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Diazidobis(2,2′-bipyridine)zinc(II) monohydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.039
wR factor = 0.084
Data-to-parameter ratio = 10.3

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

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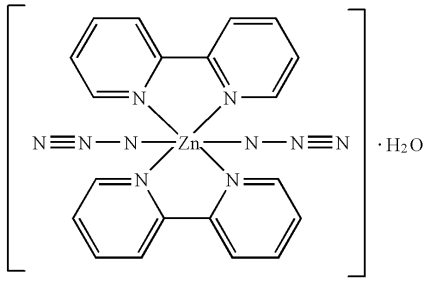
In the title compound, $[Zn(N_3)_2(C_{10}H_8N_2)_2]\cdot H_2O$, the zinc(II) ion is coordinated by two N atoms from two azide groups and four N atoms from two 2,2′-bipyridine ligands. The coordination geometry of the zinc(II) ion is slightly distorted octahedral. In the solid state, the title compound forms a network structure *via* hydrogen bonds.

Comment

Zinc is a relatively abundant element in biological organisms, and plays an essential role in a large number of enzymatic reactions (Liljas *et al.*, 1972). Although zinc(II), being a d^{10} ion, provides few spectroscopic signatures for the monitoring of structure, the structure of the zinc binding site can be elucidated by X-ray crystallography. Furthermore, the azide anion is a good inorganic ligand in the synthesis of coordination compounds. It has been selected for the versatility of this ligand, to allow ferro- or antiferromagnetic coupling according to its coordination mode (end-on EO or end-to-end EE) to transition metals. In this paper, we report the crystal structure of the diazidobis(2,2′-bipyridine)zinc(II) monohydrate complex, (I).



(I)

In (I), the Zn atom is chelated by two 2,2′-bipyridine ligands and two azide anions in a *cis* arrangement. The zinc ion has an octahedral coordination geometry. The two 2,2′-bipyridine ligands are each bonded to zinc in bidentate mode, forming five-membered chelate rings. Each five-membered chelate ring is essentially planar, the deviation of the Zn atom from the least-squares plane through the chelate ring being 0.000 (1) and 0.002 (1) Å for Zn1/N1/C5/C6/N2 and Zn1/N3/C15/C16/N4, respectively. The dihedral angle formed by the two chelate rings is 88.7 (1)°. The Zn—N bond distances are slightly longer than those found in other N-coordinated zinc(II) complexes (Chen *et al.*, 1995). The Zn—N1 and Zn—N3 bond distances *trans* to the two azide anions are slightly longer than the Zn—N2 and Zn—N4 bond distances *cis* to the two azide anions.

In the crystal structure, there are some intramolecular hydrogen bonds and weak intermolecular C—H···*Y* (*Y* = N or

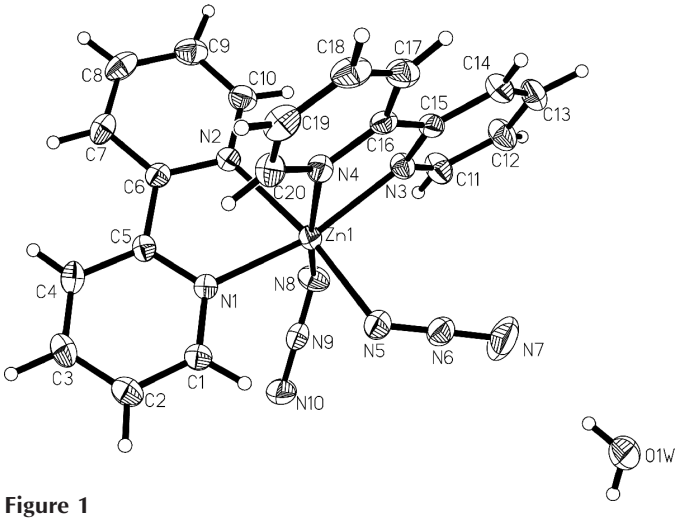


Figure 1
The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

O) hydrogen-bond interactions (Table 2), all of which stabilize the crystal structure.

Experimental

The title compound was prepared by the reaction of 2,2′-bipyridine (1.56 g, 10 mmol) with $ZnCl_2$ (0.68 g, 5 mmol) and sodium azide (0.66 g, 10 mmol) by means of hydrothermal synthesis in a stainless steel reactor with a Teflon liner at 393 K for 24 h.

Crystal data

$[Zn(N_3)_2(C_{10}H_8N_2)_2]\cdot H_2O$
M_r = 479.81
Triclinic, $P\overline{1}$
a = 8.3030 (17) Å
b = 10.334 (2) Å
c = 13.251 (3) Å
α = 83.74 (3)°
β = 86.98 (3)°
γ = 69.58 (3)°
V = 1059.0 (4) Å^3
Z = 2
D_x = 1.505 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 2–11°
μ = 1.20 mm^{-1}
T = 293 (2) K
Block, yellow
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.793, T_{max} = 0.887
3995 measured reflections
3710 independent reflections
2736 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 25.3°
$h = 0 \rightarrow 9$
$k = -11 \rightarrow 12$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.085
S = 1.02
3710 reflections
361 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 0.0239P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N8	2.110 (3)	Zn1—N4	2.233 (3)
Zn1—N5	2.131 (3)	N5—N6	1.172 (4)
Zn1—N1	2.140 (3)	N6—N7	1.154 (4)
Zn1—N3	2.159 (3)	N8—N9	1.183 (4)
Zn1—N2	2.192 (3)	N9—N10	1.158 (4)
N8—Zn1—N5	94.27 (13)	N8—Zn1—N3	94.38 (11)
N8—Zn1—N1	96.86 (11)	N5—Zn1—N3	93.09 (11)
N5—Zn1—N1	94.83 (11)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···N10^{i}	0.83 (4)	2.07 (4)	2.895 (4)	177 (4)
O1W—H2W1···N7	0.82 (5)	2.16 (5)	2.957 (6)	165 (5)
C1—H1A···N5	0.94 (4)	2.59 (3)	3.226 (5)	126 (3)
C7—H7A···N10^{ii}	0.94 (4)	2.60 (4)	3.278 (6)	129 (3)
C11—H11A···N8	0.90 (4)	2.61 (4)	3.205 (5)	124 (3)
C14—H14A···O1W^{iii}	0.92 (4)	2.43 (4)	3.346 (5)	176 (3)
C17—H17A···O1W^{iii}	0.91 (3)	2.52 (3)	3.396 (5)	160 (2)

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

The ranges of the O—H and C—H distances are 0.82 (4)–0.83 (5) and 0.90 (4)–0.99 (4) Å, respectively.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT* and *SHELXTL-PC* (Sheldrick, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-PC*; software used to prepare material for publication: *SHELXTL-PC*.

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References

Chen, X.-M., Wang, R.-Q. & Yu, X.-L. (1995). *Acta Cryst.* C**51**, 1545–1547.
Liljas, A., Kanman, K. K., Bergsten, P. C., Waara, I., Fridborg, K., Strandberg, B., Caribom, V., Jarup, L., Lovgren, S. & Petef, M. (1972). *Nature New Biol.* **235**, 131–137.
Sheldrick, G. M. (1990). *SHELXTL-PC*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.