

Triaqua(2,2'-bipyridine)maleatonickel(II)
monohydrateMingtian Li,^a Xucheng Fu^b and
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Key indicators

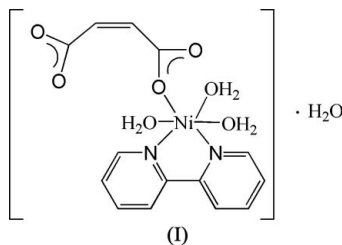
Single-crystal X-ray study
T = 292 K
Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$
R factor = 0.051
wR factor = 0.141
Data-to-parameter ratio = 13.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title complex, $[\text{Ni}(\text{C}_4\text{H}_2\text{O}_4)(\text{C}_{10}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_3]\cdot\text{H}_2\text{O}$, the Ni atom has a distorted NiO_4N_2 octahedral coordination, formed by one maleate dianion, one bipyridine and three water molecules. The crystal structure is stabilized by $\pi-\pi$ stacking and hydrogen-bonding interactions.

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Comment

Metal complexes with the maleate ligand have been studied extensively because of their wide applications (Marioka *et al.*, 1993; Ma *et al.*, 2003). Here we report the crystal structure of the title Ni^{II} complex, (I).



The molecular structure of (I) is shown in Fig. 1. The Ni atom has a distorted octahedral coordination, formed by one bipyridine ligand, three water molecules and one maleate dianion. The Ni—N bond distances and Ni—O bond distances (Table 1) are normal.

An extensive hydrogen-bonding network occurs in the crystal structure of (I) (Table 2). The centroid-to-centroid separation of 3.998 (2) Å suggests weak $\pi-\pi$ stacking between neighbouring pyridine rings. These molecular interactions help to stabilize the crystal structure.

Experimental

$\text{Ni}(\text{NO}_3)_2\cdot 6\text{H}_2\text{O}$ (0.290 g, 1 mmol) was added slowly to an aqueous solution (15 ml) of maleic acid (0.116 g, 1 mmol). The mixture was stirred for 1 h at 353 K, then an ethanol solution (5 ml) of 2,2'-

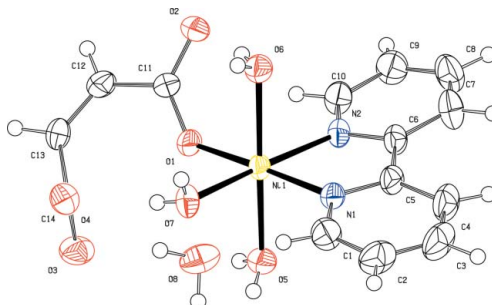


Figure 1
The molecular structure of (I), with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

bipyridine (0.156 g, 1 mmol) was added slowly with stirring. The solution was adjusted to pH = 7 with NaOH solution and stirred for 1.5 h at 353 K. The solution was then cooled to room temperature and filtered. Single crystals of (I) were obtained from the filtrate after two weeks.

Crystal data

[Ni(C₄H₂O₄)(C₁₀H₈N₂)₂·(H₂O)₃]·H₂O
M_r = 401.01
 Monoclinic, *P*2₁/*c*
a = 9.4941 (19) Å
b = 7.6031 (15) Å
c = 23.408 (5) Å
 β = 97.73 (3)°
V = 1674.3 (6) Å³
Z = 4

D_x = 1.591 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 3123 reflections
 θ = 2.6–27.8°
 μ = 1.20 mm⁻¹
T = 292 (2) K
 Needle, green
 0.40 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan *SADABS* (Sheldrick, 2002)
T_{min} = 0.642, *T_{max}* = 0.890
 10268 measured reflections

3438 independent reflections
 2764 reflections with *I* > 2σ(*I*)
R_{int} = 0.040
 θ_{max} = 26.5°
h = -11 → 7
k = -9 → 9
l = -20 → 29

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.051
wR(*F*²) = 0.141
S = 1.05
 3438 reflections
 250 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0815P)^2 + 0.6287P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} = 0.001
 Δρ_{max} = 0.97 e Å⁻³
 Δρ_{min} = -0.37 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ni1—O1	1.940 (2)	Ni1—O7	2.169 (3)
Ni1—O5	2.067 (2)	Ni1—N1	1.963 (3)
Ni1—O6	2.089 (3)	Ni1—N2	2.146 (3)
O1—Ni1—N1	176.36 (10)	O5—Ni1—N2	90.84 (10)
O1—Ni1—O6	89.16 (9)	N1—Ni1—O7	89.11 (12)

Table 2

Hydrogen-bond 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>
O5—H5A···O8	0.81 (2)	1.86 (2)	2.671 (4)	173 (4)
O5—H5B···O4 ⁱ	0.81 (3)	2.14 (4)	2.928 (4)	165 (3)
O6—H6A···O2	0.82 (2)	1.85 (2)	2.633 (4)	160 (3)
O6—H6B···O4 ⁱⁱ	0.81 (3)	2.04 (3)	2.804 (4)	157 (3)
O7—H7A···O4	0.81 (4)	1.89 (4)	2.691 (4)	174 (3)
O7—H7B···O3 ⁱⁱ	0.83 (4)	1.92 (4)	2.724 (4)	163 (4)
O8—H8A···O3	0.83 (3)	2.13 (3)	2.918 (4)	159 (3)
O8—H8B···O2 ⁱⁱⁱ	0.82 (2)	1.94 (2)	2.725 (3)	159 (5)

Symmetry codes: (i) -*x* + 1, *y* - ½, -*z* + ½; (ii) -*x* + 1, *y* + ½, -*z* + ½; (iii) *x*, *y* - 1, *z*.

Water H atoms were initially located in a difference Fourier map and then refined with O—H = restrained to 0.809 (10)–0.828 (10) Å and *U*_{iso}(H) = 1.5*U*_{eq}(O). Other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93 Å, and *U*_{iso}(H) = 1.2*U*_{eq}(C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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