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Tetraaquabis(4,6-dioxidopyrimidin-1-ium-κN^3)-nickel(II)

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.002 Å
R factor = 0.016
wR factor = 0.049
Data-to-parameter ratio = 8.9

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

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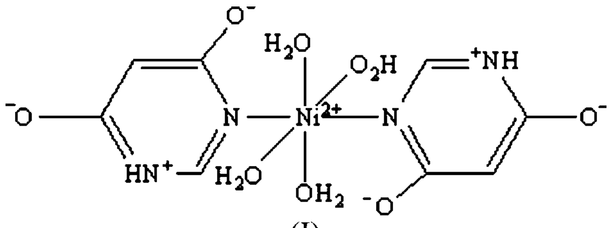
In the title compound, $[Ni(C_4H_3N_2O_2)_2(H_2O)_4]$ or $[Ni(HDHPM)_2(H_2O)_4]$ (H_2DHPM = 4,6-dihydroxypyrimidine), the Ni^{II} atom, on an inversion centre, is six-coordinated by two N atoms from two $HDMPM^-$ ligands and four O atoms from four water molecules. A three-dimensional supramolecular structure is formed through π–π and hydrogen-bonding interactions.

Comment

There has been a continuous interest in the chemistry of metal complexes of N-donor heterocycles. As a series of ligands containing N-donor heterocycles, pyrimidines and their derivatives have attracted much attention in the research field of coordination chemistry in recent years. During the past couple of years, a large number of transition metal complexes with pyrimidines were prepared due to their rich structural, biological, thermal, magnetic and sorptive properties (Masciocchi *et al.*, 1997, 1998, 2003; Tabares *et al.*, 2001; Santra *et al.*, 2001; Nedelec & Rochon, 2001; Li *et al.*, 2005). However, there are very few papers in the literature on transition metal complexes with the 4,6-dihydroxypyrimidine ligand (Boyle *et al.*, 2003; Tabassum *et al.*, 2003). As a result, the information about their structural behaviour is very limited. In a project to obtain more information on the coordination chemistry of metal ions with the ligand, we report here the crystal structure of the title complex, (I).



(I)

Crystals of $[Ni(HDHPM)_2(H_2O)_4]$ (H_2DHPM = 4,6-dihydroxypyrimidine), (I), contain mononuclear *trans*-octahedral NiN_2O_4 units in which the nickel(II) ion, on an inversion centre, is bound to two N atoms from two $HDMPM^-$ ligands and four water molecules (Fig. 1). Each H_2DHPM is partly deprotonated and acts as a monodentate ligand. The Ni1—N1 bond length of 2.1415 (15) Å is consistent with those reported for octahedral Ni^{II} ions (Barea *et al.*, 2005). The Ni—O bond distances are 2.0807 (12) Å for Ni1—O3 and 2.0608 (12) Å for Ni1—O4. The dihedral angle between the two coordinated pyrimidine rings is 38.18 (4)°. Though mononuclear, the molecules of (I) are interconnected by an extended network of intermolecular hydrogen bonds (Fig. 2

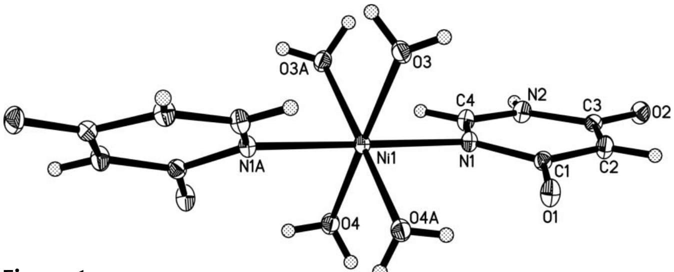


Figure 1
Molecular structure of [Ni(HDHPM)$_2$(H$_2$O)$_4$] with the labelling scheme. Displacement parameters were drawn at the 50% level. [Symmetry code: (A) $-x + 1, y, -z + \frac{3}{2}$.]

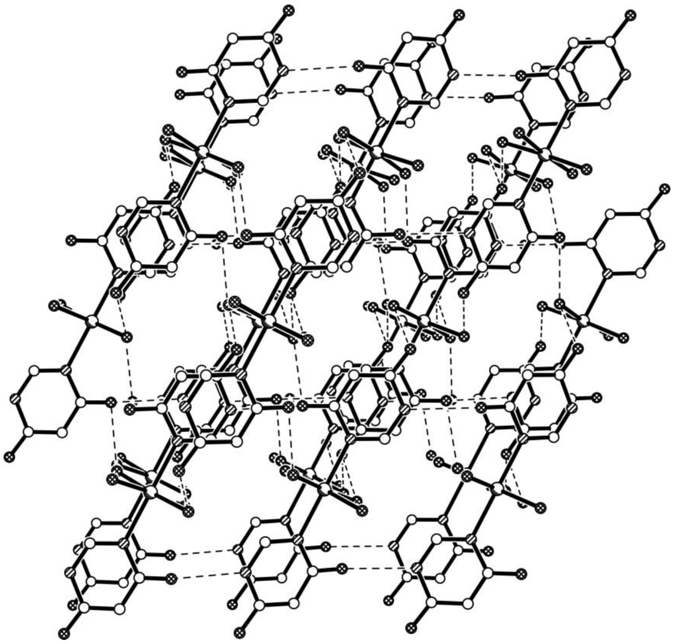


Figure 2
Packing diagram of (I), showing hydrogen bonding as dashed lines. H atoms have been omitted.

and Table 1); four water O atoms interact with the adjacent HDMPM$^-$ ligands *via* the two non-coordinated O atoms and ligands interact with each other *via* hydrogen bonds between uncoordinated N atoms and O atoms of the neighbouring ligands. Furthermore, from Fig. 2, one can easily detect the presence of π–π stacked aromatic rings. The distances of neighbouring parallel pyrimidinyl rings are 3.3879 (14) and 3.4099 (14) Å alternately (Fig. 3), indicating a strong edge-to-face offset π–π stacking interaction. Non-covalent interactions, such as hydrogen-bonding and π–π stacking interactions, play important roles in the formation of multi-dimensional frameworks. In (I), the combination of hydrogen bonding and π–π stacking leads to the formation of a three-dimensional network structure (Janiak, 2000).

Experimental

4,6-Dihydroxypyrimidine was used as received from a commercial source (Aldrich) without further purification. The complex [Ni(HDHPM)$_2$(H$_2$O)$_4$] was synthesized as follows: 4,6-dihydroxypyrimidine (0.112 g, 1 mmol) was added to warm water (10 ml) and the resulting solution was adjusted to pH 7.0 by aqueous triethylamine. Ni(SO$_4$)·6H$_2$O (0.1314 g, 0.5 mmol) was added to the above solution, and the mixture was stirred for 30 min and filtered. After three days, blue single crystals suitable of (I) for X-ray analysis were obtained. Analysis calculated for C$_8$H$_{14}$N$_4$NiO$_8$: C 27.20, H 3.97, N 15.87%; found: C 27.13, H 3.85, N 15.94%.

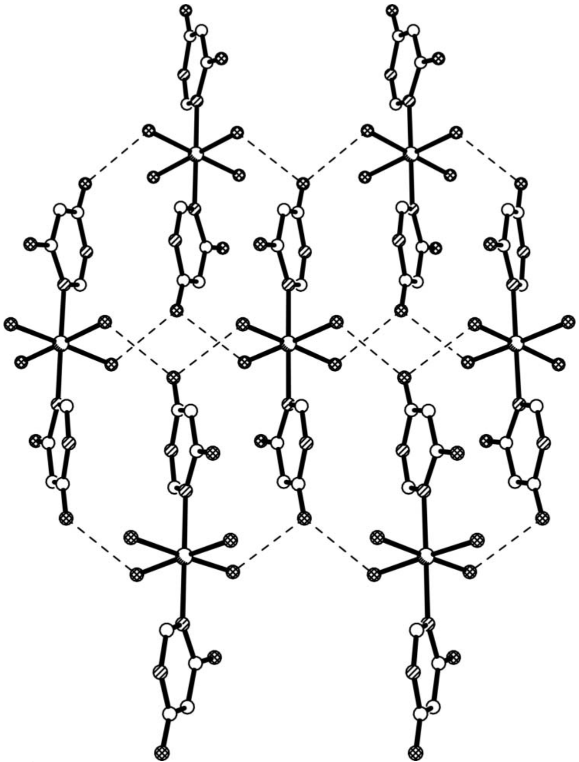


Figure 3
Packing diagram of (I), showing π-π stacking interactions. Hydrogen bonds are shown as dashed lines. H atoms have been omitted.

Crystal data

[Ni(C$_4$H$_3$N$_2$O$_2$)$_2$(H$_2$O)$_4$]
M_r = 352.94
Monoclinic, $C2/c$
a = 13.491 (3) Å
b = 7.1934 (14) Å
c = 13.025 (3) Å
β = 109.79 (3)°
V = 1189.4 (4) Å^3
Z = 4
D_x = 1.971 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.69 mm^{-1}
T = 291 (2) K
Prism, blue
0.20 × 0.18 × 0.16 mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.729, $T_{\max}$ = 0.774
4196 measured reflections
1043 independent reflections
1023 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.010
$\theta_{\max}$ = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.049
S = 1.12
1043 reflections
117 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0283P)^2 + 1.0265P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 0.26 e Å^{-3}
$\Delta\rho_{\min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0017 (4)

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Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O4—H4$F\cdots$O2^{i}	0.78 (2)	1.99 (2)	2.7557 (18)	166 (2)
O3—H3$F\cdots$O2^{ii}	0.83 (3)	1.92 (3)	2.7489 (18)	174 (2)
O4—H4$E\cdots$O1^{iii}	0.77 (2)	1.94 (2)	2.6472 (18)	153 (2)
N2—H2$C\cdots$O1^{iv}	0.80 (2)	2.10 (2)	2.8939 (19)	170 (2)
O3—H3$E\cdots$O1^{v}	0.74 (2)	2.13 (2)	2.8479 (17)	164 (2)

Symmetry codes: (i) $-x+\frac{1}{2}, -y+\frac{3}{2}, -z+1$; (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x+1, y, -z+\frac{3}{2}$; (iv) $x, -y+1, z-\frac{1}{2}$; (v) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

The H atoms of the water molecules and the N atom were located in a difference Fourier map and refined freely. Other H atoms were placed in idealized locations as riding atoms, with C—H distances of 0.93 Å and an isotropic displacement parameter equal to $1.2U_{\rm eq}$ of the parent atom.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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