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Key indicators

Single-crystal X-ray study
T = 295 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
R factor = 0.043
wR factor = 0.093
Data-to-parameter ratio = 16.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Tris(benzimidazole)(iminodiacetato)nickel(II) dihydrate

The title complex, $[\text{Ni}(\text{C}_4\text{H}_5\text{NO}_4)(\text{C}_7\text{H}_6\text{N}_2)_3] \cdot 2\text{H}_2\text{O}$, assumes a distorted octahedral geometry about Ni^{II} , involving one iminodiacetate dianion and three benzimidazole molecules. The tridentate iminodiacetate dianion chelates the Ni^{II} atom in the facial mode. The crystal packing is influenced by $\text{O}-\text{H} \cdots \text{O}$ and $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds and $\text{C}-\text{H} \cdots \pi$ interactions, the latter occurring between neighboring benzimidazole ring systems.

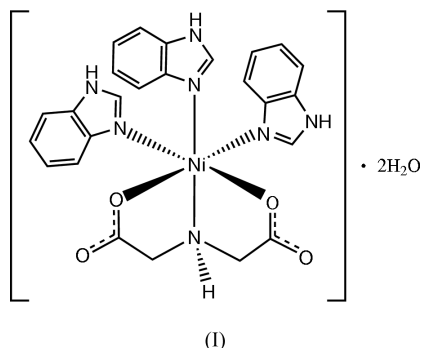
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Comment

As part of our investigations on non-covalent interactions in metal complexes, the title Ni^{II} complex incorporating benzimidazole (BZIM), (I), has been prepared and its crystal structure is presented here.



The molecular structure of (I) is illustrated in Fig. 1. The Ni^{II} cation assumes distorted octahedral coordination geometry (Table 1), involving three BZIM molecules and an iminodiacetate dianion (IDA). The tridentate IDA chelates the Ni^{II} atom in the facial configuration, which is similar to the coordination mode of IDA found in the Co analog (Su & Xu, 2004). Both chelate rings have an envelope configuration, with the Ni atom in the flap position and displaced from the mean planes formed by the other four atoms by 0.277 (4) and 0.629 (4) \AA , respectively.

The three BZIM molecules coordinating to the same Ni atom display different orientations in the crystal structure. Aromatic $\pi-\pi$ stacking between BZIM ring systems has been commonly observed in metal complexes (Xue *et al.*, 2003; Liu *et al.*, 2004), but does not occur in (I). The $\text{C}-\text{H} \cdots \pi$ interactions occur between neighboring BZIM ring systems (Fig. 2). The distances between H atoms and benzene rings range from 2.73 to 2.75 \AA , and the $\text{C}-\text{H} \cdots \text{C}_g$ (C_g = benzene centroid) angles range from 138 to 148°.

Complex molecules are linked to each other *via* hydrogen bonding between BZIM and carboxyl groups from neigh-

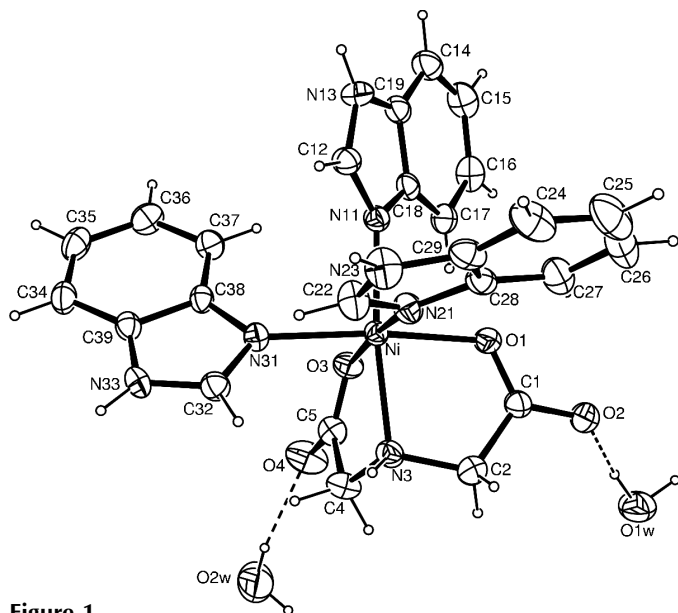


Figure 1
The molecular structure of (I), with 40% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

boring molecules (Table 2). The uncoordinated water molecules are hydrogen bonded to uncoordinated O atoms of IDA (Fig. 1).

Experimental

All reagents were commercially available and of analytical grade. Nickel dichloride hexahydrate (0.24 g, 1 mmol), benzimidazole (0.24 g, 2 mmol), iminodiacetic acid (0.13 g, 1 mmol) and sodium carbonate (0.11 g, 1 mmol) were dissolved in a water (8 ml)/ethanol (2 ml) mixture. The solution was refluxed for 5 h until a small amount of precipitate appeared and was filtered. The filtrate was kept at 353 K. Green single crystals were obtained from the filtrate after 2 d.

Crystal data

$[\text{Ni}(\text{C}_4\text{H}_5\text{NO}_4)(\text{C}_7\text{H}_6\text{N}_2)_3] \cdot 2\text{H}_2\text{O}$	$D_x = 1.483 \text{ Mg m}^{-3}$
$M_r = 580.25$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 12159 reflections
$a = 13.4711 (5) \text{ \AA}$	$\theta = 2.5\text{--}26.0^\circ$
$b = 10.2873 (4) \text{ \AA}$	$\mu = 0.80 \text{ mm}^{-1}$
$c = 19.2982 (6) \text{ \AA}$	$T = 295 (2) \text{ K}$
$\beta = 103.719 (1)^\circ$	Prism, green
$V = 2598.07 (16) \text{ \AA}^3$	$0.31 \times 0.20 \times 0.10 \text{ mm}$
$Z = 4$	

Data collection

Rigaku R-Axis RAPID diffractometer	5941 independent reflections
ω scans	4681 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$R_{\text{int}} = 0.045$
$T_{\text{min}} = 0.84$, $T_{\text{max}} = 0.92$	$\theta_{\text{max}} = 27.5^\circ$
24193 measured reflections	$h = -17 \rightarrow 17$
	$k = -13 \rightarrow 13$
	$l = -23 \rightarrow 25$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0393P)^2 + 1.3635P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.093$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.08$	$\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$
5941 reflections	$\Delta\rho_{\text{min}} = -0.31 \text{ e \AA}^{-3}$
352 parameters	
H-atom parameters constrained	

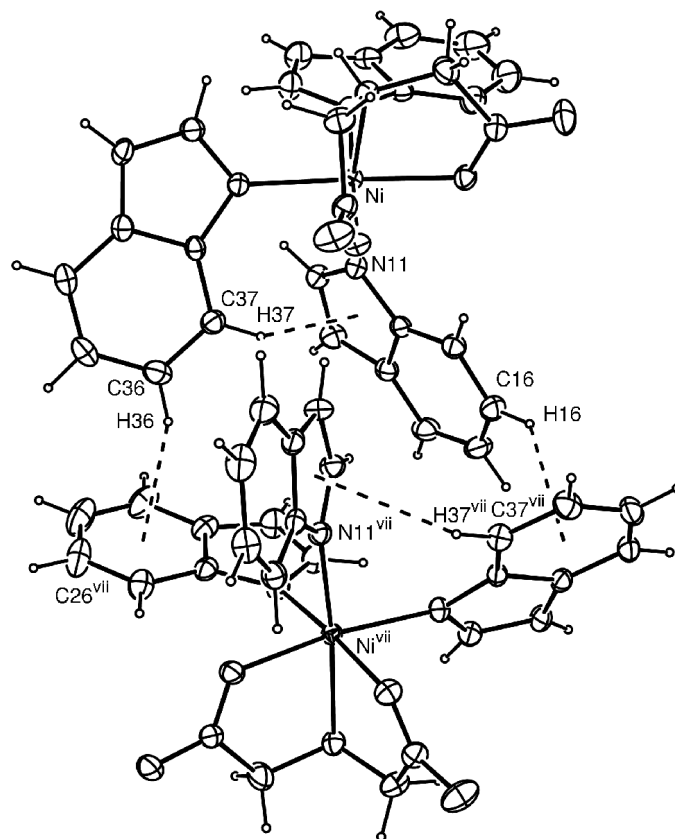


Figure 2
A diagram showing the intramolecular and intermolecular C—H... π interactions (dashed lines) in (I). [Symmetry code: (vii) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$.]

Table 1

Selected bond distances (\AA).

Ni—O1	2.0593 (15)	Ni—N11	2.0648 (18)
Ni—O3	2.1452 (16)	Ni—N21	2.1496 (19)
Ni—N3	2.1214 (18)	Ni—N31	2.1065 (17)

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
O1W—H1A...O2	0.98	1.85	2.808 (3)	168
O1W—H1B...O2W ⁱ	0.93	1.94	2.806 (3)	154
O2W—H2C...O4	0.89	1.96	2.797 (3)	156
O2W—H2D...O2 ⁱⁱ	0.83	2.21	2.994 (3)	160
N3—H3...O1W ⁱⁱⁱ	0.91	2.08	2.990 (3)	173
N13—H13...O3 ^{iv}	0.86	2.23	3.084 (2)	171
N23—H23...O4 ^v	0.86	1.92	2.767 (3)	167
N33—H33...O2 ^{vi}	0.86	1.98	2.827 (3)	168

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

The water molecule H atoms were located in difference Fourier maps and included in the refinement with fixed positional and isotropic displacement parameters [$U_{\text{iso}}(\text{H}) = 0.05 \text{ \AA}^2$]. The other H atoms were placed in calculated positions, with C—H = 0.93 (aromatic) or 0.97 \AA (methylene) and N—H = 0.86 (aromatic) or 0.91 \AA (imino), and were refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier atom})$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/ MSC, 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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