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Key indicators

Single-crystal X-ray study
 T = 295 K
 Mean $\sigma(C-C)$ = 0.007 Å
 R factor = 0.058
 wR factor = 0.101
 Data-to-parameter ratio = 12.2

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

catena-Poly[[[aquabis(1*H*-benzimidazole- κ N³)-nickel(II)]- μ -isophthalato- κ^2 O:O'] hemihydrate]

In the title polymeric complex, $[\text{Ni}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_7\text{H}_6\text{N}_2)_2(\text{H}_2\text{O})] \cdot 0.5\text{H}_2\text{O}$, the Ni^{II} atoms assume a distorted octahedral coordination geometry, formed by two isophthalate (ISOP) ions, two benzimidazole (BZIM) molecules and one water molecule. The ISOP dianions bridge the Ni^{II} atoms through terminal carboxy groups to form zigzag polymeric chains, which are linked to each other *via* hydrogen bonds. π - π stacking occurs between BZIM rings and between ISOP rings in the crystal structure.

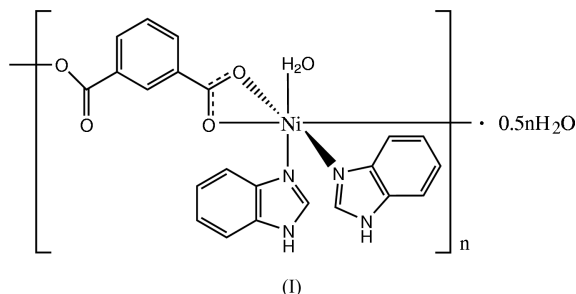
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Comment

As part of an investigation of aromatic stacking in metal complexes (Liu *et al.*, 2003; Su & Xu, 2004), the title polymeric Ni^{II} complex, (I), bridged by an isophthalate dianion (ISOP), incorporating benzimidazole (BZIM), has been prepared in the laboratory and its crystal structure is presented here.



The asymmetric unit of (I) contains two Ni^{II} complex units and one uncoordinated water molecule. Each Ni^{II} atom displays a similar coordination geometry, as shown in Fig. 1.

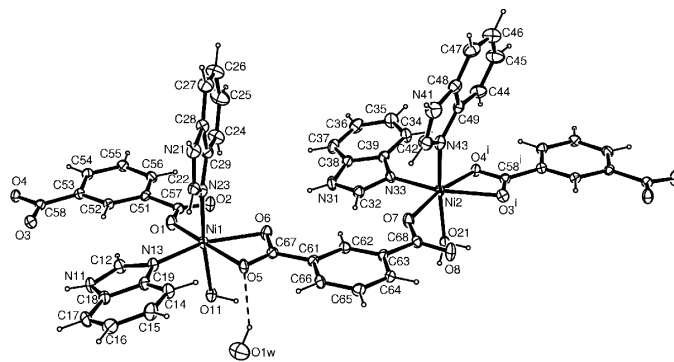
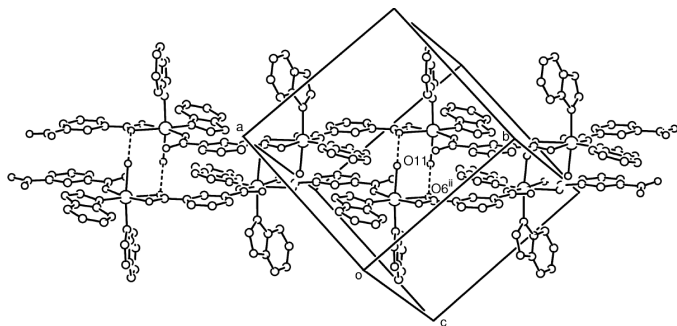


Figure 1
 Part of the polymeric structure of (I), with 30% probability displacement ellipsoids. The dashed line indicates a hydrogen bond. [Symmetry code: (i) 1 + x, -1 + y, z.]

**Figure 2**

The molecular packing, showing polymeric complex chains. [Symmetry code: (ii) $1 - x, 1 - y, 1 - z$.]

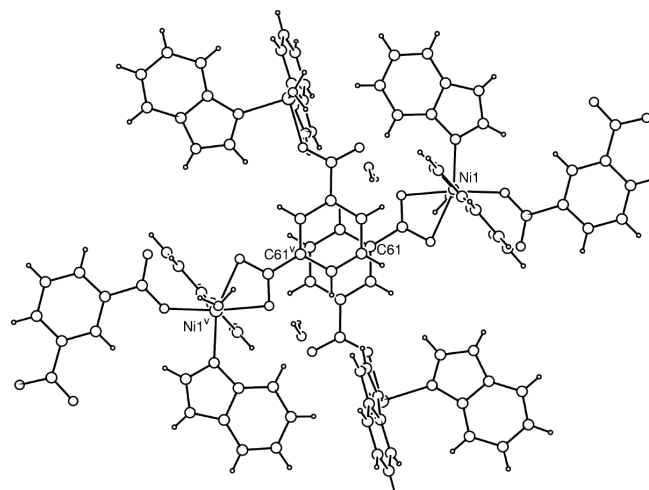
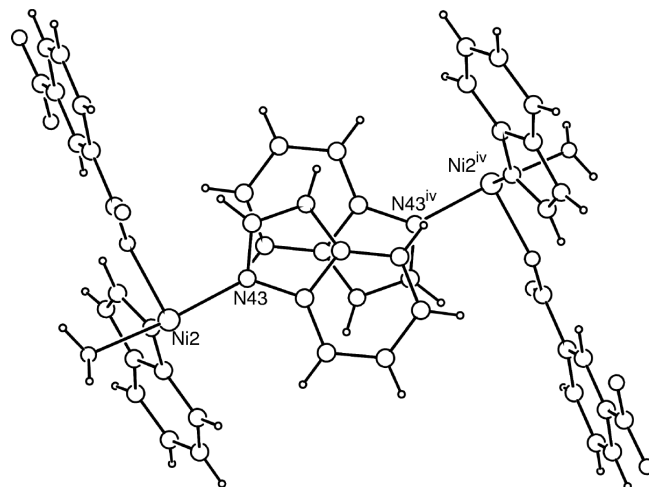
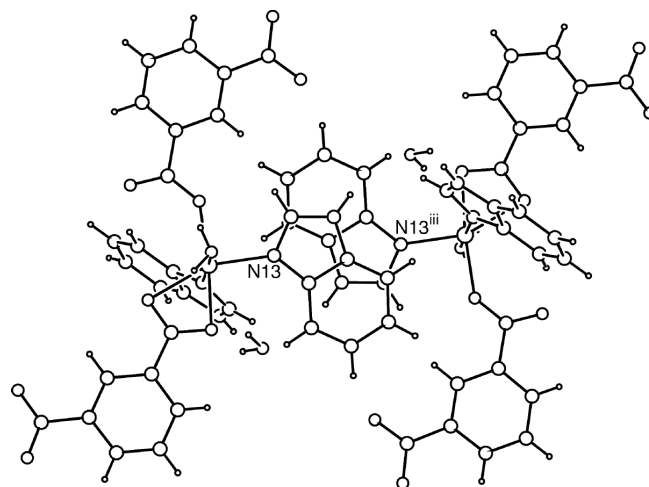
Two BZIM coordinate *cis* to an Ni atom, while two ISOP coordinate to the Ni atom in monodentate and chelate modes, respectively. One water molecule coordinates to the Ni atom to complete the distorted octahedral coordination geometry (Table 1). The uncoordinated water molecule is hydrogen bonded with carboxy groups coordinating to atom Ni1 (Table 2), but no uncoordinated water molecule links to the Ni2 complex unit.

Both ISOP groups have a nearly planar configuration, with a maximum dihedral angle of $10.0(6)^\circ$ between the C51-benzene and C58-carboxy planes. The ISOP dianions bridge neighboring Ni atoms to form zigzag polymeric complex chains extending along the crystallographic $[1\bar{1}0]$ direction, as shown in Fig. 2. Adjacent chains are linked to each other *via* an extensive hydrogen-bonding network (Table 2).

An overlap between parallel BZIM rings and between parallel ISOP rings is observed in the crystal structure, as shown in Fig. 3. The distances between parallel N11-BZIM and N11-BZIMⁱⁱⁱ mean planes [symmetry code: (iii) $1 - x, 2 - y, 1 - z$] and between N41-BZIM and N41-BZIM^{iv} mean planes [symmetry code: (iv) $2 - x, 1 - y, -z$] are $3.40(3)$ and $3.53(3)$ Å, respectively. The distance between parallel C61-benzene and C61^v-benzene rings [symmetry code: (v) $2 - x, 1 - y, 1 - z$] is $3.28(4)$ Å. These distances clearly suggest the existence of π - π stacking in the crystal. π - π stacking also occurs between nearly parallel aromatic rings in the crystal structure (Fig. 4), as evidenced by the following data: the centroid-to-centroid distance of $3.394(3)$ Å and dihedral angle of $10.4(4)^\circ$ between N11-imidazole and N33-imidazoleⁱⁱ rings [symmetry code: (ii) $1 - x, 1 - y, 1 - z$]; the centroid-to-centroid distance of $3.526(2)$ Å and dihedral angle of $2.0(3)^\circ$ between C53-benzene and C63ⁱⁱ-phenyl rings.

Experimental

An ethanol solution (10 ml) of BZIM (0.24 g, 2 mmol) was mixed with an aqueous solution (4 ml) of NiCl₂·6H₂O (0.47 g, 2 mmol), and the mixture was refluxed for 25 min. An aqueous solution (8 ml) containing isophthalic acid (0.33 g, 2 mmol) and NaOH (0.16 g, 4 mmol) was then added to the above mixture, and the solution was refluxed for a further 3 h. After cooling to room temperature, the solution was filtered. Green single crystals were obtained from the filtrate after one week.

**Figure 3**

π - π stacking between parallel aromatic rings. [Symmetry codes: (iii) $1 - x, 2 - y, 1 - z$; (iv) $2 - x, 1 - y, -z$; (v) $2 - x, 1 - y, 1 - z$.]

Crystal data

[Ni(C₈H₄O₄)(C₇H₆N₂)₂·(H₂O)]·0.5H₂O
M_r = 486.12
 Triclinic, *P* $\bar{1}$
a = 12.1060 (6) Å
b = 13.7927 (8) Å
c = 13.8994 (9) Å
 α = 60.813 (3)°
 β = 88.719 (3)°
 γ = 80.625 (2)°
V = 1994.7 (2) Å³

Z = 4
D_x = 1.619 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 8095 reflections
 θ = 2.2–24.0°
 μ = 1.02 mm⁻¹
T = 295 (2) K
 Plate, green
 0.20 × 0.15 × 0.10 mm

Data collection

Rigaku R-Axis RAPID diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
T_{min} = 0.81, *T_{max}* = 0.90
 15 366 measured reflections

7148 independent reflections
 4851 reflections with *I* > 2σ(*I*)
R_{int} = 0.068
 θ_{max} = 25.2°
h = -14 → 14
k = -16 → 16
l = -16 → 16

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.058
wR (*F*²) = 0.101
S = 1.05
 7148 reflections
 586 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2 + 1.5337P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.34 \text{ e \AA}^{-3}$
 $\Delta\rho_{min} = -0.34 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Ni1—O1	2.042 (3)	Ni2—O3 [†]	2.267 (3)
Ni1—O5	2.089 (3)	Ni2—O4 [†]	2.098 (3)
Ni1—O6	2.224 (3)	Ni2—O7	2.039 (3)
Ni1—O11	2.152 (3)	Ni2—O21	2.134 (3)
Ni1—N13	2.064 (3)	Ni2—N33	2.075 (3)
Ni1—N23	2.068 (4)	Ni2—N43	2.096 (4)
O1—Ni1—O6	112.62 (11)	O7—Ni2—O3 [†]	113.16 (11)

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

Table 2

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1W—H1A...O5	0.87	2.08	2.868 (4)	151
O1W—H1B...O2 ⁱⁱ	0.88	2.32	3.004 (5)	136
O11—H11A...O6 ⁱⁱ	0.87	1.94	2.728 (4)	150
O11—H11B...O2 ⁱⁱ	0.89	1.87	2.714 (4)	158
O21—H21A...O3 ⁱⁱ	0.93	1.96	2.788 (3)	147
O21—H21B...O8 ^{vi}	0.94	1.69	2.619 (5)	172
N11—H11...O21 ⁱⁱ	0.86	2.16	2.890 (4)	142
N21—H21...O4 ^{vii}	0.86	2.19	3.038 (5)	168
N31—H31...O11 ⁱⁱ	0.86	2.33	3.014 (5)	137
N41—H41...O1W ^v	0.86	2.25	2.958 (6)	139

Symmetry codes: (ii) 1 - *x*, 1 - *y*, 1 - *z*; (v) 2 - *x*, 1 - *y*, 1 - *z*; (vi) 2 - *x*, -*y*, 1 - *z*; (vii) 1 + *x*, *y*, *z*.

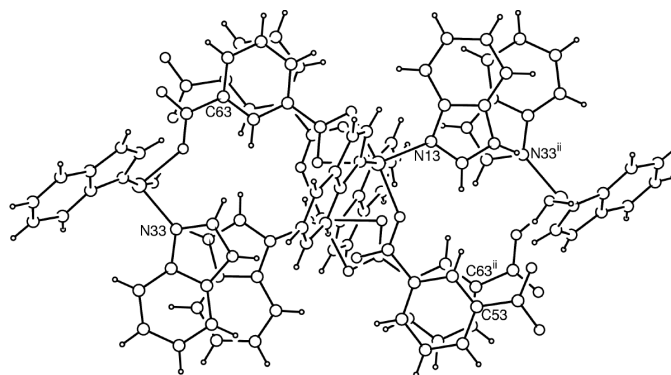


Figure 4

π-π stacking between nearly parallel aromatic rings. [Symmetry code: (ii) 1 - *x*, 1 - *y*, 1 - *z*.]

Water H atoms were located in a difference Fourier map and included in the refinement with fixed positional (O—H = 0.869–0.939 Å) and isotropic displacement parameters (0.05 Å²). All other H atoms were placed in calculated positions (C—H = 0.93 Å and N—H = 0.86 Å) and refined as riding, with *U_{iso}*(H) = 1.2*U_{eq}*(carrier atom).

Data collection: *PROCESS-AUTO* (Rigaku Corporation, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK and Rigaku Corporation, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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