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Bis[μ-1,3-bis(imidazol-1-yl)benzene-$\kappa^2N^3:N^{3'}$]-bis[diazidozinc(II)]

Wei-Dong Xu and Mou-Hai Shu*

School of Chemistry and Chemical Technology, Shanghai Jiao Tong University, Shanghai 200240, People's Republic of China

Correspondence e-mail: mhshu@sjtu.edu.cn

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In the molecule of the title complex, $[Zn_2(N_3)_4(C_{12}H_{10}N_4)_2]$, each Zn^{II} ion has a distorted tetrahedral geometry formed by two imidazolyl N atoms and two azide N atoms. Two Zn^{II} ions are bridged by a pair of 1,3-bis(imidazol-1-yl)benzene ligands, resulting in a macrocyclic complex, located across an inversion center.

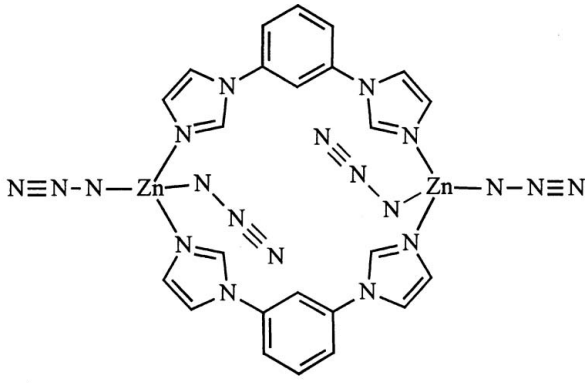
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.037
wR factor = 0.138
Data-to-parameter ratio = 12.4

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

Comment

1,4-Bis(imidazol-1-yl)benzene (bib) has been used in the construction of infinite frameworks of metal complexes (Vargas *et al.*, 2003). We present here the structure of the title macrocyclic Zn^{II} complex, (I), in which bib plays the role of a bridging ligand.



(I)

The molecular structure of (I) is shown in Fig. 1. The Zn^{II} cation has a distorted tetrahedral coordination geometry, formed by four N atoms from bib ligands and azide anions. Bond angles at Zn are in the range 104.78 (15) to 113.8 (2)° (Table 1). Two bib molecules bridge two Zn^{II} ions, forming a macrocyclic metal complex, located across an inversion center. The Zn···Zn separation is 9.859 (4) Å. Within the bib ligand, the benzene ring is twisted with respect to the imidazole rings, making dihedral angles of 34.2 (2) and 35.2 (2)° with the N1- and N4-imidazole rings, respectively.

Weak C—H···N hydrogen bonding is observed between macrocyclic molecules (Table 2).

Experimental

A mixture of $Zn(OAc)_2{\cdot}2H_2O$ (0.044 g, 0.2 mmol) and NaN_3(0.026 g, 0.4 mmol) in water (10 ml) was stirred for 10 min and introduced into a straight glass tube (30 ml). A methanol solution (5 ml) of bib (0.042 g, 0.2 mmol) was layered carefully on to the solution in the glass tube and the tube was covered. Single crystals of (I) were obtained after two weeks (yield 0.058 g, 81%).

Crystal data

$[Zn_2(N_3)_4(C_{12}H_{10}N_4)_2]$
M_r = 719.34
Triclinic, $P\overline{1}$
a = 7.4056 (9) Å
b = 8.9749 (10) Å
c = 11.4207 (13) Å
α = 93.867 (2)°
β = 105.193 (2)°
γ = 99.152 (2)°
V = 718.46 (14) Å^3
Z = 1
D_x = 1.663 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.73 mm^{-1}
T = 293 (2) K
Block, colorless
0.34 × 0.25 × 0.19 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.572, T_{max} = 0.730
3728 measured reflections
2574 independent reflections
2267 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 25.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.138
S = 1.22
2574 reflections
208 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn—N1	2.005 (3)	Zn—N5	1.953 (4)
Zn—N4^{i}	2.012 (3)	Zn—N8	1.930 (4)
N8—Zn—N5	113.8 (2)	N8—Zn—N4^{i}	104.78 (15)
N8—Zn—N1	112.16 (15)	N5—Zn—N4^{i}	105.99 (15)
N5—Zn—N1	111.59 (15)	N1—Zn—N4^{i}	107.95 (13)

Symmetry code: (i) $-x+2, -y+1, -z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···N7^{ii}	0.93	2.47	3.384 (6)	167
C10—H10···N7^{iii}	0.93	2.56	3.431 (6)	156
C11—H11···N9^{iv}	0.93	2.62	3.245 (6)	125

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

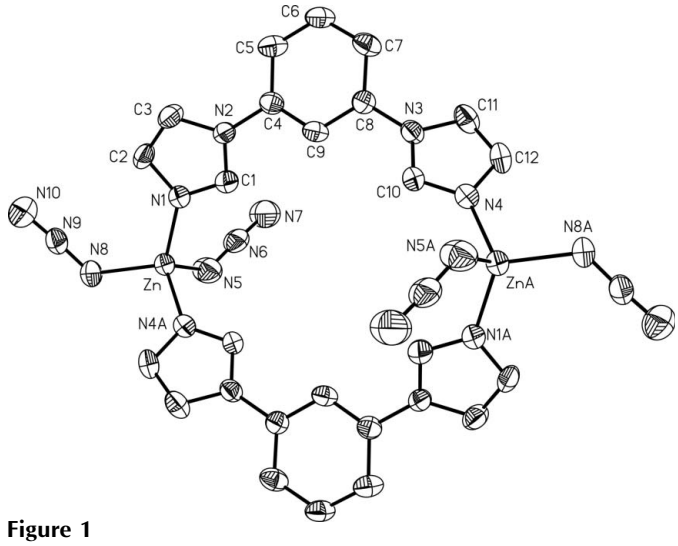


Figure 1
The molecular structure of (I), shown with 50% probability displacement ellipsoids. H atoms have been omitted for clarity. [Symmetry code: (A) $-x+2, -y+1, -z+1$.]

H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(C).

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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