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{[*N*,*N*′-Bis(4-methoxybenzyl)ethane-1,2-diyldiimino]diacetato-κ^4O,N,N',O'}-bis(1*H*-imidazole-κN^3)zinc(II)

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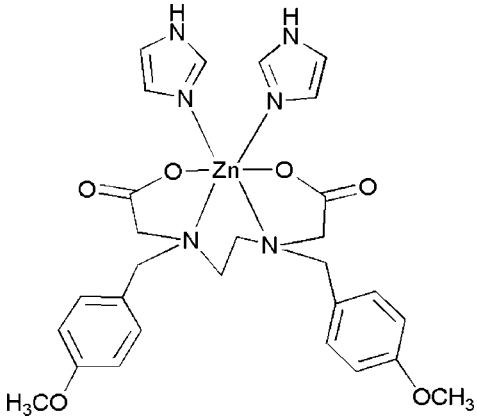
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.054; wR factor = 0.147; data-to-parameter ratio = 16.1.

In the title complex, $[Zn(C_{22}H_{26}N_2O_6)(C_3H_4N_2)_2]$, the Zn^{II} atom is in a distorted octahedral coordination environment defined by the bond lengths and angles formed by an N_4O_2 donor set. In the crystal structure, intermolecular N—H···O hydrogen bonds link molecules into chains of rings. The atoms of one 4-methoxybenzyl group are disordered over two sites in approximately a 0.7:0.3 ratio.

Related literature

We have recently determined the structure of the Ni^{II} analog of the title compound (Zhang *et al.*, 2007).

For related literature, see: Suresh *et al.* (2006).



Experimental

Crystal data

$[Zn(C_{22}H_{26}N_2O_6)(C_3H_4N_2)_2]$
M_r = 615.98
Orthorhombic, *Pcab*
a = 15.3277 (6) Å
b = 16.3989 (6) Å
c = 24.8735 (10) Å
V = 6252.1 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.83 mm^{-1}
T = 299 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.851, T_{max} = 0.921
67264 measured reflections
6826 independent reflections
3459 reflections with $I > 2\sigma(I)$
R_{int} = 0.098

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.147
S = 0.86
6826 reflections
424 parameters
53 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N5	2.099 (2)	Zn1—O2	2.1261 (18)
Zn1—N3	2.103 (2)	Zn1—N1	2.281 (2)
Zn1—O5	2.1086 (18)	Zn1—N2	2.287 (2)
N5—Zn1—N3	97.89 (9)	O5—Zn1—N1	96.89 (8)
N5—Zn1—O5	98.14 (8)	O2—Zn1—N1	75.98 (7)
N3—Zn1—O5	88.30 (8)	N5—Zn1—N2	93.68 (8)
N5—Zn1—O2	88.14 (8)	N3—Zn1—N2	161.94 (8)
N3—Zn1—O2	96.37 (8)	O5—Zn1—N2	76.32 (7)
O5—Zn1—O2	171.62 (8)	O2—Zn1—N2	97.83 (8)
N5—Zn1—N1	161.68 (8)	N1—Zn1—N2	79.75 (9)
N3—Zn1—N1	92.98 (8)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O3^{i}	0.86	1.87	2.722 (3)	171
N6—H6A···O6^{ii}	0.86	1.86	2.716 (3)	171
C23—H23···O5	0.93	2.47	2.979 (4)	115
C26—H26···O2	0.93	2.48	2.974 (3)	114

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2393).

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Suresh, J., Alex Raja, V. P., Perumal, S. & Natarajan, S. (2006). *Acta Cryst.* E**62**, o3307–o3309.
Zhang, M., Weng, H.-L. & Xu, X.-M. (2007). *Acta Cryst.* E**63**, m1465–m1466.

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supplementary materials

Acta Cryst. (2007). E**63**, m1797 [**doi:10.1107/S1600536807026037**]

{[*N*,*N*'-Bis(4-methoxybenzyl)ethane-1,2-diyldiimino]diacetato-κ^4*O*,*N*,*N*',*O*'}bis(1*H*-imidazole-κ*N*^{3})zinc(II)

M. Zhang, H.-L. Weng, B. Hu and X.-M. Xu

Comment

This work is a part of a study of the synthesis and structural characterization of metal complexes with the [*N*,*N*'-bis(4-methoxybenzyl) ethane-1,2-diyldiimino]diacetate ligand. In this paper, we report the structure of a new Zn(II) complex, Zn(L_a)(L_b)$_2$(L_a=[*N*,*N*'-bis(4-methoxybenzyl) ethane-1,2-diyldiimino]diacetate, L_b=imidazole)(1). In (1) (Fig 1), the Zn^{II} atom is in a distorted octahedral coordination environment defined by a N_4O_2 donor set, from two amine N atoms (N1,N2), two carboxyl O atoms (O2,O5), and two imidazole N atoms (N3, N5). In the crystal structure (Fig 2), C—H···O and N—H···O hydrogen bonds (Table 2) consolidate the crystal packing into a chain of rings.

Experimental

The title complex was prepared according to the literature method (Zhang *et al.*, 2007). Crystals were obtained by slow evaporation (one month) of a methanol solution (15 ml) of the title complex (0.06 g,0.1 mmol).

Refinement

H atoms bound to C atoms were placed in calculated positions and refined in the riding-model approximation, with C—H = 0.93–97Å and U_{iso}(H) = 1.2U_{eq}(C) or C—H = 0.96Å and U_{iso} (H) = 1.5U_{eq}(C) for the methyl groups. Similarly H atoms bonded to N atoms were refined with N—H = 0.86 Å, and U_{iso}(H) = 1.2U_{eq}(N). The atoms of the 4-methoxybenzyl group were refined as disordered over two sites with refined occupancies 0.706 (8) and 0.294 (4) for the major and minor components. The largest peak in the final difference Fourier of 1.278 e A°$^{-3}$ is located 1.87Å from atom H11B. During the refinement of the structure, electron density peaks were located that were believed to be highly disordered solvent molecules (possibly methanol). Attempts made to model the solvent molecule were not successful. The SQUEEZE option in *PLATON* (Spek, 2003) indicated there was a solvent cavity of volume 98 Å^3 containing approximately 18 electrons. In the final cycles of refinement, this contribution to the electron density was removed from the observed data. The density, the F(000) value, the molecular weight and the formula are given without taking into account the results obtained with the SQUEEZE option *PLATON* (Spek, 2003). A similar treatment of disordered solvent molecules was carried out by (Suresh *et al.*, 2006; and references cited threin)

Figures

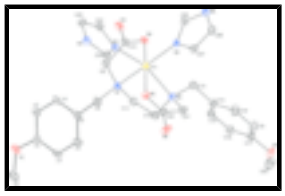

Fig. 1. Molecular structure of (I) showing 30% probability displacement ellipsoids.

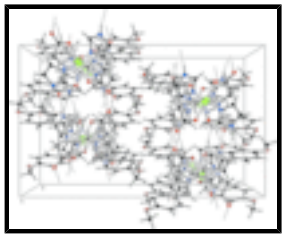

Fig. 2. Part of the crystal structure of the title compound. Dashed lines denote hydrogen bonds.

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Crystal data

$[Zn(C_{22}H_{26}N_2O_6)(C_3H_4N_2)_2]$	F_{000} = 2576
M_r = 615.98	D_x = 1.309 Mg m^{-3}
Orthorhombic, *Pcab*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2bc 2ac	Cell parameters from 9349 reflections
a = 15.3277 (6) Å	θ = 2.5–23.3º
b = 16.3989 (6) Å	μ = 0.83 mm^{-1}
c = 24.8735 (10) Å	*T* = 299 (2) K
V = 6252.1 (4) Å^3	Block, colorless
Z = 8	0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer	6826 independent reflections
Radiation source: fine-focus sealed tube	3459 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.098
T = 299(2) K	θ_{max} = 27.0º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −19→19
T_{min} = 0.851, T_{max} = 0.921	*k* = −20→20
67264 measured reflections	*l* = −31→31

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.054$

$wR(F^2) = 0.147$

$S = 0.86$

6826 reflections

424 parameters

53 restraints

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0892P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 1.28$ e Å^{-3}

$\Delta\rho_{min} = -0.45$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.872846 (19)	0.15880 (2)	0.249200 (12)	0.05098 (14)	
O1	1.0598 (3)	−0.2030 (3)	0.4822 (2)	0.1087 (18)	0.706 (8)
C1	1.1068 (5)	−0.2738 (5)	0.4709 (3)	0.126 (3)	0.706 (8)
H1A	1.0758	−0.3055	0.4447	0.188*	0.706 (8)
H1B	1.1138	−0.3051	0.5032	0.188*	0.706 (8)
H1C	1.1631	−0.2594	0.4569	0.188*	0.706 (8)
C2	1.0426 (3)	−0.1459 (3)	0.4402 (2)	0.0715 (17)	0.706 (8)
C3	1.0004 (4)	−0.0748 (3)	0.45597 (16)	0.108 (3)	0.706 (8)
H3	0.9875	−0.0661	0.4921	0.130*	0.706 (8)
C4	0.9776 (5)	−0.0166 (3)	0.4178 (2)	0.102 (3)	0.706 (8)
H4	0.9494	0.0310	0.4284	0.122*	0.706 (8)
C5	0.9970 (4)	−0.0296 (3)	0.36391 (19)	0.061 (2)	0.706 (8)
C6	1.0391 (3)	−0.1007 (3)	0.34812 (17)	0.0608 (14)	0.706 (8)
H6	1.0521	−0.1094	0.3120	0.073*	0.706 (8)
C7	1.0619 (3)	−0.1589 (2)	0.3863 (2)	0.0652 (17)	0.706 (8)
H7	1.0901	−0.2065	0.3757	0.078*	0.706 (8)
O1'	1.0884 (9)	−0.2337 (7)	0.4386 (5)	0.152 (6)	0.294 (8)
C1'	1.1133 (19)	−0.220 (2)	0.4934 (7)	0.170 (12)	0.294 (8)
H1'1	1.1421	−0.1678	0.4962	0.254*	0.294 (8)
H1'2	1.1522	−0.2620	0.5050	0.254*	0.294 (8)
H1'3	1.0622	−0.2196	0.5158	0.254*	0.294 (8)

C2'	1.0549 (7)	−0.1642 (5)	0.4130 (5)	0.063 (5)	0.294 (8)
C3'	1.0248 (9)	−0.0965 (7)	0.4410 (4)	0.075 (4)	0.294 (8)
H3'	1.0174	−0.0991	0.4781	0.091*	0.294 (8)
C4'	1.0059 (10)	−0.0248 (6)	0.4136 (5)	0.076 (5)	0.294 (8)
H4'	0.9858	0.0206	0.4324	0.091*	0.294 (8)
C5'	1.0169 (11)	−0.0208 (7)	0.3582 (5)	0.050 (4)	0.294 (8)
C6'	1.0470 (11)	−0.0886 (9)	0.3302 (4)	0.124 (8)	0.294 (8)
H6'	1.0543	−0.0859	0.2932	0.148*	0.294 (8)
C7'	1.0659 (8)	−0.1603 (6)	0.3576 (5)	0.092 (6)	0.294 (8)
H7'	1.0860	−0.2056	0.3389	0.110*	0.294 (8)
C8	0.98219 (17)	0.04199 (18)	0.32373 (13)	0.0644 (8)	
H8A	1.0013	0.0924	0.3404	0.077*	
H8B	1.0181	0.0330	0.2921	0.077*	
C9	0.83192 (19)	0.07064 (18)	0.35121 (12)	0.0628 (8)	
H9A	0.8630	0.1046	0.3767	0.075*	
H9B	0.8157	0.0206	0.3694	0.075*	
C10	0.74994 (19)	0.11460 (19)	0.33311 (13)	0.0581 (7)	
C11	0.8554 (2)	−0.01970 (18)	0.27802 (14)	0.0645 (8)	
H11A	0.7923	−0.0197	0.2802	0.077*	
H11B	0.8765	−0.0688	0.2955	0.077*	
C12	0.88233 (19)	−0.02103 (18)	0.21974 (14)	0.0663 (9)	
H12A	0.9454	−0.0252	0.2175	0.080*	
H12B	0.8576	−0.0688	0.2025	0.080*	
C13	0.76025 (17)	0.04746 (19)	0.17132 (12)	0.0609 (8)	
H13A	0.7231	0.0375	0.2022	0.073*	
H13B	0.7442	0.1003	0.1568	0.073*	
C14	0.74011 (17)	−0.01576 (18)	0.12971 (12)	0.0576 (7)	
C15	0.70541 (19)	−0.09060 (19)	0.14364 (12)	0.0625 (8)	
H15	0.6956	−0.1022	0.1797	0.075*	
C16	0.68473 (18)	−0.14911 (18)	0.10515 (13)	0.0650 (8)	
H16	0.6611	−0.1991	0.1153	0.078*	
C17	0.6999 (2)	−0.1316 (2)	0.05166 (13)	0.0669 (8)	
C18	0.7343 (2)	−0.0585 (2)	0.03745 (13)	0.0862 (11)	
H18	0.7452	−0.0471	0.0014	0.103*	
C19	0.7529 (2)	−0.0013 (2)	0.07575 (13)	0.0797 (10)	
H19	0.7749	0.0490	0.0650	0.096*	
C20	0.6471 (3)	−0.2624 (3)	0.02183 (18)	0.1185 (16)	
H20A	0.6910	−0.2961	0.0381	0.178*	
H20B	0.6273	−0.2875	−0.0108	0.178*	
H20C	0.5989	−0.2564	0.0461	0.178*	
C21	0.91426 (18)	0.06929 (18)	0.14722 (12)	0.0636 (8)	
H21A	0.8870	0.1059	0.1216	0.076*	
H21B	0.9279	0.0188	0.1287	0.076*	
C22	0.9984 (2)	0.1077 (2)	0.16797 (13)	0.0632 (8)	
C23	1.00997 (18)	0.26933 (18)	0.29940 (11)	0.0565 (7)	
H23	1.0477	0.2566	0.2713	0.068*	
C24	0.89875 (19)	0.27488 (18)	0.35004 (12)	0.0595 (7)	
H24	0.8432	0.2662	0.3639	0.071*	
C25	0.9610 (2)	0.32244 (17)	0.37273 (12)	0.0644 (8)	

H25	0.9563	0.3521	0.4044	0.077*
C26	0.73884 (17)	0.27658 (18)	0.20333 (11)	0.0549 (7)
H26	0.7033	0.2674	0.2330	0.066*
C27	0.84577 (19)	0.27410 (18)	0.14814 (11)	0.0585 (7)
H27	0.8995	0.2622	0.1326	0.070*
C28	0.7846 (2)	0.32259 (17)	0.12664 (12)	0.0625 (8)
H28	0.7879	0.3498	0.0939	0.075*
N1	0.88931 (14)	0.05132 (14)	0.30650 (9)	0.0537 (6)
N2	0.85342 (14)	0.05256 (14)	0.19088 (9)	0.0531 (6)
N3	0.93063 (14)	0.24140 (13)	0.30321 (9)	0.0503 (6)
N4	1.03098 (16)	0.31812 (15)	0.34020 (10)	0.0626 (7)
H4A	1.0801	0.3424	0.3449	0.075*
N5	0.81647 (14)	0.24446 (13)	0.19703 (8)	0.0494 (6)
N6	0.71714 (15)	0.32427 (14)	0.16178 (10)	0.0604 (6)
H6A	0.6693	0.3510	0.1581	0.072*
O2	0.75060 (12)	0.15092 (11)	0.28925 (7)	0.0597 (5)
O3	0.68863 (15)	0.11563 (16)	0.36534 (9)	0.0894 (8)
O4	0.68267 (16)	−0.18484 (16)	0.01018 (9)	0.0913 (7)
O5	0.99491 (11)	0.14794 (12)	0.21076 (8)	0.0614 (5)
O6	1.06393 (15)	0.09949 (16)	0.13974 (10)	0.0995 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0416 (2)	0.0579 (2)	0.0534 (2)	−0.00057 (15)	−0.00030 (14)	−0.00093 (15)
O1	0.109 (4)	0.127 (4)	0.090 (4)	0.042 (3)	0.007 (3)	0.034 (3)
C1	0.141 (6)	0.131 (7)	0.104 (6)	0.053 (6)	−0.015 (5)	0.045 (5)
C2	0.078 (4)	0.075 (4)	0.062 (4)	0.025 (3)	−0.005 (3)	−0.011 (4)
C3	0.149 (7)	0.109 (5)	0.066 (4)	0.074 (5)	−0.015 (4)	−0.007 (4)
C4	0.113 (7)	0.106 (5)	0.086 (5)	0.057 (4)	−0.051 (4)	−0.012 (4)
C5	0.030 (4)	0.054 (4)	0.100 (6)	−0.005 (3)	−0.011 (3)	0.002 (3)
C6	0.035 (2)	0.055 (3)	0.093 (4)	0.007 (2)	0.009 (2)	0.007 (3)
C7	0.044 (3)	0.068 (4)	0.084 (6)	0.020 (2)	0.005 (3)	0.006 (3)
O1'	0.176 (12)	0.123 (10)	0.157 (13)	0.057 (9)	0.035 (11)	0.066 (10)
C1'	0.166 (14)	0.178 (15)	0.164 (14)	0.014 (10)	0.001 (9)	0.017 (9)
C2'	0.067 (7)	0.054 (7)	0.067 (9)	0.009 (6)	0.000 (6)	−0.005 (6)
C3'	0.096 (8)	0.058 (7)	0.072 (7)	0.044 (6)	0.002 (6)	−0.029 (6)
C4'	0.078 (8)	0.074 (8)	0.075 (8)	0.047 (6)	−0.010 (6)	−0.018 (7)
C5'	0.027 (6)	0.055 (7)	0.069 (7)	−0.019 (5)	0.002 (5)	−0.003 (6)
C6'	0.121 (11)	0.108 (11)	0.142 (11)	0.014 (8)	0.015 (8)	0.018 (8)
C7'	0.090 (8)	0.095 (8)	0.091 (8)	0.008 (6)	−0.002 (6)	−0.002 (6)
C8	0.0454 (17)	0.067 (2)	0.081 (2)	0.0041 (15)	−0.0143 (15)	0.0021 (17)
C9	0.0549 (19)	0.073 (2)	0.0608 (19)	0.0061 (15)	0.0032 (16)	0.0126 (16)
C10	0.0509 (18)	0.0616 (19)	0.062 (2)	0.0048 (14)	0.0054 (15)	0.0128 (16)
C11	0.0653 (19)	0.0550 (19)	0.073 (2)	−0.0045 (15)	−0.0095 (16)	0.0015 (17)
C12	0.062 (2)	0.065 (2)	0.072 (2)	0.0006 (16)	−0.0128 (16)	−0.0070 (17)
C13	0.0399 (15)	0.074 (2)	0.0686 (19)	−0.0006 (14)	−0.0069 (14)	−0.0111 (16)
C14	0.0423 (16)	0.071 (2)	0.0596 (19)	−0.0053 (15)	−0.0056 (14)	−0.0067 (16)

C15	0.0515 (17)	0.084 (2)	0.0520 (18)	−0.0102 (16)	−0.0007 (14)	−0.0027 (16)
C16	0.0485 (17)	0.073 (2)	0.074 (2)	−0.0130 (15)	−0.0007 (16)	−0.0053 (17)
C17	0.0559 (19)	0.084 (2)	0.061 (2)	−0.0030 (17)	−0.0037 (15)	−0.0150 (18)
C18	0.102 (3)	0.106 (3)	0.0504 (19)	−0.037 (2)	−0.0023 (19)	−0.001 (2)
C19	0.091 (3)	0.081 (2)	0.066 (2)	−0.0291 (19)	−0.0129 (19)	0.0095 (19)
C20	0.155 (4)	0.097 (3)	0.104 (4)	−0.035 (3)	−0.018 (3)	−0.025 (3)
C21	0.0512 (18)	0.073 (2)	0.067 (2)	−0.0071 (15)	0.0017 (15)	−0.0204 (16)
C22	0.0516 (19)	0.071 (2)	0.067 (2)	−0.0018 (16)	0.0056 (16)	−0.0123 (17)
C23	0.0519 (18)	0.0651 (19)	0.0526 (18)	−0.0026 (15)	0.0053 (14)	−0.0067 (15)
C24	0.0548 (17)	0.0640 (19)	0.0597 (19)	0.0039 (16)	0.0062 (15)	−0.0003 (16)
C25	0.073 (2)	0.065 (2)	0.0554 (19)	0.0057 (17)	0.0048 (17)	−0.0060 (15)
C26	0.0473 (17)	0.0606 (18)	0.0568 (18)	−0.0018 (14)	0.0042 (14)	0.0077 (15)
C27	0.0533 (17)	0.0663 (19)	0.0558 (19)	−0.0067 (16)	0.0095 (15)	−0.0013 (15)
C28	0.067 (2)	0.070 (2)	0.0514 (18)	−0.0135 (16)	−0.0019 (16)	0.0087 (15)
N1	0.0449 (13)	0.0547 (14)	0.0616 (15)	−0.0004 (11)	−0.0081 (12)	0.0006 (12)
N2	0.0444 (13)	0.0610 (15)	0.0540 (14)	−0.0020 (11)	0.0007 (11)	−0.0074 (12)
N3	0.0420 (13)	0.0561 (14)	0.0530 (14)	0.0007 (11)	0.0013 (11)	−0.0030 (11)
N4	0.0559 (15)	0.0636 (16)	0.0684 (17)	−0.0061 (12)	−0.0052 (13)	−0.0045 (13)
N5	0.0448 (13)	0.0556 (14)	0.0478 (14)	−0.0018 (11)	−0.0008 (11)	0.0030 (10)
N6	0.0473 (14)	0.0643 (16)	0.0694 (17)	−0.0009 (12)	−0.0029 (12)	0.0085 (13)
O2	0.0492 (11)	0.0718 (13)	0.0581 (12)	0.0055 (9)	0.0036 (9)	0.0159 (10)
O3	0.0672 (15)	0.1196 (19)	0.0814 (17)	0.0266 (14)	0.0225 (13)	0.0384 (14)
O4	0.106 (2)	0.1000 (18)	0.0676 (15)	−0.0186 (16)	−0.0063 (13)	−0.0219 (14)
O5	0.0448 (11)	0.0736 (14)	0.0658 (13)	−0.0060 (9)	0.0019 (9)	−0.0164 (11)
O6	0.0589 (14)	0.135 (2)	0.105 (2)	−0.0228 (14)	0.0235 (14)	−0.0598 (16)

Geometric parameters (Å, °)

Zn1—N5	2.099 (2)	C11—H11A	0.9700
Zn1—N3	2.103 (2)	C11—H11B	0.9700
Zn1—O5	2.1086 (18)	C12—N2	1.472 (4)
Zn1—O2	2.1261 (18)	C12—H12A	0.9700
Zn1—N1	2.281 (2)	C12—H12B	0.9700
Zn1—N2	2.287 (2)	C13—C14	1.497 (4)
O1—C1	1.395 (7)	C13—N2	1.511 (3)
O1—C2	1.428 (5)	C13—H13A	0.9700
C1—H1A	0.9600	C13—H13B	0.9700
C1—H1B	0.9600	C14—C19	1.377 (4)
C1—H1C	0.9600	C14—C15	1.382 (4)
C2—C3	1.3900	C15—C16	1.392 (4)
C2—C7	1.3900	C15—H15	0.9300
C3—C4	1.3900	C16—C17	1.381 (4)
C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.3900	C17—C18	1.357 (4)
C4—H4	0.9300	C17—O4	1.377 (4)
C5—C6	1.3900	C18—C19	1.366 (4)
C5—C8	1.558 (4)	C18—H18	0.9300
C6—C7	1.3900	C19—H19	0.9300
C6—H6	0.9300	C20—O4	1.414 (4)

C7—H7	0.9300	C20—H20A	0.9600
O1'—C2'	1.402 (8)	C20—H20B	0.9600
O1'—C1'	1.435 (10)	C20—H20C	0.9600
C1'—H1'1	0.9600	C21—N2	1.458 (3)
C1'—H1'2	0.9600	C21—C22	1.525 (4)
C1'—H1'3	0.9600	C21—H21A	0.9700
C2'—C3'	1.3900	C21—H21B	0.9700
C2'—C7'	1.3900	C22—O6	1.233 (3)
C3'—C4'	1.3900	C22—O5	1.253 (3)
C3'—H3'	0.9300	C23—N3	1.303 (3)
C4'—C5'	1.3900	C23—N4	1.332 (3)
C4'—H4'	0.9300	C23—H23	0.9300
C5'—C6'	1.3900	C24—C25	1.355 (4)
C5'—C8	1.443 (7)	C24—N3	1.377 (3)
C6'—C7'	1.3900	C24—H24	0.9300
C6'—H6'	0.9300	C25—N4	1.346 (4)
C7'—H7'	0.9300	C25—H25	0.9300
C8—N1	1.495 (3)	C26—N5	1.311 (3)
C8—H8A	0.9700	C26—N6	1.338 (3)
C8—H8B	0.9700	C26—H26	0.9300
C9—N1	1.453 (3)	C27—C28	1.341 (4)
C9—C10	1.517 (4)	C27—N5	1.384 (3)
C9—H9A	0.9700	C27—H27	0.9300
C9—H9B	0.9700	C28—N6	1.354 (3)
C10—O3	1.235 (3)	C28—H28	0.9300
C10—O2	1.243 (3)	N4—H4A	0.8600
C11—N1	1.459 (4)	N6—H6A	0.8600
C11—C12	1.507 (5)		
N5—Zn1—N3	97.89 (9)	C11—C12—H12B	109.2
N5—Zn1—O5	98.14 (8)	H12A—C12—H12B	107.9
N3—Zn1—O5	88.30 (8)	C14—C13—N2	117.1 (2)
N5—Zn1—O2	88.14 (8)	C14—C13—H13A	108.0
N3—Zn1—O2	96.37 (8)	N2—C13—H13A	108.0
O5—Zn1—O2	171.62 (8)	C14—C13—H13B	108.0
N5—Zn1—N1	161.68 (8)	N2—C13—H13B	108.0
N3—Zn1—N1	92.98 (8)	H13A—C13—H13B	107.3
O5—Zn1—N1	96.89 (8)	C19—C14—C15	116.9 (3)
O2—Zn1—N1	75.98 (7)	C19—C14—C13	121.7 (3)
N5—Zn1—N2	93.68 (8)	C15—C14—C13	121.4 (3)
N3—Zn1—N2	161.94 (8)	C14—C15—C16	121.8 (3)
O5—Zn1—N2	76.32 (7)	C14—C15—H15	119.1
O2—Zn1—N2	97.83 (8)	C16—C15—H15	119.1
N1—Zn1—N2	79.75 (9)	C17—C16—C15	118.7 (3)
C1—O1—C2	119.5 (6)	C17—C16—H16	120.6
C3—C2—C7	120.0	C15—C16—H16	120.6
C3—C2—O1	115.4 (4)	C18—C17—O4	116.1 (3)
C7—C2—O1	124.5 (4)	C18—C17—C16	120.0 (3)
C4—C3—C2	120.0	O4—C17—C16	123.9 (3)
C4—C3—H3	120.0	C17—C18—C19	120.4 (3)

C2—C3—H3	120.0	C17—C18—H18	119.8
C3—C4—C5	120.0	C19—C18—H18	119.8
C3—C4—H4	120.0	C18—C19—C14	122.1 (3)
C5—C4—H4	120.0	C18—C19—H19	118.9
C4—C5—C6	120.0	C14—C19—H19	118.9
C4—C5—C8	118.2 (3)	O4—C20—H20A	109.5
C6—C5—C8	121.2 (3)	O4—C20—H20B	109.5
C7—C6—C5	120.0	H20A—C20—H20B	109.5
C7—C6—H6	120.0	O4—C20—H20C	109.5
C5—C6—H6	120.0	H20A—C20—H20C	109.5
C6—C7—C2	120.0	H20B—C20—H20C	109.5
C6—C7—H7	120.0	N2—C21—C22	111.5 (2)
C2—C7—H7	120.0	N2—C21—H21A	109.3
C2'—O1'—C1'	113.5 (19)	C22—C21—H21A	109.3
O1'—C1'—H1'1	109.5	N2—C21—H21B	109.3
O1'—C1'—H1'2	109.5	C22—C21—H21B	109.3
H1'1—C1'—H1'2	109.5	H21A—C21—H21B	108.0
O1'—C1'—H1'3	109.5	O6—C22—O5	125.1 (3)
H1'1—C1'—H1'3	109.5	O6—C22—C21	116.8 (3)
H1'2—C1'—H1'3	109.5	O5—C22—C21	118.0 (3)
C3'—C2'—C7'	120.0	N3—C23—N4	112.4 (2)
C3'—C2'—O1'	122.9 (10)	N3—C23—H23	123.8
C7'—C2'—O1'	116.3 (10)	N4—C23—H23	123.8
C2'—C3'—C4'	120.0	C25—C24—N3	109.4 (3)
C2'—C3'—H3'	120.0	C25—C24—H24	125.3
C4'—C3'—H3'	120.0	N3—C24—H24	125.3
C5'—C4'—C3'	120.0	N4—C25—C24	106.3 (3)
C5'—C4'—H4'	120.0	N4—C25—H25	126.9
C3'—C4'—H4'	120.0	C24—C25—H25	126.9
C4'—C5'—C6'	120.0	N5—C26—N6	111.6 (2)
C4'—C5'—C8	125.3 (10)	N5—C26—H26	124.2
C6'—C5'—C8	113.3 (10)	N6—C26—H26	124.2
C5'—C6'—C7'	120.0	C28—C27—N5	109.4 (3)
C5'—C6'—H6'	120.0	C28—C27—H27	125.3
C7'—C6'—H6'	120.0	N5—C27—H27	125.3
C6'—C7'—C2'	120.0	C27—C28—N6	106.8 (3)
C6'—C7'—H7'	120.0	C27—C28—H28	126.6
C2'—C7'—H7'	120.0	N6—C28—H28	126.6
C5'—C8—N1	126.5 (7)	C9—N1—C11	109.3 (2)
N1—C8—C5	113.6 (3)	C9—N1—C8	112.3 (2)
C5'—C8—H8A	104.0	C11—N1—C8	113.4 (2)
N1—C8—H8A	108.9	C9—N1—Zn1	104.05 (17)
C5—C8—H8A	108.9	C11—N1—Zn1	105.91 (17)
C5'—C8—H8B	99.5	C8—N1—Zn1	111.33 (17)
N1—C8—H8B	108.9	C21—N2—C12	109.0 (2)
C5—C8—H8B	108.9	C21—N2—C13	112.0 (2)
H8A—C8—H8B	107.7	C12—N2—C13	113.3 (2)
N1—C9—C10	112.2 (2)	C21—N2—Zn1	104.23 (16)
N1—C9—H9A	109.2	C12—N2—Zn1	106.03 (17)

C10—C9—H9A	109.2	C13—N2—Zn1	111.68 (16)
N1—C9—H9B	109.2	C23—N3—C24	104.6 (2)
C10—C9—H9B	109.2	C23—N3—Zn1	124.95 (19)
H9A—C9—H9B	107.9	C24—N3—Zn1	130.35 (19)
O3—C10—O2	124.7 (3)	C23—N4—C25	107.3 (2)
O3—C10—C9	116.4 (3)	C23—N4—H4A	126.4
O2—C10—C9	118.8 (3)	C25—N4—H4A	126.4
N1—C11—C12	112.4 (2)	C26—N5—C27	105.0 (2)
N1—C11—H11A	109.1	C26—N5—Zn1	124.67 (19)
C12—C11—H11A	109.1	C27—N5—Zn1	130.1 (2)
N1—C11—H11B	109.1	C26—N6—C28	107.3 (2)
C12—C11—H11B	109.1	C26—N6—H6A	126.4
H11A—C11—H11B	107.9	C28—N6—H6A	126.4
N2—C12—C11	112.0 (2)	C10—O2—Zn1	116.58 (18)
N2—C12—H12A	109.2	C17—O4—C20	119.4 (3)
C11—C12—H12A	109.2	C22—O5—Zn1	117.84 (18)
N2—C12—H12B	109.2		
C1—O1—C2—C3	−175.9 (6)	N3—Zn1—N1—C8	−54.73 (19)
C1—O1—C2—C7	6.7 (8)	O5—Zn1—N1—C8	33.9 (2)
C7—C2—C3—C4	0.0	O2—Zn1—N1—C8	−150.6 (2)
O1—C2—C3—C4	−177.5 (5)	N2—Zn1—N1—C8	108.6 (2)
C2—C3—C4—C5	0.0	C22—C21—N2—C12	−76.9 (3)
C3—C4—C5—C6	0.0	C22—C21—N2—C13	156.9 (2)
C3—C4—C5—C8	−171.6 (5)	C22—C21—N2—Zn1	36.0 (3)
C4—C5—C6—C7	0.0	C11—C12—N2—C21	151.0 (2)
C8—C5—C6—C7	171.3 (5)	C11—C12—N2—C13	−83.5 (3)
C5—C6—C7—C2	0.0	C11—C12—N2—Zn1	39.4 (3)
C3—C2—C7—C6	0.0	C14—C13—N2—C21	59.1 (3)
O1—C2—C7—C6	177.3 (5)	C14—C13—N2—C12	−64.7 (3)
C1'—O1'—C2'—C3'	−18 (2)	C14—C13—N2—Zn1	175.6 (2)
C1'—O1'—C2'—C7'	152.0 (17)	N5—Zn1—N2—C21	69.48 (18)
C7'—C2'—C3'—C4'	0.0	N3—Zn1—N2—C21	−60.4 (4)
O1'—C2'—C3'—C4'	169.5 (13)	O5—Zn1—N2—C21	−28.01 (17)
C2'—C3'—C4'—C5'	0.0	O2—Zn1—N2—C21	158.10 (17)
C3'—C4'—C5'—C6'	0.0	N1—Zn1—N2—C21	−127.76 (18)
C3'—C4'—C5'—C8	165.5 (14)	N5—Zn1—N2—C12	−175.58 (17)
C4'—C5'—C6'—C7'	0.0	N3—Zn1—N2—C12	54.6 (3)
C8—C5'—C6'—C7'	−167.1 (13)	O5—Zn1—N2—C12	86.93 (17)
C5'—C6'—C7'—C2'	0.0	O2—Zn1—N2—C12	−86.96 (17)
C3'—C2'—C7'—C6'	0.0	N1—Zn1—N2—C12	−12.82 (17)
O1'—C2'—C7'—C6'	−170.1 (12)	N5—Zn1—N2—C13	−51.68 (19)
C4'—C5'—C8—N1	−74.9 (12)	N3—Zn1—N2—C13	178.5 (2)
C6'—C5'—C8—N1	91.5 (9)	O5—Zn1—N2—C13	−149.2 (2)
C4'—C5'—C8—C5	−61 (3)	O2—Zn1—N2—C13	36.94 (19)
C6'—C5'—C8—C5	105 (3)	N1—Zn1—N2—C13	111.07 (19)
C4—C5—C8—C5'	111 (3)	N4—C23—N3—C24	−0.1 (3)
C6—C5—C8—C5'	−60 (3)	N4—C23—N3—Zn1	−177.41 (18)
C4—C5—C8—N1	−80.7 (4)	C25—C24—N3—C23	0.2 (3)
C6—C5—C8—N1	107.9 (4)	C25—C24—N3—Zn1	177.30 (19)

N1—C9—C10—O3	162.8 (3)	N5—Zn1—N3—C23	−91.8 (2)
N1—C9—C10—O2	−21.7 (4)	O5—Zn1—N3—C23	6.2 (2)
N1—C11—C12—N2	−58.1 (3)	O2—Zn1—N3—C23	179.2 (2)
N2—C13—C14—C19	−84.7 (4)	N1—Zn1—N3—C23	103.0 (2)
N2—C13—C14—C15	97.2 (3)	N2—Zn1—N3—C23	37.5 (4)
C19—C14—C15—C16	0.4 (4)	N5—Zn1—N3—C24	91.6 (2)
C13—C14—C15—C16	178.6 (3)	O5—Zn1—N3—C24	−170.4 (2)
C14—C15—C16—C17	0.3 (4)	O2—Zn1—N3—C24	2.6 (2)
C15—C16—C17—C18	−0.1 (5)	N1—Zn1—N3—C24	−73.6 (2)
C15—C16—C17—O4	179.5 (3)	N2—Zn1—N3—C24	−139.1 (3)
O4—C17—C18—C19	179.4 (3)	N3—C23—N4—C25	0.0 (3)
C16—C17—C18—C19	−1.0 (5)	C24—C25—N4—C23	0.2 (3)
C17—C18—C19—C14	1.8 (6)	N6—C26—N5—C27	0.1 (3)
C15—C14—C19—C18	−1.4 (5)	N6—C26—N5—Zn1	−175.02 (17)
C13—C14—C19—C18	−179.7 (3)	C28—C27—N5—C26	−0.3 (3)
N2—C21—C22—O6	156.1 (3)	C28—C27—N5—Zn1	174.41 (19)
N2—C21—C22—O5	−26.9 (4)	N3—Zn1—N5—C26	−87.8 (2)
N3—C24—C25—N4	−0.2 (3)	O5—Zn1—N5—C26	−177.2 (2)
N5—C27—C28—N6	0.4 (3)	O2—Zn1—N5—C26	8.4 (2)
C10—C9—N1—C11	−77.8 (3)	N1—Zn1—N5—C26	38.0 (4)
C10—C9—N1—C8	155.5 (2)	N2—Zn1—N5—C26	106.1 (2)
C10—C9—N1—Zn1	35.0 (3)	N3—Zn1—N5—C27	98.3 (2)
C12—C11—N1—C9	153.2 (2)	O5—Zn1—N5—C27	8.9 (2)
C12—C11—N1—C8	−80.7 (3)	O2—Zn1—N5—C27	−165.5 (2)
C12—C11—N1—Zn1	41.7 (3)	N1—Zn1—N5—C27	−135.8 (3)
C5'—C8—N1—C9	66.0 (8)	N2—Zn1—N5—C27	−67.8 (2)
C5—C8—N1—C9	62.6 (4)	N5—C26—N6—C28	0.2 (3)
C5'—C8—N1—C11	−58.5 (8)	C27—C28—N6—C26	−0.4 (3)
C5—C8—N1—C11	−61.9 (4)	O3—C10—O2—Zn1	167.9 (3)
C5'—C8—N1—Zn1	−177.8 (8)	C9—C10—O2—Zn1	−7.2 (4)
C5—C8—N1—Zn1	178.8 (3)	N5—Zn1—O2—C10	−168.1 (2)
N5—Zn1—N1—C9	−60.0 (3)	N3—Zn1—O2—C10	−70.4 (2)
N3—Zn1—N1—C9	66.46 (18)	N1—Zn1—O2—C10	21.1 (2)
O5—Zn1—N1—C9	155.10 (17)	N2—Zn1—O2—C10	98.4 (2)
O2—Zn1—N1—C9	−29.37 (17)	C18—C17—O4—C20	179.7 (3)
N2—Zn1—N1—C9	−130.20 (18)	C16—C17—O4—C20	0.2 (5)
N5—Zn1—N1—C11	55.2 (3)	O6—C22—O5—Zn1	176.3 (3)
N3—Zn1—N1—C11	−178.36 (18)	C21—C22—O5—Zn1	−0.4 (4)
O5—Zn1—N1—C11	−89.71 (18)	N5—Zn1—O5—C22	−75.3 (2)
O2—Zn1—N1—C11	85.81 (18)	N3—Zn1—O5—C22	−173.1 (2)
N2—Zn1—N1—C11	−15.02 (18)	N1—Zn1—O5—C22	94.2 (2)
N5—Zn1—N1—C8	178.8 (2)	N2—Zn1—O5—C22	16.5 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4A···O3^{i}	0.86	1.87	2.722 (3)	171
N6—H6A···O6^{ii}	0.86	1.86	2.716 (3)	171
C23—H23···O5	0.93	2.47	2.979 (4)	115

C26—H26···O2	0.93	2.48	2.974 (3)	114

Symmetry codes: (i) *x*+1/2, −*y*+1/2, *z*; (ii) *x*−1/2, −*y*+1/2, *z*.

Fig. 1

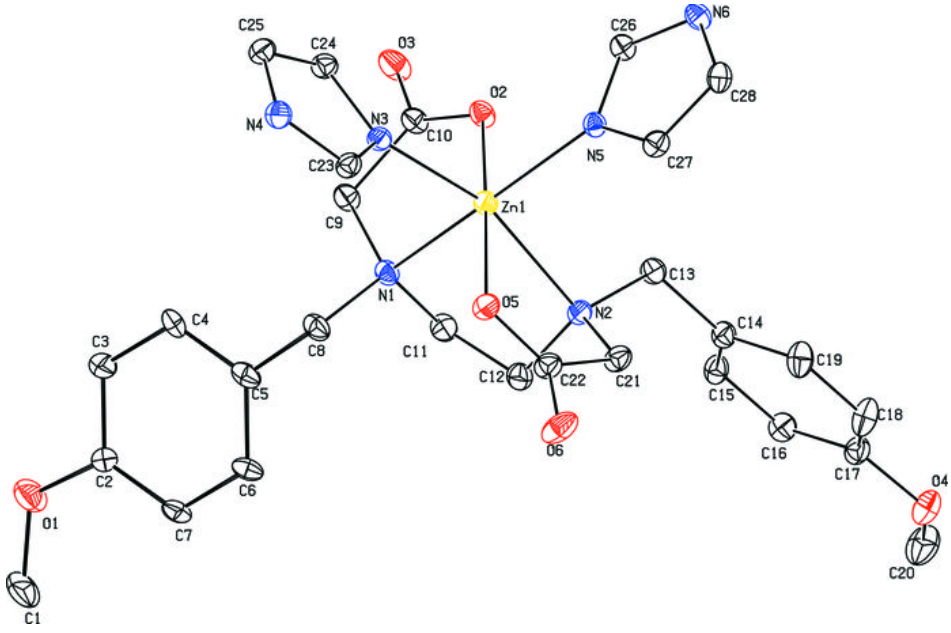

Fig. 2