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## Key indicators

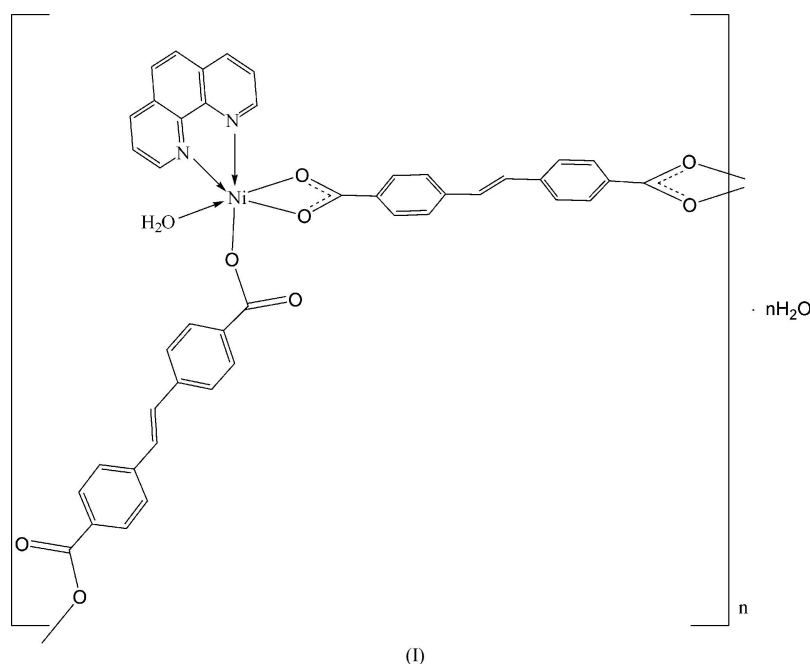
Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.042  
 $wR$  factor = 0.124  
Data-to-parameter ratio = 15.6For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Poly[[[aqua(1,10-phenanthroline- $\kappa^2N,N'$ )-  
nickel(II)]- $\mu_3$ -4,4'-(ethene-1,2-diyl)dibenzoato-  
 $\mu_2$ -4,4'-(ethene-1,2-diyl)dibenzoato] monohydrate]

In the title complex,  $\{[\text{Ni}(\text{C}_{16}\text{H}_{10}\text{O}_4)(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})] \cdot \text{H}_2\text{O}\}_n$ , the  $\text{Ni}^{\text{II}}$  ion is in a distorted octahedral geometry and coordinated by two N atoms of a 1,10-phenanthroline (phen) ligand, three carboxylate O atoms of two different bpea $^{2-}$  ligands and one water molecule. The  $[\text{Ni}(\text{phen})\text{H}_2\text{O}]$  units are connected by two different 4,4'-(ethene-1,2-diyl)dibenzoate (bpea $^{2-}$ ) bridges, forming a one-dimensional zigzag chain structure. One bpea $^{2-}$  ligand coordinates to Ni in a bis-monodentate fashion, while the other acts as a bis-bidentate chelate.

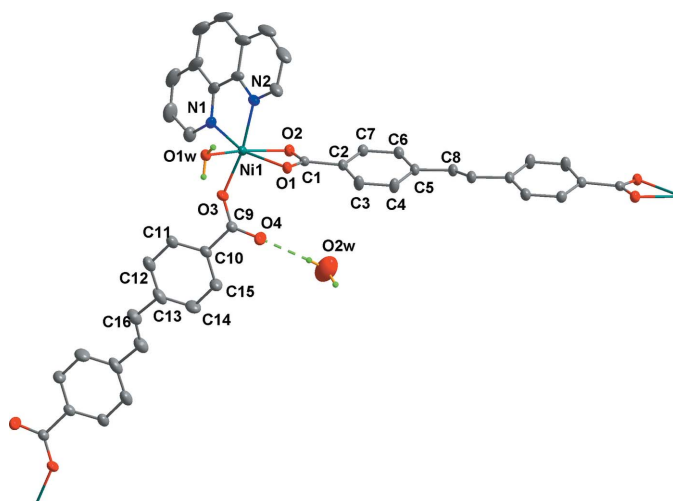
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## Comment

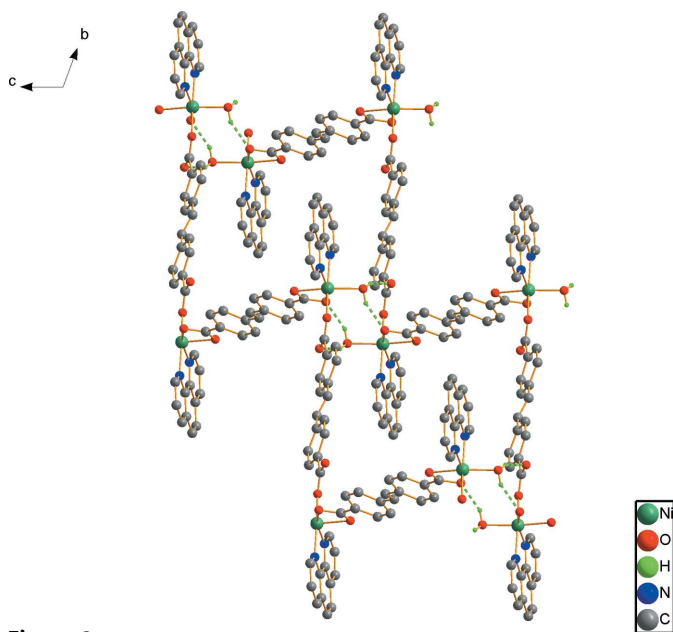
The construction of coordination polymers and networks by the self-assembly of organic ligands and metal ions is a rapidly growing area of research, not only because of their intriguing structural motifs, but also because of their promising technological applications (Evans & Lin, 2002).



Many new complexes have been synthesized using polycarboxylates combined with specific transition metal ions by introducing neutral  $N$ -heterocyclic ligands (He *et al.*, 2005). Recently, we have investigated the ligand 4,4'-(ethene-1,2-diyl)dibenzoate (bpea $^{2-}$ ), whose coordination chemistry, to the best of our knowledge, had not been investigated previously (Wang *et al.*, 2004, 2006). We report here the synthesis and structure of a new one-dimensional nickel complex,  $\{[\text{Ni}(\text{bpea})(\text{phen})(\text{H}_2\text{O})] \cdot \text{H}_2\text{O}\}_n$ , (I) (Fig. 1).


**Figure 1**

Part of the structure of (I), with displacement ellipsoids drawn at the 30% probability level and with a hydrogen bond shown as a dashed line. Unlabelled atoms are related to labelled atoms by the symmetry operations  $(-x, 1 - y, 2 - z)$  for C8 and  $(2 - x, -y, 1 - z)$  for C16. H atoms have been omitted except on water molecules.


**Figure 2**

Packing diagram for (I), with hydrogen bonds shown as dashed lines. H atoms have been omitted except on water molecules.

The complex is an infinite one-dimensional chain polymer with an Ni<sup>II</sup> ion, half each of two bpea<sup>2-</sup> ligands, a phen ligand, a coordinated water molecule and one uncoordinated water molecule in the asymmetric unit. The Ni<sup>II</sup> ion is coordinated by three carboxylate O atoms from two different bpea<sup>2-</sup> ligands, the two N atoms of a phen ligand, and one coordinated water molecule in a distorted octahedral geometry (Table 1). The uncoordinated water molecule forms a single hydrogen bond to the complex through atom O4 (Table 2). One bpea<sup>2-</sup> ligand coordinates to Ni in a bis-monodentate fashion, while the other acts as a bis-bidentate chelate, linking

the Ni<sup>II</sup> ions into a one-dimensional zigzag chain structure along  $(2\bar{1}1)$ . The chains are further interconnected through intermolecular hydrogen bonds, forming a two-dimensional supramolecular network (Table 2 and Fig. 2).

## Experimental

A mixture of NiCl<sub>2</sub>·6H<sub>2</sub>O (0.29 g, 1 mmol), phen (0.198 g, 1 mmol), H<sub>2</sub>bpea (0.268 g, 1 mmol) and water (10 ml) was stirred for 15 min in air, then transferred and sealed in a 23 ml Parr Teflon-lined stainless steel vessel, heated to 433 K for 5 d, and then cooled to room temperature. The resulting green crystals were filtered off, washed and dried in air. Analysis calculated for C<sub>28</sub>H<sub>22</sub>NiN<sub>2</sub>O<sub>6</sub>: C 62.14, H 4.10, N 5.18%; found: C 62.10, H 4.09, N 5.13%.

### Crystal data

[Ni(C<sub>16</sub>H<sub>10</sub>O<sub>4</sub>)(C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>)·(H<sub>2</sub>O)]·H<sub>2</sub>O  
*M<sub>r</sub>* = 541.19  
 Triclinic, *P* $\bar{1}$   
*a* = 10.055 (4) Å  
*b* = 11.476 (5) Å  
*c* = 11.793 (5) Å  
 $\alpha$  = 104.101 (19)°  
 $\beta$  = 103.065 (16)°

$\gamma$  = 107.632 (16)°  
*V* = 1189.8 (9) Å<sup>3</sup>  
*Z* = 2  
*D<sub>x</sub>* = 1.511 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 $\mu$  = 0.86 mm<sup>-1</sup>  
*T* = 295 (2) K  
 Block, green  
 0.36 × 0.25 × 0.15 mm

### Data collection

Rigaku R-Axis RAPID  
 diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan  
 (ABSCOR; Higashi, 1995)  
*T<sub>min</sub>* = 0.746, *T<sub>max</sub>* = 0.881

11792 measured reflections  
 5413 independent reflections  
 4576 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.020  
 $\theta_{\max}$  = 27.5°

### Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.042  
*wR* (*F*<sup>2</sup>) = 0.124  
*S* = 1.08  
 5413 reflections  
 346 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.078P)^2 + 0.3494P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 1.11 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.65 \text{ e } \text{Å}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Ni—O3	2.0254 (18)	Ni—N2	2.096 (2)
Ni—O1W	2.0499 (19)	Ni—O1	2.1090 (18)
Ni—N1	2.071 (2)	Ni—O2	2.1109 (18)
O3—Ni—O1W	85.52 (8)	N1—Ni—O1	160.00 (8)
O3—Ni—N1	90.86 (9)	N2—Ni—O1	88.47 (8)
O1W—Ni—N1	94.87 (8)	O3—Ni—O2	98.42 (7)
O3—Ni—N2	169.40 (8)	O1W—Ni—O2	163.75 (7)
O1W—Ni—N2	90.81 (8)	N1—Ni—O2	100.81 (8)
N1—Ni—N2	79.53 (9)	N2—Ni—O2	87.86 (8)
O3—Ni—O1	102.00 (7)	O1—Ni—O2	62.49 (6)
O1W—Ni—O1	101.29 (7)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1W-H1W1\cdots O4^i$	0.853 (10)	1.838 (14)	2.650 (3)	158 (2)
$O1W-H1W2\cdots O1^i$	0.844 (10)	1.941 (16)	2.706 (3)	150 (2)
$O2W-H2W1\cdots O4$	0.88 (7)	2.07 (7)	2.882 (5)	154 (6)

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

Water H atoms were located in a difference map and refined with O—H and H $\cdots$ H distance restraints of 0.85 (1) and 1.39 (1) Å, respectively, and with  $U_{iso}(H) = 1.5U_{eq}(O)$ . All other H atoms were placed in calculated positions, with C—H = 0.93 Å (aromatic) and  $U_{iso}(H) = 1.2U_{eq}(C)$ , and were refined in the riding-model approximation. The highest electron-density peak is located 0.94 (2) Å from atom C16.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:

*ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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