

Poly[bis[aquaneodymium(III)]- μ_2 -oxalato-di- μ_4 -succinato]

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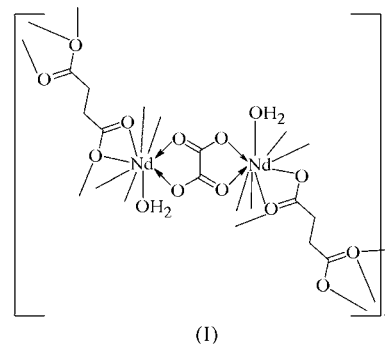
In the title compound, $[\text{Nd}_2(\text{C}_4\text{H}_4\text{O}_4)_2(\text{C}_2\text{O}_4)(\text{H}_2\text{O})_2]_n$, the flexible succinate anion assumes the *gauche* conformation and bridges the nine-coordinate Nd atoms to generate two-dimensional layers parallel to (010). The coordination polymer layers are linked into a three-dimensional framework by the rigid oxalate ligands. The oxalate ions are located on a center of inversion.

Comment

Great effort has been devoted to the design and synthesis of functional materials, an area of intense activity and tremendous potential significance (Bradshaw *et al.*, 2005; Kitagawa *et al.*, 2004; Rao *et al.*, 2004). Weak intermolecular forces, such as hydrogen bonding, π - π stacking, dipole-dipole attractions and van der Waals interactions, have been studied in depth and can be used in the design of molecular solids with specific supramolecular structures and functions (Fujita *et al.*, 2005; Noveron *et al.*, 2002; Bourne *et al.*, 2001). The self-assemblies of supramolecular complexes can be achieved by controlling the noncovalent interactions among the ligands, which are, in most cases, organic groups (Hunks *et al.*, 2002; Braga *et al.*, 2000)

Utilization of rigid aromatic dicarboxylate ligands has become an interesting strategy for constructing neutral nanoporous coordination polymers (Serre *et al.*, 2002; Li *et al.*, 1999; Chui *et al.*, 1999). Unlike the rigid dicarboxylate spacer ligands, saturated aliphatic dicarboxylate ligands exhibit conformational and coordination versatility due to their single-bonded carbon chains, which are viewed as important flexible spacer ligands. Under mild ambient and hydrothermal conditions, self-assembly of metal cations with α,ω -dicarboxylate anions such as succinate afforded a variety of supramolecular motifs, where the discrete metal-oxygen polyhedra could be interconnected by organic linkers into polymeric layers and three-dimensional frameworks. Unfortunately, such three-dimensional frameworks exhibit normally little porosity (Zhang *et al.*, 2006; Guillou *et al.*, 2003; Forster & Cheetham, 2002). To overcome this problem, our recent

research has been intensively focused on simultaneous utilization of rigid dicarboxylate and flexible α,ω -dicarboxylate ligands to construct coordination polymers. We report here a novel lanthanide coordination polymer, $[\text{Nd}_2(\text{C}_4\text{H}_4\text{O}_4)_2(\text{C}_2\text{O}_4)(\text{H}_2\text{O})_2]_n$ (I), containing oxalate ligands, one of the simplest rigid dicarboxylate ligands, and flexible succinate ligands.



In (I), the Nd atoms are bridged by flexible succinate ligands to generate two-dimensional layers, which are pillared by rigid oxalate ligands into higher-dimensional frameworks. As shown in Fig. 1, the asymmetric unit consists of one Nd^{3+} cation, one succinate anion, one-half of an oxalate anion and one aqua ligand. The Nd atoms are each coordinated by nine O atoms of five succinate anions, one oxalate anion and one aqua ligand to complete a distorted tricapped trigonal-prismatic geometry. The succinate anions assume a *gauche* conformation, in which both carboxylate groups function similarly; each carboxylate group chelates one Nd atom, with one O atom (O1 and O4) additionally bonded to another Nd atom. The $\text{Nd1}^{\text{iii}}-\text{O4}$ bond distance is 2.925 (5) Å (symmetry code as in Table 1); however, the other $\text{Nd1}-\text{O}$ bond distances range from 2.372 (5) to 2.580 (5) Å, which means that only very weak coordination interactions exist between atoms O4 and Nd1^{iii} . Through the terminal carboxylate bridging interactions, the polyhedra are edged-shared to generate metal-oxygen chains extending infinitely along the [001] direction, in which the adjacent $\text{Nd}\cdots\text{Nd}$ distances are 4.447 (2) and 4.190 (1) Å. Along the [100] direction, the chains are linked by the *gauche* succinate anions into layers parallel

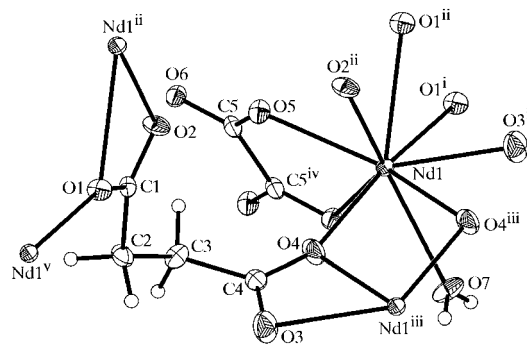


Figure 1
The structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry codes: (i) $x + 1, y, z + 1$; (ii) $-x + 1, -y, -z$; (iii) $-x + 2, -y, -z$; (iv) $-x + 2, -x + 2, -y + 1, -z + 1$; (v) $x - 1, y, z - 1$.]

to (010) (Fig. 2). Both lengths and angles within the succinate anions exhibit normal values (Seguaini *et al.*, 2004). The oxalate ions are located on a center of inversion and act as double bidentate (tetradentate) ligands in a linear chain that connects two Nd atoms in two different layers to form a three-dimensional framework (Fig. 3). The aqua ligands donate H atoms to carboxylate atoms O2 and O5 to form hydrogen bonds (Table 2), which make a significant contribution to the stabilization of the crystal structure.

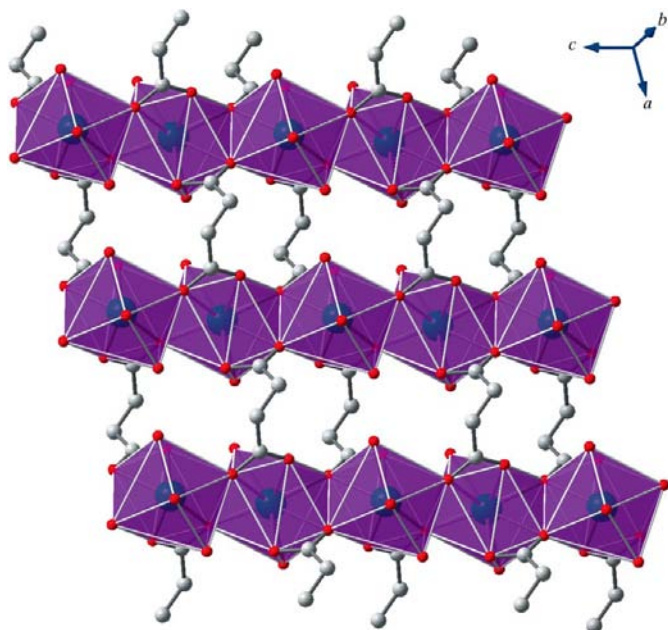


Figure 2
The two-dimensional layer structure formed by the connectivity between Nd atoms and succinate ligands in the title compound. H atoms attached to C atoms have been omitted for clarity.

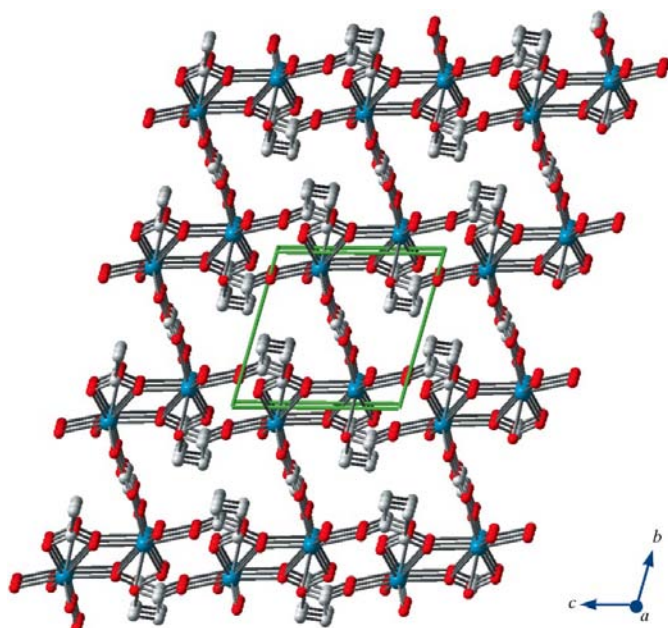


Figure 3
The three-dimensional framework of the title compound.

Experimental

A mixture of $\text{NdCl}_3 \cdot 6\text{H}_2\text{O}$ (1.00 mmol, 0.36 g), oxalic acid (0.50 mmol, 0.05 g), succinic acid (0.50 mmol, 0.06 g), NaOH (2.00 mmol, 0.08 g) and water (10.0 ml) was heated in a 23 ml stainless steel reactor with a Teflon liner at 443 K for 48 h. The orange plate-like crystals which formed were filtered off and washed with water and acetone (yield 46% based on Nd).

Crystal data

$[\text{Nd}_2(\text{C}_4\text{H}_4\text{O}_4)_2(\text{C}_2\text{O}_4)(\text{H}_2\text{O})_2]$	$\gamma = 101.422 (1)^\circ$
$M_r = 322.34$	$V = 385.23 (4) \text{ \AA}^3$
Triclinic, $P\bar{1}$	$Z = 2$
$a = 6.8792 (4) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 7.6203 (5) \text{ \AA}$	$\mu = 6.74 \text{ mm}^{-1}$
$c = 8.0401 (5) \text{ \AA}$	$T = 291 (2) \text{ K}$
$\alpha = 102.281 (2)^\circ$	$0.23 \times 0.17 \times 0.06 \text{ mm}$
$\beta = 104.125 (1)^\circ$	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	2232 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	1572 independent reflections
$T_{\min} = 0.259, T_{\max} = 0.662$	1487 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$	119 parameters
$wR(F^2) = 0.113$	H-atom parameters constrained
$S = 1.10$	$\Delta\rho_{\text{max}} = 0.40 \text{ e \AA}^{-3}$
1572 reflections	$\Delta\rho_{\text{min}} = -0.85 \text{ e \AA}^{-3}$

Table 1

Selected bond lengths (\AA).

Nd1—O1 ⁱ	2.443 (4)	Nd1—O4 ⁱⁱⁱ	2.925 (5)
Nd1—O1 ⁱⁱ	2.580 (5)	Nd1—O5	2.498 (4)
Nd1—O2 ⁱⁱⁱ	2.523 (5)	Nd1—O6 ^{iv}	2.449 (5)
Nd1—O3 ⁱⁱⁱ	2.469 (5)	Nd1—O7	2.460 (5)
Nd1—O4	2.372 (5)		

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

Table 2

Hydrogen-bond geometry ($\text{ \AA}, ^\circ$).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
$\text{O7---H7A}\cdots\text{O2}^{\text{vi}}$	0.85	1.90	2.745 (6)	177
$\text{O7---H7B}\cdots\text{O5}^{\text{vi}}$	0.85	2.00	2.777 (6)	151

Symmetry code: (vi) $x + 1, y, z$.

H atoms attached to C atoms were included at calculated positions and treated as riding atoms [$\text{C---H} = 0.97 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$]. The water H atoms were found in a difference map, relocated in idealized positions ($\text{O---H} = 0.85 \text{ \AA}$) and refined as riding atoms [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$].

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2004); 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: SK3164). Services for accessing these data are described at the back of the journal.

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