Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Bis(biguanido-κ^2N,N')palladium(II) dihydrate

Ying-Lan Su[a,b] and Miao-Li Zhu[a*]

[a]Institute of Molecular Science, Key Laboratory of Chemical Biology and Molecular Engineering of the Education Ministry, Shanxi University, Taiyuan, Shanxi 0300061, People's Republic of China, and [b]Chemistry Group of Basic Department, Shanxi Coal, Vocational and Technical College, Taiyuan, Shanxi 030031People's Republic of China

Correspondence e-mail: miaoli@sxu.edu.cn

Received 26 April 2006
Accepted 26 April 2006

Key indicators

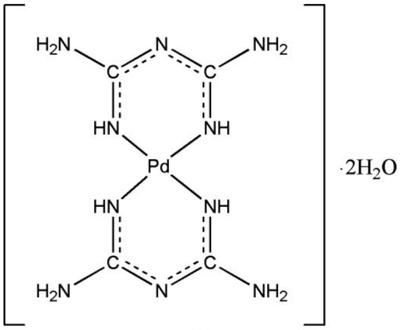
Single-crystal X-ray study
$T = 298$ K
Mean σ(N–C) = 0.005 Å
R factor = 0.038
wR factor = 0.084
Data-to-parameter ratio = 12.5

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

In the title compound, $[Pd(C_2H_6N_5)_2]\cdot 2H_2O$, the Pd atom is coordinated by four N atoms from two bidentate biguanide ligands in a square-planar arrangement. A network of O—H···N, N—H···N and N—H···O hydrogen bonds helps to consolidate the crystal packing. The Pd atom occupies a special position with $\overline{1}$ site symmetry.

Comment

In previous work, the crystal structures of the biguanide ($C_2H_6N_5^-$) anion coordinated to Cu^{2+} and Ni^{2+} were reported (Su, Lu, Li & Zhu, 2005; Su, Lu & Zhu, 2005). Pd^{2+} and Ni^{2+} ions have the same d^8 electron configuration, so we set out to investigate the coordination behaviour of Pd^{2+} with the biguanide ligand, resulting in the title compound, (I) (Fig. 1).



(I)

Compound (I) consists of a square-planar $[Pd(C_2H_6N_5)_2]$ complex (Pd site symmetry $\overline{1}$) and two uncoordinated water molecules. In the complex, Pd is coordinated by four N atoms from two bidentate ligands (Table 1). This coordination geometry is consistent with that seen in the Cu^{2+} and Ni^{2+} analogues noted above. The ligand is close to planar. Compared with the previous complexes, we notice that the Pd—N coordinated bond distances are longer than the equivalent distances in $[Cu(C_2H_6N_5)_2]\cdot 2H_2O$ [1.927 (3) and 1.954 (3) Å; Su, Lu, Li & Zhu, 2005] and $[Ni(C_2H_6N_5)_2]\cdot 2H_2O$ [1.849 (2) and 1.859 (2) Å; Su, Lu & Zhu, 2005].

In addition, deprotonation of the ligand in (I) produces an increase of the π conjugation in the central C—N—C system, decreasing the bond angle at the bridging N atom to 122.3 (4)°, compared with 124.9 (8)–127.7 (5)° for the neutral ligand (Bentefrit *et al.*, 1997; Lemoine *et al.*, 1996).

The structure of (I) is stabilized by extensive hydrogen-bonding interactions involving all the N atoms and all O atoms of the water molecules (Fig. 2 and Table 2)

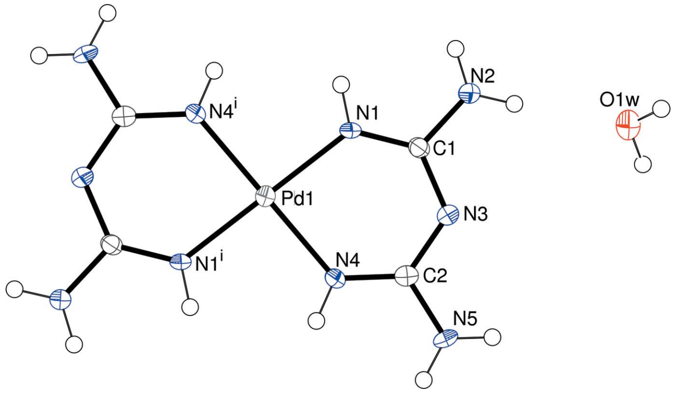


Figure 1
The structure of (I), with displacement ellipsoids drawn at the 30% probability level for non-H atoms. [Symmetry code: (i) $1 - x, -y, 1 - z$.]

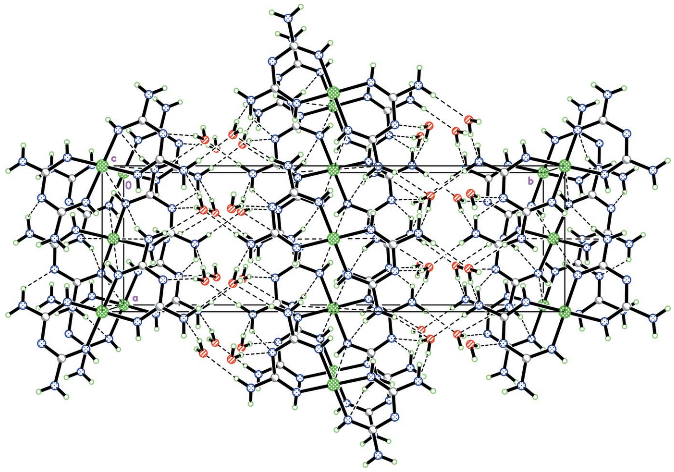


Figure 2
The packing of (I), with hydrogen bonds shown as dashed lines.

Experimental

An aqueous solution of $PdCl_2$ was added dropwise to an alkaline aqueous solution of the ligand with stirring, in a 1:2 molar ratio. The colourless solution was filtered, and the filtrate was left to stand at room temperature. Colourless crystals of (I) formed after a few days.

Crystal data

$[Pd(C_2H_6N_5)_2]\cdot 2H_2O$
$M_r = 342.67$
Orthorhombic, *Pbca*
$a = 7.1450$ (12) Å
$b = 22.663$ (4) Å
$c = 6.9532$ (11) Å
$V = 1125.9$ (3) Å^3
$Z = 4$
$D_x = 2.022$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.66$ mm^{-1}
$T = 298$ (2) K
Plate, colourless
0.21 × 0.14 × 0.02 mm

Data collection

Bruker SMART 1K CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
$T_{min} = 0.722$, $T_{max} = 0.968$
5096 measured reflections
991 independent reflections
819 reflections with $I > 2\sigma(I)$
$R_{int} = 0.069$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.084$
$S = 1.11$
991 reflections
79 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0261P)^2 + 3.5974P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.76$ e Å^{-3}
$\Delta\rho_{min} = -0.97$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pd1—N1	1.979 (3)	Pd1—N4	1.990 (3)
N1—Pd1—N4	87.36 (14)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1B···N2^{ii}	0.85	2.19	3.014 (5)	163
O1W—H1A···N3^{iii}	0.85	2.16	2.978 (5)	164
N5—H5B···O1W^{ii}	0.86	2.30	3.080 (5)	150
N5—H5A···N4^{iv}	0.86	2.61	3.349 (5)	144
N2—H2A···N3^{v}	0.86	2.56	3.136 (5)	125
N1—H1···N3^{v}	0.86	2.69	3.322 (5)	131

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

N-bound H atoms were placed in geometrically idealized positions, with N—H = 0.86 Å, and refined as riding with $U_{iso}(H) = 1.2U_{eq}(N)$. H atoms attached to O were located in a difference Fourier map and then treated as riding, with O—H = 0.85 Å and $U_{iso}(H) = 1.5U_{eq}(O)$.

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*.

We thank the National and Shanxi Provincial Natural Science Foundation of China (grant Nos. 20471033 and 20051013) for financial support.

References

Bentefrit, F., Morgant, G., Viossat, B., Leonce, S., Guilbaud, N., Pierre, A., Atassi, G. & Dung, N.-H. (1997). *J. Inorg. Biochem.* **68**, 53–59.
Bruker (2000). *SMART* (Version 5.0) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Lemoine, P., Chiadmi, M., Bissery, V., Tomas, A. & Viossat, B. (1996). *Acta Cryst.* C**52**, 1430–1436.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1999). *SHELXTL/PC*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2000). *SADABS*. University of Göttingen, Germany.
Su, Y.-L., Lu, L.-P., Li, X.-M. & Zhu, M.-L. (2005). *Acta Cryst.* E**61**, m910–m912.
Su, Y.-L., Lu, L.-P. & Zhu, M.-L. (2005). *Acta Cryst.* E**61**, m2531–m2533.