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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(C-C) = 0.003$ Å
 R factor = 0.025
 wR factor = 0.067
Data-to-parameter ratio = 11.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Diaquaazido(3,5-diaminobenzoato- κN)-(1,10-phenanthroline- $\kappa^2 N, N'$)zinc(II) monohydrate

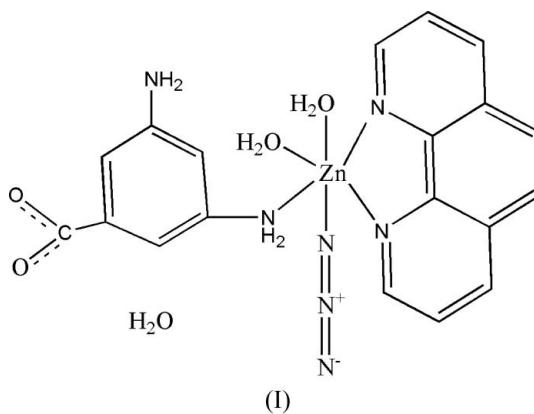
The reaction of 3,5-diaminobenzoic acid, 1,10-phenanthroline, NaN_3 and Zn^{II} in basic aqueous solution gave rise to the title compound, $[\text{Zn}(\text{C}_7\text{H}_7\text{N}_2\text{O}_2)(\text{N}_3)(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2]\cdot\text{H}_2\text{O}$. The Zn^{II} atom is six-coordinate with a distorted octahedral geometry. The two aqua ligands are in *cis* positions and the 3,5-diaminobenzoate ligand binds to the central Zn atom through one of its amino groups.

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Comment

The construction of crystalline solids using polydentate organic ligands and transition metal ions has become a very active research field in recent years (Erxleben, 2003). 3,5-Diaminobenzoic acid, with its carboxyl group and two amino groups, can act as a polydentate ligand and therefore has a large potential for the formation of coordination polymers and supramolecular compounds. Recently, the preparation and structure of several coordination compounds with the 3,5-diaminobenzoate ligand have been reported (Wei *et al.*, 2005, 2006; Ye *et al.*, 2005). We present here the crystal structure of the title mononuclear complex, (I) (Fig. 1).



The Zn atom of (I) is coordinated octahedrally by four N and two O atoms, with the Zn–O and Zn–N bond lengths in the range 2.1060 (13)–2.2061 (16) Å (Table 1). The 3,5-diaminobenzoate ion acts as a monodentate ligand and binds to the central Zn atom through one of its amino groups. The two coordinating water molecules are *cis* oriented, with an O1–Zn–O2 angle of 83.93 (6)°. The azide group acts as a monodentate ligand and coordinates nonlinearly to Zn^{II} , with a Zn1–N3–N4 angle of 120.28 (16)° (Miao *et al.*, 2006). 1,10-Phenanthroline binds to the central Zn atom in a typical chelating mode.

The crystal packing of (I) is determined by a network of hydrogen bonds between the complex molecule and the non-

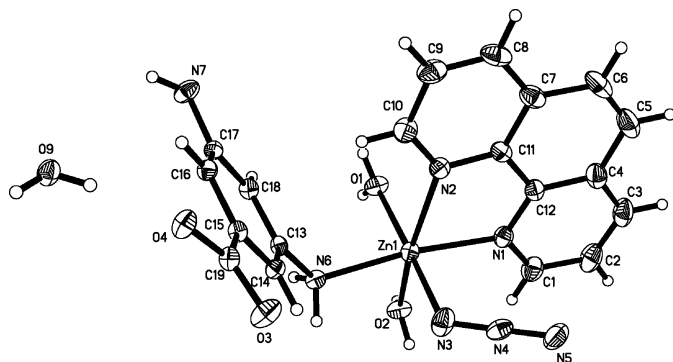


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radii.

coordinated water molecule (Table 2) and by stacking interactions between 1,10-phenanthroline ligands, with an interplanar spacing of 3.20 Å.

Experimental

A mixture of 3,5-diaminobenzoic acid (1.0 mmol) and piperidine (1.0 mmol) was added, with stirring, to a solution of $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (1.0 mmol) in water (15 ml). 1,10-Phenanthroline (1.0 mmol) and NaN_3 (1.0 mmol) were then added successively. The resulting mixture was refluxed for 5 h and then filtered. The resulting light-yellow solution was kept at room temperature to evaporate slowly. After 3 d, light-yellow single crystals of (I) suitable for X-ray diffraction were obtained.

Crystal data

$[\text{Zn}(\text{C}_7\text{H}_7\text{N}_2\text{O}_2)(\text{N}_3)(\text{C}_{12}\text{H}_8\text{N}_2) \cdot (\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$	$\gamma = 77.786 (1)^\circ$
$M_r = 492.80$	$V = 1033.20 (3) \text{ \AA}^3$
Triclinic, $P\bar{1}$	$Z = 2$
$a = 7.8039 (1) \text{ \AA}$	$D_x = 1.584 \text{ Mg m}^{-3}$
$b = 10.1720 (2) \text{ \AA}$	Mo $K\alpha$ radiation
$c = 13.4728 (2) \text{ \AA}$	$\mu = 1.24 \text{ mm}^{-1}$
$\alpha = 81.959 (1)^\circ$	$T = 293 (2) \text{ K}$
$\beta = 85.029 (1)^\circ$	Block, colourless
	$0.30 \times 0.20 \times 0.16 \text{ mm}$

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	10775 measured reflections
φ and ω scans	3629 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	3307 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.708$, $T_{\max} = 0.827$	$R_{\text{int}} = 0.022$
	$\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.067$
 $S = 1.07$
 3629 reflections
 318 parameters
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.035P)^2 + 0.2809P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\text{max}} = 0.002$$

$$\Delta\rho_{\text{max}} = 0.31 \text{ e \AA}^{-3}$$

$$\Delta\rho_{\text{min}} = -0.33 \text{ e \AA}^{-3}$$

Table 1
Selected bond lengths (Å).

Zn1—O2	2.1060 (13)	Zn1—N1	2.1558 (16)
Zn1—O1	2.1255 (15)	Zn1—N6	2.1568 (15)
Zn1—N3	2.1539 (18)	Zn1—N2	2.2061 (16)

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N7—H7A \cdots N3 ⁱ	0.79 (3)	2.52 (3)	3.260 (3)	157 (2)
N7—H7B \cdots O3 ⁱ	0.83 (3)	2.43 (3)	3.223 (2)	160 (2)
O1—H1WA \cdots O4 ⁱⁱⁱ	0.77 (3)	1.95 (3)	2.719 (2)	178 (3)
O9—H9WA \cdots O4 ⁱⁱⁱ	0.79 (3)	2.00 (3)	2.788 (2)	174 (3)
O1—H1WB \cdots N5 ⁱ	0.80 (3)	2.00 (3)	2.799 (3)	177 (3)
O1—H1WB \cdots N4 ⁱ	0.80 (3)	2.66 (3)	3.410 (2)	159 (2)
O2—H2WB \cdots O3 ⁱⁱ	0.87 (3)	1.86 (3)	2.7334 (19)	179 (2)
O9—H9WB \cdots O4	0.82 (3)	1.93 (3)	2.742 (2)	174 (3)
N6—H6A \cdots O9 ^{iv}	0.90	2.07	2.957 (2)	170
N6—H6B \cdots O3 ^v	0.90	2.47	3.291 (2)	152
O2—H2WA \cdots O9 ^{vi}	0.82	1.90	2.678 (2)	157

Symmetry codes: (i) $x-1, y, z$; (ii) $x, y-1, z$; (iii) $-x+1, -y+2, -z+2$; (iv) $-x+1, -y+1, -z+2$; (v) $-x+2, -y+1, -z+2$; (vi) $x+1, y-1, z$.

Water atom H2WA, H atoms bound to C atoms and H atoms of the coordinating NH_2 group were positioned geometrically and constrained to ride on their parent atoms, with $C-H = 0.93$, $N-H = 0.90$ and $O-H = 0.82$ Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$, or $1.5U_{\text{eq}}(\text{O})$. The remaining H atoms were identified in difference Fourier syntheses and refined freely; $O-H = 0.77 (3)$ – $0.87 (3)$ Å, $N-H = 0.79 (3)$ – $0.83 (3)$ Å.

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 (Sheldrick, 2000); software used to prepare material for publication: SHELXTL.

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