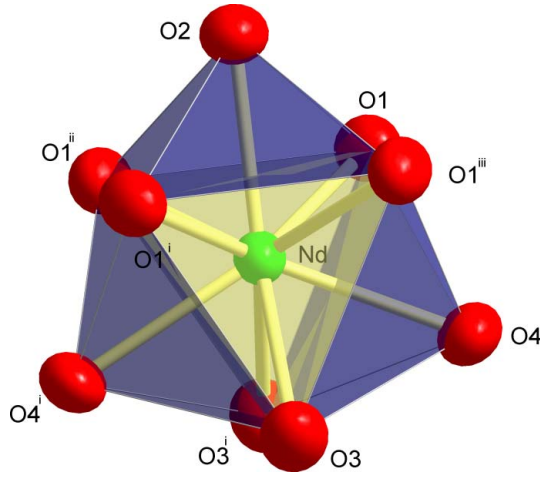

Figure 2
Coordination of neodymium by water in $NdI_3·9H_2O$. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $\frac{1}{2} - x, \frac{3}{2} - y, z$; (ii) $\frac{1}{2} - x, y, z$; (iii) $x, \frac{3}{2} - y, z$.]

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1996); software used to prepare material for publication: *SHELXL97*.

References

Arenz, S., Babai, A., Binnemans, K., Driesen, Ch., Giernoth, R., Mudring, A.-V. & Nockemann, P. (2005). *Chem. Phys. Lett.* **402**, 75–79.
Brandenburg, K. (1996). *DIAMOND*. Release 2.1. Crystal Impact GbR, Bonn, Germany.
Heinio, O., Leskelä, M. & Niinistö, L. (1980). *Acta Chem. Scand. A*, **34**, 207–211.
Kwestroo, W. & von Hal, A. H. M. (1976). *J. Inorg. Nucl. Chem.* **38**, 1019–1022.
Lim, K. C., Skelton, B. W. & White, A. H. (2000). *Aust. J. Chem.* **53**, 867–873.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Stoe & Cie (1999). *X-SHAPE*. Version 1.0.1. Stoe & Cie, Darmstadt, Germany.
Stoe & Cie (2002). *X-AREA*. Version 1.18. Stoe & Cie, Darmstadt, Germany.