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Diaquatris(4-pyridylcarboxylato)neodymium(III)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.029
wR factor = 0.074
Data-to-parameter ratio = 10.7

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

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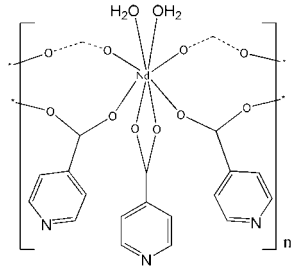
The isonicotinate (4-pyridylcarboxylate) ligand was used to synthesize the title compound, $[Nd(C_6H_4NO_2)_3(H_2O)_2]$. It has a one-dimensional chain structure. The Nd atom lies on a crystallographic twofold axis. The Nd^{III} center is in an infinite chain, coordinated by four carboxylate O atoms of bridging isonicotinate groups, two carboxylate O atoms of the chelating isonicotinate group, and two water molecules. Weak interactions between pyridine H and N atoms generate a three-dimensional framework.

Comment

There has been intense interest in the synthesis and construction of lanthanide complexes with carboxylate ligands, owing to their potential application as luminescent sensor materials in biological devices (Choppin & Bünzli, 1989), and numerous lanthanide complexes have been studied (Bünzli & Piguet, 2002). Most of them have been found to possess a variety of dimeric or infinite chain structures in which the carboxylate groups act as bridges between metal atoms (Pan *et al.*, 2000). In this context, we have attempted to construct neutral lanthanide coordination polymers using the anionic bifunctional isonicotinate linking group, with the aim of obtaining a three-dimensional framework and functional solid based on molecular building blocks by both metal–ligand coordination and hydrogen-bond interactions.



(I)

The title compound, (I), crystallizes in the monoclinic space group $P2_1/c$. This compound has a one-dimensional, infinite zigzag chain structure along the *a*-axis direction, with a double carboxylate bridge. The Nd metal center lies on a crystallographic twofold axis. At each metal center, there is a chelating carboxylate group. There are also two water molecules bound to the metal center, giving eight-coordination. The Nd center is coordinated by four carboxylate O atoms of bridging isonicotinate groups [O3, $O4^{i}$, O5 and $O6^{ii}$; symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x+1, -y+1, -z$], two carboxylate O atoms of the chelating isonicotinate group (O1 and O2), and two water molecules (O1*W* and O2*W*). The Nd center has a distorted dodecahedral coordination geometry,

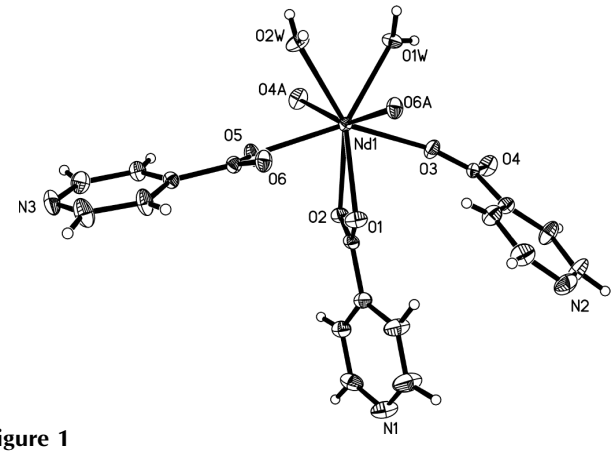


Figure 1
View of compound (I), showing the atom-labelling scheme. H atoms are represented by circles of arbitrary size. Ellipsoids are drawn at the 30% probability level.

with O—Nd—O angles ranging from 50.51 (10) to 154.96 (13)° (Table 1). The distances between adjacent Nd atoms are 4.7339 (10) and 4.8254 (11) Å. There are O—H···N interactions between pyridyl N atoms and coordinated water O atoms (O1*W*—H1*WB*···N3^{iii} and O2*W*—H2*WB*···N2^{iv}; symmetry codes: (iii) $1-x, -\frac{1}{2}+y, -\frac{1}{2}-z$; (iv) $x, y, -1+z$]. The interchain hydrogen bonds formed between pyridine N atoms of isonicotinate bridging groups and coordinated water molecules determine the assembly of the crystal structure. Hydrogen-bond interactions extend the one-dimensional chains into a three-dimensional framework.

Experimental

Sodium isonicotinate (4-pyridylcarboxylate) was prepared as follows: 20 mmol isonicotinate acid and 20 mmol sodium bicarbonate were mixed together in 20 ml water. The mixture was stirred at room temperature. After the reaction was completed, the solution was concentrated to obtain the sodium salt of the ligand. Neodymium(III) nitrate hexahydrate (1 mmol) and sodium isonicotinate (3 mmol) were mixed in water (10 ml). The solution was filtered, and purple single crystals of the title complex, (I), were obtained by evaporation of the solvent at room temperature.

Crystal data

$[Nd(C_6H_4NO_2)_3(H_2O)_2]$
M_r = 546.58
Monoclinic, $P2_1/c$
a = 9.526 (2) Å
b = 19.053 (4) Å
c = 10.787 (2) Å
β = 92.19 (3)°
V = 1956.4 (7) Å^3
Z = 4
D_x = 1.856 Mg m^{-3}
Mo Kα radiation
Cell parameters from 27 reflections
θ = 2.6–26.1°
μ = 2.71 mm^{-1}
T = 293 (2) K
Block, purple
0.40 × 0.37 × 0.22 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: ψ scan (*XCAD*4; Harms & Wocadlo, 1995)
T_{min} = 0.352, T_{max} = 0.551
3656 measured reflections
3441 independent reflections
2830 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 25.0°
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 22$
$l = -12 \rightarrow 12$
3 standard reflections
every 200 reflections
intensity decay: none

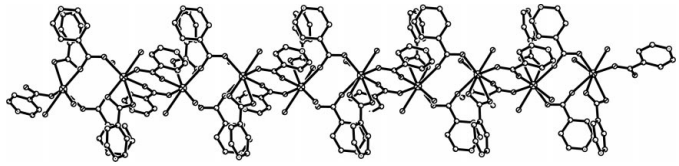


Figure 2
The infinite one-dimensional zigzag chain structure along the *a*-axis direction. H atoms bonded to C atoms have been omitted for clarity.

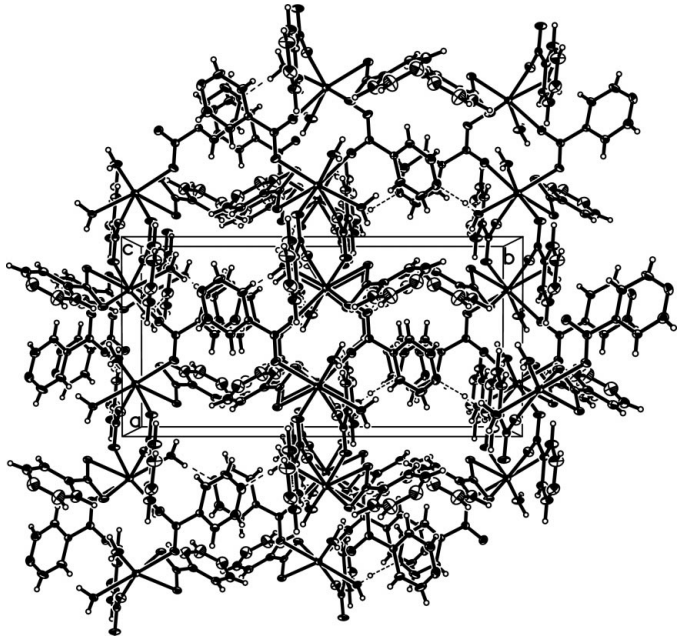


Figure 3
The molecular packing of (I), viewed along the *c* axis. Dashed lines indicate hydrogen-bonding interactions. Ellipsoids are drawn at the 30% probability level.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.074
S = 1.07
3441 reflections
323 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 1.6679P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −1.16 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Nd1—O6^{ii}	2.397 (3)	Nd1—O2*W*	2.480 (3)
Nd1—O4^{i}	2.406 (3)	Nd1—O1*W*	2.490 (3)
Nd1—O3	2.417 (3)	Nd1—O1	2.497 (3)
Nd1—O5	2.446 (3)	Nd1—O2	2.631 (3)
O6^{ii}—Nd1—O4^{i}	154.96 (13)	O2—C6—C1	121.1 (4)
O6^{ii}—Nd1—O3	84.14 (12)	O1—C6—C1	117.5 (4)
O4^{i}—Nd1—O3	105.38 (12)	O4—C12—O3	123.4 (4)
O6^{ii}—Nd1—O5	108.91 (11)	O4—C12—C7	117.6 (4)
O4^{i}—Nd1—O5	76.28 (12)	O3—C12—C7	118.9 (4)
O3—Nd1—O5	145.91 (12)	O6—C13—O5	123.9 (4)
O2*W*—Nd1—O1*W*	71.20 (11)	O6—C13—C14	119.4 (4)
O1—Nd1—O2	50.51 (10)	O5—C13—C14	116.6 (4)
O2—C6—O1	121.3 (4)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O2^{i}	0.81	2.01	2.782 (4)	160
O1W—H1WB···N3^{iii}	0.92	1.87	2.791 (5)	173
O2W—H2WA···O1^{ii}	0.84	1.94	2.746 (5)	162
O2W—H2WB···N2^{iv}	0.79	2.01	2.790 (6)	170

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

All the H atoms were located in a difference Fourier map and refined isotropically. The deepest hole is located 0.97 Å from Nd1.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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