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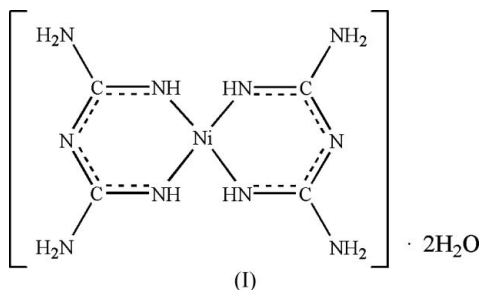
Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{N}-\text{C}) = 0.004$ Å
 R factor = 0.036
 wR factor = 0.086
Data-to-parameter ratio = 14.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Bis(biguanido- $\kappa^2\text{N},\text{N}'$)nickel(II) dihydrate

In the title compound, $[\text{Ni}(\text{C}_2\text{H}_6\text{N}_5)_2] \cdot 2\text{H}_2\text{O}$, the Ni cation (site symmetry $\bar{1}$) is coordinated by four N atoms from two bidentate ligands in a square-planar arrangement. A network of $\text{O}-\text{H} \cdots \text{N}$, $\text{N}-\text{H} \cdots \text{N}$ and $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds helps to consolidate the crystal packing.

Comment

Biguanidine ($\text{C}_2\text{H}_7\text{N}_5$) and its derivatives are moderately strong bases, forming well defined salts and possessing excellent capacity for coordination with transition metals, giving rise to highly coloured bidentate chelate complexes. Various metal complexes have been studied, such as $[\text{PtCl}_4(\text{C}_4\text{H}_{11}\text{N}_5)(\text{DMSO})]$ (DMSO is dimethyl sulfoxide; Bentefrit *et al.*, 1997), $[\text{Co}(\text{C}_4\text{H}_{12}\text{N}_5)\text{Cl}_3]$ (Lemoine *et al.*, 1996), $[\text{Zn}(\text{C}_4\text{H}_{12}\text{N}_5)\text{Cl}_3]$ (Zhu *et al.*, 2002), $[\text{Cu}(\text{C}_4\text{H}_{10}\text{N}_5)_2] \cdot 8\text{H}_2\text{O}$, $[\text{Ni}(\text{C}_4\text{H}_{10}\text{N}_5)_2]$ (Zhu *et al.*, 2002*a,b*), $[\text{Cu}(\text{C}_6\text{H}_{12}\text{N}_5\text{O})_2]$ (Lu & Zhu, 2003) and $[\text{Cu}(\text{C}_2\text{H}_6\text{N}_5)_2] \cdot 2\text{H}_2\text{O}$ (Su *et al.*, 2005). We report here the structure of the title nickel complex, (I), containing deprotonated biguanidine anions.



Selected geometric parameters for (I) are listed in Table 1. The molecular structure and crystal packing are illustrated in Figs. 1 and 2. Compound (I) contains square-planar $\text{Ni}(\text{C}_2\text{H}_6\text{N}_5)_2$ groups, with the Ni atom (site symmetry $\bar{1}$) coordinated by two bidentate ligands. The Ni–N bond distances in (I) are very similar to those in $[\text{Ni}(\text{C}_4\text{H}_{10}\text{N}_5)_2]$ [1.848 (2) and 1.854 (2) Å; Zhu *et al.*, 2002*b*] and in $[\text{Ni}(\text{C}_4\text{H}_{11}\text{N}_5)_2](\text{Cl})(\text{OH})$ [1.863 (5) and 1.866 (5) Å; Lemoine *et al.*, 1996].

All the C–N bonds in (I) have some double-bond character (Table 1), with the C1–N1 and C2–N4 pairs bonded to Ni being the shortest bonds. In addition, deprotonation of the ligand significantly decreases the bond angle at the bridging N atom to 119.9 (2)°, compared with 124.9 (8) and 127.7 (5)° for neutral ligands (Bentefrit *et al.*, 1997; Lemoine *et al.*, 1996).

The molecules in the crystal structure are held together by a number of intermolecular hydrogen bonds involving the non-coordinated water molecules and the ligand N atoms (Table 2).

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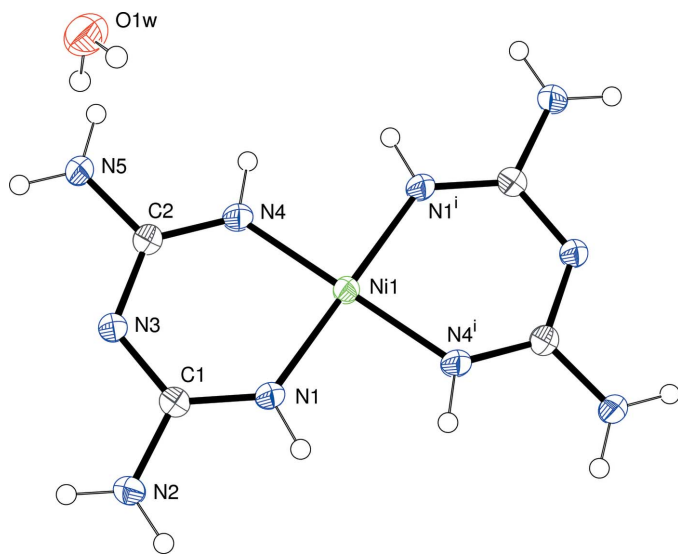


Figure 1
The structure of (I), with displacement ellipsoids drawn at the 30% probability level. [Symmetry code: (i) $1 - x, 1 - y, -z$.]

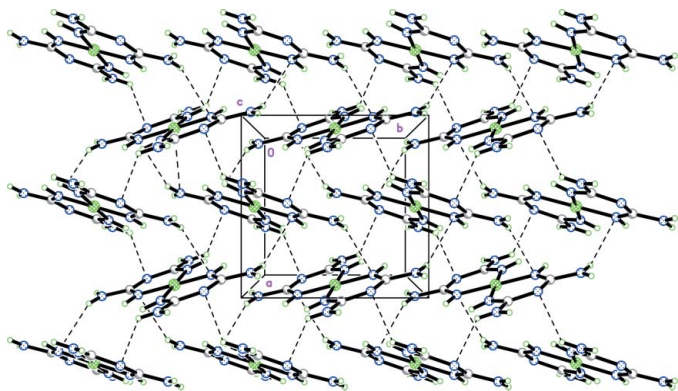


Figure 2
The packing of (I). Dashed lines indicate hydrogen bonds.

Experimental

An aqueous solution of $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ was added dropwise to a KOH solution (pH 9) of biguanidine with stirring, in a 1:2 molar ratio. The yellow solution was filtered, and the filtrate was left at room temperature. Yellow crystals of the title complex formed after about one month.

Crystal data

$[\text{Ni}(\text{C}_2\text{H}_6\text{N}_5)_2] \cdot 2\text{H}_2\text{O}$
 $M_r = 294.98$
 Orthorhombic, $Pbca$
 $a = 6.964$ (5) Å
 $b = 7.139$ (5) Å
 $c = 22.193$ (15) Å
 $V = 1103.3$ (13) Å³
 $Z = 4$
 $D_x = 1.776$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 1226 reflections
 $\theta = 4.2$ – 25.2°
 $\mu = 1.77$ mm⁻¹
 $T = 298$ (2) K
 Plate, yellow
 $0.20 \times 0.20 \times 0.02$ mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2000)
 $T_{\min} = 0.718, T_{\max} = 0.965$
 5222 measured reflections

1154 independent reflections
 761 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.064$
 $\theta_{\max} = 26.9^\circ$
 $h = -8 \rightarrow 7$
 $k = -9 \rightarrow 8$
 $l = -27 \rightarrow 27$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.086$
 $S = 0.89$
 1154 reflections
 79 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0452P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.38$ e Å⁻³
 $\Delta\rho_{\min} = -0.37$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ni1—N4	1.849 (2)	N3—C1	1.347 (4)
Ni1—N1	1.859 (2)	N3—C2	1.349 (3)
N1—C1	1.315 (4)	N4—C2	1.311 (4)
N2—C1	1.362 (3)	N5—C2	1.362 (4)
C1—N3—C2	119.9 (2)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1W—H2W ⁱ ···N5	0.81	2.23	3.022 (3)	166
O1W—H1W ⁱⁱ ···N3 ⁱ	0.80	2.17	2.958 (3)	167
N5—H5B ⁱⁱⁱ ···O1W ⁱⁱ	0.86	2.12	2.967 (3)	168
N5—H5A ⁱⁱⁱ ···N3 ⁱⁱⁱ	0.86	2.52	3.106 (3)	127
N2—H2B ^{iv} ···O1W ^{iv}	0.86	2.29	3.076 (4)	152
N2—H2A ^v ···N1 ^v	0.86	2.58	3.306 (4)	143

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

H atoms attached to N were positioned geometrically ($N-H = 0.86$ Å) and refined as riding with the constraint $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$. H atoms attached to O were located in a difference map and refined as riding in their as-found relative positions, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

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/PC (Sheldrick, 1999); software used to prepare material for publication: SHELXTL/PC.

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