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Poly[di-μ_4-1,4-benzenedicarboxylato-μ_6-succinato-dineodymium(III)]

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The title compound, $[Nd_2(C_4H_4O_4)(C_8H_4O_4)_2]_n$, was synthesized by hydrothermal synthesis. The Nd atom is coordinated by four O atoms from four 1,4-benzenedicarboxylate ligands and four O atoms from three succinate anions, in a distorted square-antiprismatic coordination geometry. The antiprisms are bridged by the 1,4-benzenedicarboxylate and succinate ligands, forming a three-dimensional network. The succinate ion is located on a centre of inversion.

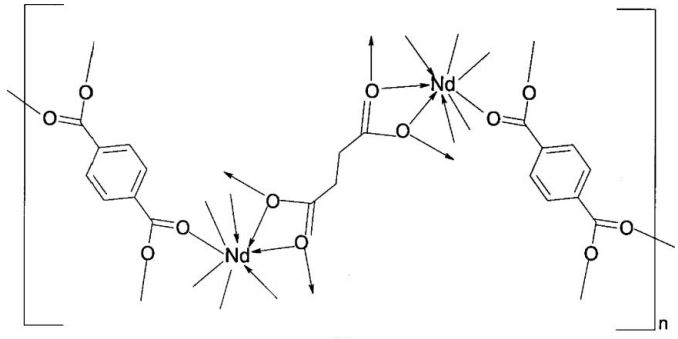
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.024
wR factor = 0.081
Data-to-parameter ratio = 16.6

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

Comment

The title compound, (I), is isostructural with its $[M_2(C_4H_4O_4)(C_8H_4O_4)_2]_n$ [M = Gd (Wang & Li, 2005) or Dy (Li & Wang, 2005)] analogues. As illustrated in Fig. 1, the Nd atom possesses square-antiprismatic coordination geometry (Table 1), in which the Nd—O bond distances range from 2.3306 (18) to 2.6225 (17) Å, with an average bond distance of 2.464 Å, similar to those found in the previously reported isostructural complexes.



(I)

In (I), the succinate ligand is located on an inversion centre and functions as an octadentate ligand, bis-chelating two Nd atoms with each O atom bridging to another Nd atom. In this mode, the Nd atoms are linked into a two-dimensional polymeric sheet parallel to the *ab* plane. These sheets are in turn bridged *via* 1,4-benzenedicarboxylate ligands, forming a three-dimensional framework.

Experimental

A mixture of $NdCl_3{\cdot}6H_2O$ (1.00 mmol, 0.36 g), 1,4-benzenedicarboxylic acid (0.55 mmol, 0.09 g), succinic acid (0.51 mmol, 0.06 g), NaOH (2.00 mmol, 0.08 g) and H_2O (10.0 ml) was heated in a 23 ml stainless steel reactor with a Teflon liner at 443 K for 48 h. The resulting red column-like crystals of (I) were filtered off and washed with water and acetone. Yield: 43% based on Nd.

Crystal data

$[Nd_2(C_4H_4O_4)(C_8H_4O_4)_2]$
M_r = 732.78
Orthorhombic, *Pbca*
a = 14.0586 (3) Å
b = 6.9445 (1) Å
c = 21.9664 (5) Å
V = 2144.58 (7) Å^3
Z = 4
D_x = 2.270 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 512 reflections
θ = 3.3–26.7°
μ = 4.86 mm^{-1}
T = 292 (2) K
Column, red
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.385, T_{max} = 0.422
12052 measured reflections
2579 independent reflections
2433 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 28.0°
$h = -18 \rightarrow 17$
$k = -9 \rightarrow 9$
$l = -25 \rightarrow 28$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.081
S = 1.01
2579 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0672P)^2 + 1.0685P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0076 (3)

Table 1
Selected bond lengths (Å).

Nd—O1	2.3858 (18)	Nd—O5	2.6225 (17)
Nd—O2^{i}	2.3306 (18)	Nd—O5^{iv}	2.521 (2)
Nd—O3^{ii}	2.4042 (19)	Nd—O6	2.5639 (19)
Nd—O4^{iii}	2.3931 (18)	Nd—O6^{v}	2.486 (3)

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x+\frac{3}{2}, -y+1, z+\frac{1}{2}$; (iv) $-x+\frac{3}{2}, y-\frac{1}{2}, z$; (v) $-x+\frac{3}{2}, y+\frac{1}{2}, z$.

H atoms were included in calculated positions and treated as riding atoms, with C—H distances of 0.93–0.97 Å and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (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*.

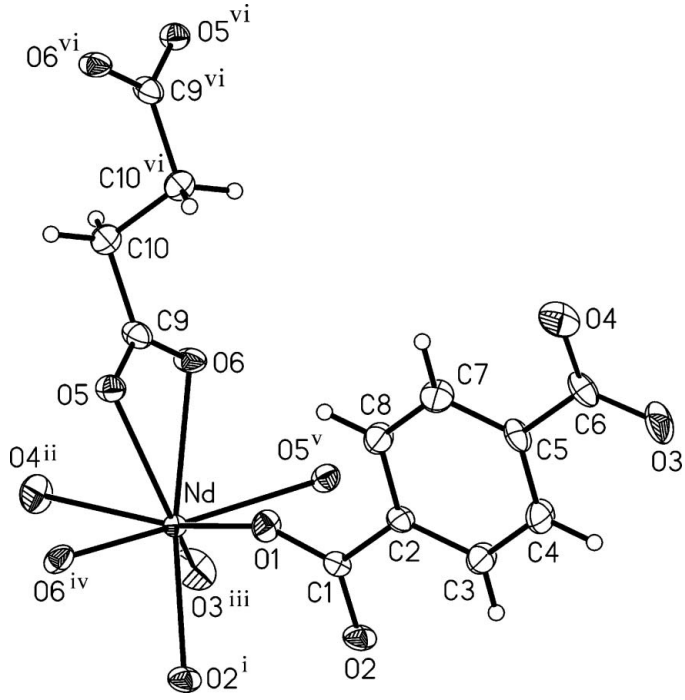


Figure 1
The coordination environment of the Nd atom of (I), with the atom-numbering scheme, showing displacement ellipsoids at the 45% probability level. [Symmetry codes: (i) $2-x, 1-y, 1-z$; (ii) $x, \frac{1}{2}-y, \frac{1}{2}+z$; (iii) $\frac{3}{2}-x, 1-y, \frac{1}{2}+z$; (iv) $\frac{3}{2}-x, y-\frac{1}{2}, z$; (v) $\frac{3}{2}-x, y+\frac{1}{2}, z$; (vi) $1-x, 1-y, 1-z$.]

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