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Poly[diaqua-μ_6-succinato-di-μ_5-succinato-dineodymium(III)]

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The title compound, $[Nd_2(C_4H_4O_4)_3(H_2O)_2]_n$, has been synthesized under hydrothermal conditions. The asymmetric unit consists of two Nd^{3+} cations, three succinate anions and two aqua ligands. The coordination polyhedron around each Nd atom is a tricapped trigonal prism; the prisms are bridged into a three-dimensional network by succinate ligands. The succinate ligands exhibit *gauche* and *anti* conformations with different coordination modes.

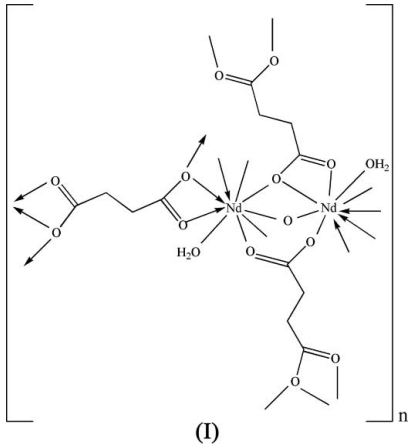
Key indicators

Single-crystal X-ray study
T = 290 K
Mean σ(C–C) = 0.003 Å
R factor = 0.014
wR factor = 0.037
Data-to-parameter ratio = 13.9

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 Ce (Seguatni *et al.*, 2004) and Dy (Wang *et al.*, 2006) analogues. The asymmetric unit consists of two Nd^{3+} cations, three succinate anions and two aqua ligands (Fig. 1). The Nd atoms are each coordinated by nine O atoms of six succinate anions and one aqua ligand, forming a tricapped trigonal prism, in which the Nd—O bond distances range from 2.4059 (17) to 2.6091 (17) Å, with an average of 2.500 Å (Table 1). The polyhedra are edge-shared, generating one-dimensional infinite chains along the [100] direction. They are further linked by the *gauche* succinate ligands into layers along [001] and parallel to (010). The tetradentate *anti* succinate anions form pillars, resulting in a three-dimensional framework. The aqua ligands further stabilize the structure through extensive O—H···O hydrogen-bonding interactions (Table 2).



(I)

Experimental

A mixture of $NdCl_3{\cdot}6H_2O$ (1.00 mmol, 0.38 g), succinic acid (1.00 mmol, 0.12 g), NaOH (2.00 ml, 1 *M*) and water (10.0 ml) was heated in a 23 ml stainless steel reactor with a Teflon liner at 443 K for 24 h. After the vessel was cooled to room temperature, a small number of orange block-like crystals were separated by filtration.

Crystal data

$[Nd_2(C_4H_4O_4)_3(H_2O)_2]$
M_r = 672.73
Triclinic, $P\overline{1}$
a = 7.843 (1) Å
b = 8.111 (1) Å
c = 14.218 (3) Å
α = 96.987 (4)°
β = 97.015 (4)°
γ = 103.514 (4)°
V = 862.2 (2) Å^3
Z = 2
D_x = 2.591 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 6.03 mm^{-1}
T = 290 (2) K
Block, orange
0.18 × 0.11 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.438, T_{max} = 0.646
5015 measured reflections
3521 independent reflections
3226 reflections with $I > 2\sigma(I)$
R_{int} = 0.009
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.014
$wR(F^2)$ = 0.037
S = 1.05
3521 reflections
254 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0189P)^2 + 0.6339P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0087 (13)

Table 1
Selected bond lengths (Å).

Nd1—O1	2.4375 (16)	Nd2—O1	2.6091 (17)
Nd1—O4^{i}	2.5163 (17)	Nd2—O2	2.5161 (18)
Nd1—O6	2.4059 (17)	Nd2—O3^{iv}	2.4078 (17)
Nd1—O7^{ii}	2.5591 (17)	Nd2—O5	2.4602 (17)
Nd1—O8^{ii}	2.5158 (18)	Nd2—O7^{ii}	2.4645 (17)
Nd1—O9	2.5441 (17)	Nd2—O9^{v}	2.4691 (17)
Nd1—O10	2.5063 (19)	Nd2—O11^{vi}	2.5200 (19)
Nd1—O12^{iii}	2.4994 (17)	Nd2—O12^{vi}	2.5948 (17)
Nd1—O13	2.5108 (19)	Nd2—O14	2.4699 (18)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O13—H13A···O5^{vii}	0.82	2.04	2.845 (3)	169
O13—H13B···O8^{vii}	0.82	2.38	2.917 (5)	124
O14—H14A···O2^{iv}	0.82	1.91	2.731 (4)	173
O14—H14B···O4^{i}	0.82	2.06	2.868 (4)	169

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

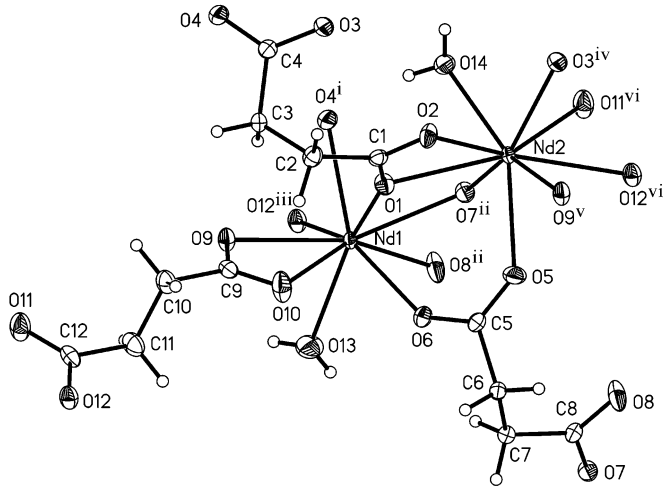


Figure 1
A part of the polymeric structure of the title compound, showing 45% probability displacement ellipsoids for non-H atoms. [Symmetry code: (i) $1-x, 1-y, 1-z$; (ii) $2-x, 1-y, 2-z$; (iii) $x, y-1, z$; (iv) $2-x, 1-y, 1-z$; (v) $1+x, y, z$; (vi) $1+x, y-1, z$.]

H atoms of the methylene groups were included at calculated positions and treated as riding with C—H distances constrained to 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C). The water H atoms were found in a difference map and then treated as riding atoms, with O—H distances of 0.82 Å and U_{iso}(H) = 0.05 Å^2.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 1998); software used to prepare material for publication: *SHELXTL*.

References

Bruker (1998). *SMART* (Version 5.16), *SAINT* (Version 6.01) and *SHELXTL* (Version 6.14). Bruker AXS Inc., Madison, Wisconsin, USA.
Seguatni, A., Fakhfakh, M., Vaauley, M. J. & Jouini, N. (2004). *J. Solid State Chem.* **177**, 3402–3410.
Sheldrick, G. M. (1996). *SADABS*. Version 2.01. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wang, C.-X., Li, Y., Zhang, Q.-H., Cai, D.-J. & Xie, X.-B. (2006). *Acta Cryst.* E**62**, m545–m547.