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catena-Poly[[(2,2′-bipyridine)nickel(II)]-*μ*-4,4′-oxydibenzoato]

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean *σ*(C–C) = 0.004 Å
R factor = 0.046
wR factor = 0.098
Data-to-parameter ratio = 13.1

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

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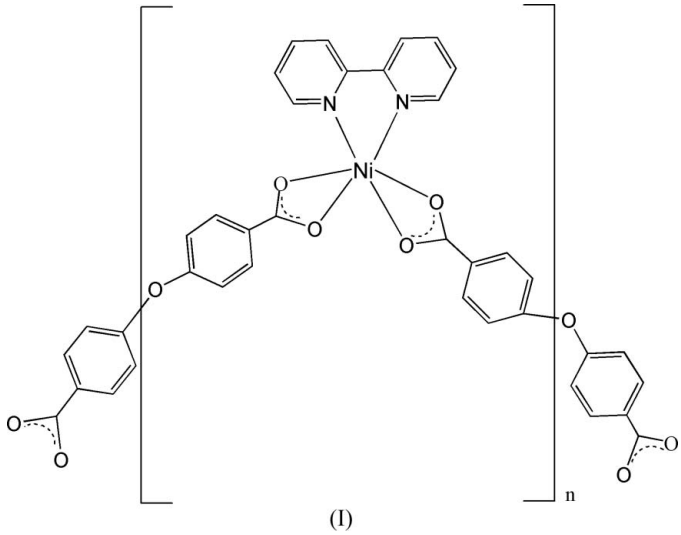
In the title compound, $[Ni(C_{14}H_8O_5)(C_{10}H_8N_2)]_n$, the Ni^{II} atom is coordinated by four O atoms of two 4,4′-oxydibenzoate (oba) dianions and two N atoms of a chelate 2,2′-bipyridine ligand to furnish a distorted octahedral coordination environment. The V-shaped oba dianion acts as a bridge between two Ni atoms to form a zigzag chain coordination polymer.

Comment

The versatility of the flexible ligand H_2oba (H_2oba is 4,4′-oxydibenzoic acid) is manifested by the interesting polymeric structures that it forms (Liu *et al.*, 2002; Skakle *et al.*, 2001; Wang *et al.*, 2004). In our previous work, the reaction of nickel(II) acetate, H_2oba and phen (phen is 1,10-phenanthroline) afforded polymeric $\{[Ni(phen)(oba)]\cdot 0.25H_2O\}_n$ (Xiao *et al.*, 2005). We used 2,2′-bipyridine (2,2′-bipy) in place of phen and obtained the title compound, (I).



(I)

In (I), the Ni^{II} atom is coordinated by four O atoms of two oba ligands and two N atoms of a chelate 2,2′-bipy ligand to furnish a distorted octahedral coordination environment (Fig. 1). The Ni^{II} atoms are linked by the oba ligands to form zigzag chains running along [201]. The 2,2′-bipy ligands protrude on both sides of the zigzag chain (Fig. 2). The dihedral angle between the planes of the two benzene rings of the oba dianion is 82.7 (1)°. The mean plane of the 2,2′-bipy ligand forms dihedral angles of 87.7 (1) and 94.1 (1)°, respectively, with the C12–C17 and C18–C23 benzene rings, indicating that the 2,2′-bipy plane is perpendicular to the two benzene rings of the oba ligand.

Experimental

The title compound was synthesized by the hydrothermal method from a mixture of 4,4′-oxybis(benzoic acid) (0.5 mmol), $Ni(CH_3COO)_2{\cdot}4H_2O$ (0.5 mmol), 2,2'-bipyridine (0.5 mmol) and water (8.0 ml) in a 15.0 ml Teflon-lined stainless steel reactor. The solution was heated at 423 K for four days. On completion of the reaction, the system was cooled slowly to room temperature, and green crystals were collected.

Crystal data

$[Ni(C_{14}H_8O_5)(C_{10}H_8N_2)]$
M_r = 471.10
Monoclinic, $P2_1/c$
a = 12.2223 (18) Å
b = 15.017 (2) Å
c = 11.3182 (16) Å
β = 92.026 (3)°
V = 2076.1 (5) Å^3
Z = 4
D_x = 1.507 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2159 reflections
θ = 2.3–22.3°
μ = 0.97 mm^{-1}
T = 298 (2) K
Block, green
0.19 × 0.16 × 0.14 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.837, T_{max} = 0.876
11 073 measured reflections
3792 independent reflections
3075 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 25.3°
$h = -13 \rightarrow 14$
$k = -13 \rightarrow 18$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.098
S = 1.06
3792 reflections
289 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 0.4839P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Extinction correction: none

Table 1
Selected geometric parameters (Å, °).

Ni1—N1	1.990 (2)	Ni1—O2	2.389 (2)
Ni1—N2	2.000 (2)	Ni1—O4^{i}	1.9885 (19)
Ni1—O1	1.993 (2)	Ni1—O5^{i}	2.418 (2)
N1—Ni1—N2	80.93 (10)	O4^{i}—Ni1—N1	163.29 (9)
N1—Ni1—O1	91.67 (9)	O4^{i}—Ni1—N2	97.19 (9)
N1—Ni1—O2	92.49 (8)	O4^{i}—Ni1—O1	96.44 (8)
N2—Ni1—O1	155.03 (8)	O4^{i}—Ni1—O2	104.22 (8)
N2—Ni1—O2	96.46 (8)	O5^{i}—Ni1—N1	105.02 (9)
O1—Ni1—O2	59.85 (8)	O5^{i}—Ni1—N2	98.02 (9)
O1—Ni1—O5^{i}	106.95 (8)	O4^{i}—Ni1—O5^{i}	58.63 (8)
O2—Ni1—O5^{i}	158.81 (7)		

Symmetry code: (i) $x+1, -y+\frac{1}{2}, z+\frac{1}{2}$.

H atoms were included in the refinement in calculated positions in the riding-model approximation [C—H = 0.93 Å and U_{iso}(H) = $1.2U_{eq}$(C)].

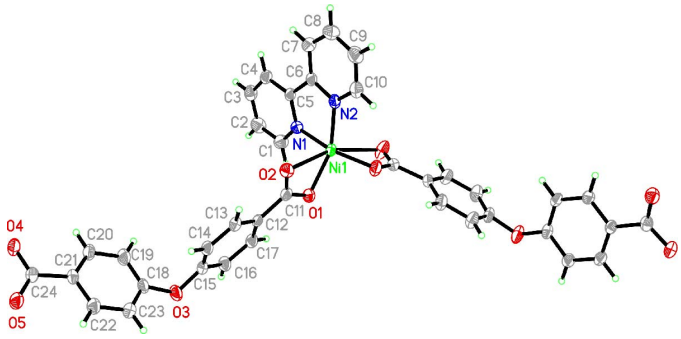


Figure 1
The coordination environment of atom Ni1 in (I), with the atom numbering, showing displacement ellipsoids at the 30% probability level.

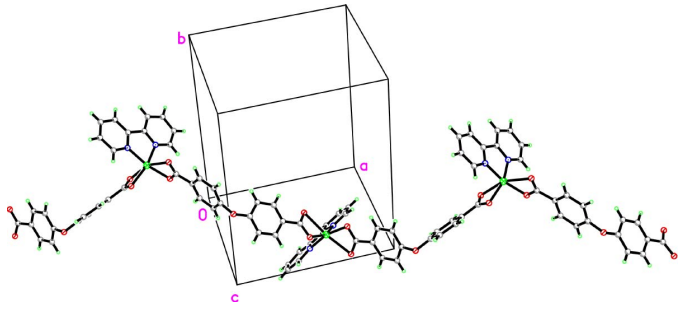


Figure 2
The zigzag chain of (I).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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