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Poly[aquaneodymium(III)-μ_5-2-oxido-5-sulfonatobenzoato]

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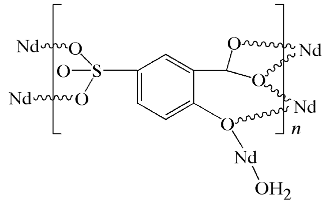
The title compound, $[Nd(C_7H_3O_6S)(H_2O)]_n$ or $[Nd(SSA)(H_2O)]_n$ (H_3SSA is 5-sulfosalicylic acid), was synthesized by the hydrothermal reaction of Nd_2O_3 with H_3SSA in water. The compound forms a three-dimensional network in which the asymmetric unit contains one Nd^{III} atom, one SSA ligand and one coordinated water molecule. The central Nd^{III} ion is eight-coordinate, bonded to seven O atoms from five different SSA ligands [Nd—O = 2.405 (4)–2.612 (4) Å] and one aqua O atom [Nd—O*W* = 2.441 (4) Å].

Comment

Owing to the high coordination numbers of lanthanide ions and the inherent flexibility of their coordination geometries, much effort has been devoted to the study of novel lanthanide metal complexes. For instance, a two-dimensional brick-wall network complex, $[Tb(oba)(Hoba)(H_2O)_2]\cdot H_2O$ [Hoba is 4,4′-oxybis(benzoic acid); Liu *et al.*, 2002], and a series of three-dimensional hybrid coordination polymers, $[Ln_2(H_2O)_4\{(1,2\text{-BDC})_2(1,4\text{-BDC})\}]$ (BDC is benzenedicarboxylate; Thirumurugan & Natarajan, 2004), have recently been reported. The H_3SSA ligand has a strong coordination ability, as it possesses three different chelating groups (SO_3H, OH and COOH). It has been used extensively to construct metal-organic coordination polymers, such as a ladder-structure complex, $[Ba_2(SSA)_4(H_2O)_{10}]$ (Ma *et al.*, 2003), and the two-dimensional complex $[Eu(SSA)_2(H_2O)_5]_n$ (Starynowicz, 2000). However, much effort has been devoted to the investigation of transition metal–SSA coordination polymers, rather than the analoguous compounds with lanthanide metals. Recently, we have become interested in the study of lanthanide metal complexes of multidentate ligands to assemble novel topological architectures. We report here the hydrothermal synthesis and crystal structure of the title complex, $[Nd(SSA)(H_2O)]_n$, (I).

The unit cell of (I) is composed of one Nd^{III} cation, one sulfosalicylate trianion and one water molecule. Each eight-coordinate Nd^{III} ion is bonded to one water molecule, two sulfonate O atoms, three carboxylate O atoms and two hydroxy O atoms from five different SSA ligands in a dodecahedral geometry [Nd—O = 2.405 (4)–2.612 (4) Å, Nd—O*W*1 = 2.441 (4) Å and O—Nd—O = 50.86 (13)–167.00 (15)°].



(I)

As shown in Fig. 1, one carboxylate group, one hydroxy group and the Nd^{III} ion form a six-membered ring. The closest Nd···Nd separation is 3.983 (5) Å, comparable with reported Nd···Nd distances (Zhang *et al.*, 2003; Wan *et al.*, 2003; Legendziewicz *et al.*, 1999), indicating a lack of direct metal–metal interaction. Each pair of adjacent Nd1 and $Nd1^i$ atoms is bridged by a pair of hydroxy groups in a μ_2-bridging coordination mode. Each pair of adjacent $Nd1^i$ and $Nd1^v$ atoms is bridged by a pair of carboxylate groups in a tridentate chelating–bridging coordination mode [symmetry codes: (i) $-x, -y, -z$; (v) $1 + x, y, z$]. Adjacent atom pairs $Nd1/Nd1^i$ and $Nd1^i/Nd1^v$ [separations of 3.983 (5) and 4.132 (5) Å, respectively] are linked alternately into covalent chains running along the *a* axis. These one-dimensional covalent chains are further interconnected, *via* a pair of sulfonate groups in the bidentate bridging coordination mode, into two-dimensional covalent networks parallel to the *ab* plane. These two-dimensional layers are further integrated by SSA ligands into a three-dimensional framework, as shown in Fig. 2.

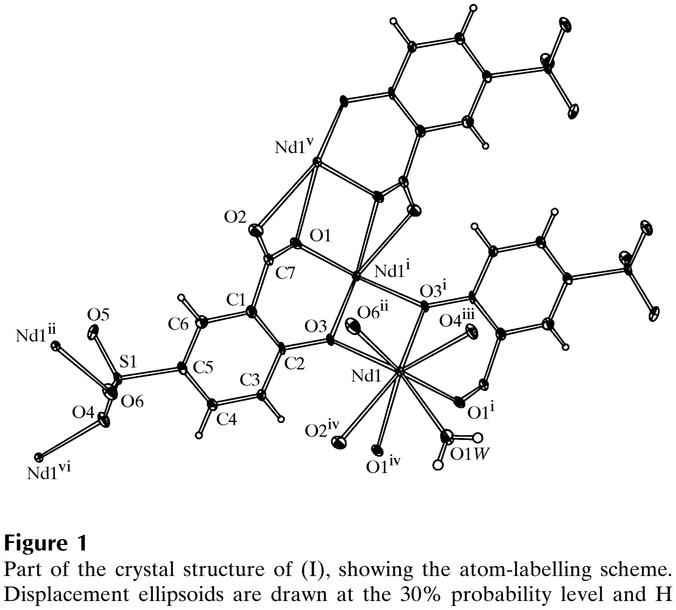


Figure 1
Part of the crystal structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry codes: (i) $-x, -y, -z$; (ii) $-x, -y, -1 - z$; (iii) $x, 1 + y, 1 + z$; (iv) $x - 1, y, z$; (v) $1 + x, y, z$; (vi) $x, y - 1, z - 1$.]

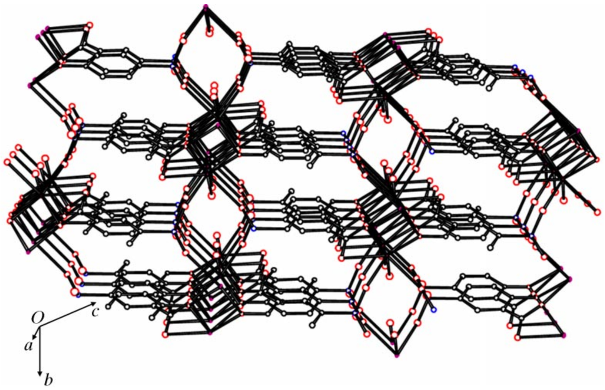


Figure 2
The packing structure of (I), viewed along [100]. H atoms have been omitted for clarity.

It is worth noting that the 5-sulfosalicylic acid ligand is completely deprotonated in (I), behaving as a μ_5-bridging ligand and linking five individual but symmetry-equivalent Nd atoms. In the three-dimensional framework, all the chelating units of SSA participate efficiently in the bonding to Nd atoms; the carboxylate group adopts a tridentate chelating–bridging mode connecting two Nd atoms, the hydroxy group acts as a μ_2-bridge and the sulfonate group adopts a bidentate bridging mode bridging two Nd atoms.

Experimental

A mixture of Nd_2O_3 (0.084 g, 0.25 mmol), 5-sulfosalicylic acid (0.110 g, 0.5 mmol) and NaOH (0.008 g, 0.2 mmol) in H_2O (16 ml) was sealed in a 25 ml Teflon-lined stainless steel vessel and heated to 433 K for 72 h. After the reaction, the vessel was cooled slowly to room temperature and purple crystals of (I) were obtained.

Crystal data

$[Nd(C_7H_3O_6S)(H_2O)]$
$M_r = 377.41$
Triclinic, $P\overline{1}$
$a = 6.0553$ (2) Å
$b = 8.2433$ (3) Å
$c = 9.96940$ (10) Å
$\alpha = 111.733$ (2)°
$\beta = 94.984$ (2)°
$\gamma = 93.813$ (2)°
$V = 457.88$ (2) Å^3
$Z = 2$
$D_x = 2.737$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2164 reflections
$\theta = 2.2$–25.0°
$\mu = 5.92$ mm^{-1}
$T = 293$ (2) K
Rhombus, purple
0.30 × 0.16 × 0.12 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.334$, $T_{\max} = 0.492$
2425 measured reflections
1621 independent reflections
1538 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.024$
$\theta_{\max} = 25.0°$
$h = -7 \rightarrow 7$
$k = -8 \rightarrow 9$
$l = -11 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.079$
$S = 1.08$
1595 reflections
151 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 2.194P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.003$
$\Delta\rho_{\max} = 1.17$ e Å^{-3}
$\Delta\rho_{\min} = -1.30$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Nd1—O1$^{\rm i}$	2.405 (4)	Nd1—O4$^{\rm iii}$	2.481 (4)
Nd1—O3	2.407 (4)	Nd1—O1$^{\rm iv}$	2.488 (4)
Nd1—O3$^{\rm i}$	2.431 (4)	Nd1—O2$^{\rm iv}$	2.612 (4)
Nd1—O1*W*	2.441 (4)	Nd1—Nd1$^{\rm i}$	3.9835 (5)
Nd1—O6$^{\rm ii}$	2.453 (4)		
O1$^{\rm i}$—Nd1—O3	108.83 (14)	O1*W*—Nd1—O1$^{\rm iv}$	74.32 (16)
O1$^{\rm i}$—Nd1—O3$^{\rm i}$	70.46 (13)	O6$^{\rm ii}$—Nd1—O1$^{\rm iv}$	127.74 (14)
O3—Nd1—O3$^{\rm i}$	69.15 (14)	O4$^{\rm iii}$—Nd1—O1$^{\rm iv}$	140.28 (15)
O1$^{\rm i}$—Nd1—O1*W*	74.01 (17)	O1$^{\rm i}$—Nd1—O2$^{\rm iv}$	111.66 (13)
O3—Nd1—O1*W*	154.36 (15)	O3—Nd1—O2$^{\rm iv}$	86.44 (14)
O3$^{\rm i}$—Nd1—O1*W*	132.59 (15)	O3$^{\rm i}$—Nd1—O2$^{\rm iv}$	154.09 (14)
O1$^{\rm i}$—Nd1—O6$^{\rm ii}$	167.00 (15)	O1*W*—Nd1—O2$^{\rm iv}$	69.45 (15)
O3—Nd1—O6$^{\rm ii}$	78.23 (15)	O6$^{\rm ii}$—Nd1—O2$^{\rm iv}$	79.14 (14)
O3$^{\rm i}$—Nd1—O6$^{\rm ii}$	103.20 (15)	O4$^{\rm iii}$—Nd1—O2$^{\rm iv}$	128.60 (14)
O1*W*—Nd1—O6$^{\rm ii}$	104.56 (18)	O1$^{\rm iv}$—Nd1—O2$^{\rm iv}$	50.86 (13)
O1$^{\rm i}$—Nd1—O4$^{\rm iii}$	87.13 (14)	O1$^{\rm i}$—Nd1—C7$^{\rm iv}$	87.63 (14)
O3—Nd1—O4$^{\rm iii}$	133.73 (14)	O3—Nd1—C7$^{\rm iv}$	87.01 (14)
O3$^{\rm i}$—Nd1—O4$^{\rm iii}$	76.71 (14)	O3$^{\rm i}$—Nd1—C7$^{\rm iv}$	139.00 (15)
O1*W*—Nd1—O4$^{\rm iii}$	71.10 (16)	O1*W*—Nd1—C7$^{\rm iv}$	67.48 (16)
O6$^{\rm ii}$—Nd1—O4$^{\rm iii}$	80.28 (15)	O6$^{\rm ii}$—Nd1—C7$^{\rm iv}$	103.88 (15)
O1$^{\rm i}$—Nd1—O1$^{\rm iv}$	64.78 (15)	O4$^{\rm iii}$—Nd1—C7$^{\rm iv}$	138.08 (16)
O3—Nd1—O1$^{\rm iv}$	83.85 (14)	O1$^{\rm iv}$—Nd1—C7$^{\rm iv}$	25.89 (15)
O3$^{\rm i}$—Nd1—O1$^{\rm iv}$	115.38 (13)	O2$^{\rm iv}$—Nd1—C7$^{\rm iv}$	25.17 (15)

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

H atoms bonded to C atoms were positioned geometrically (C—H = 0.93 Å) and allowed to ride on their parent C atoms before the final refinement cycle, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The water H atoms were located in difference maps, with O—H distances restrained to 0.82 (2) Å, and refined as riding, with $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm O})$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *XPREP* in *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: HJ1019). Services for accessing these data are described at the back of the journal.

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