

Aqua(4,4'-dimethyl-2,2'-bipyridine- κ^2N,N')(nitrate- κO)(nitrate- κ^2O,O')zinc

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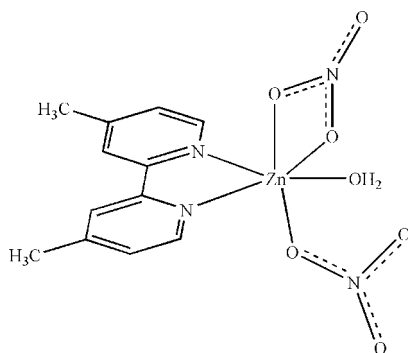
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 Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.037; wR factor = 0.084; data-to-parameter ratio = 18.5.

In the title compound, $[Zn(NO_3)_2(C_{12}H_{12}N_2)(H_2O)]$, the Zn^{II} atom is six-coordinated in a distorted octahedral geometry by two N atoms from a chelating 4,4'-dimethyl-2,2'-bipyridine ligand, one water O atom, one O atom from a monodentate nitrate anion and two O atoms from a chelating nitrate anion. In the crystal, there are aromatic $\pi-\pi$ contacts between the pyridine rings [centroid-centroid distances = 3.9577 (13) Å] and intermolecular $O-H\cdots O$ and $C-H\cdots O$ hydrogen bonds.

Related literature

For related structures, see: Ahmadi *et al.* (2008); Alizadeh *et al.* (2010); Amani *et al.* (2009); Bellusci *et al.* (2008); Hojjat Kashani *et al.* (2008); Kalateh *et al.* (2008, 2010); Sakamoto *et al.* (2004); Sofetis *et al.* (2006); Willett *et al.* (2001); Yoshikawa *et al.* (2003); Yousefi *et al.* (2008).



Experimental

Crystal data

$[Zn(NO_3)_2(C_{12}H_{12}N_2)(H_2O)]$	$V = 1559.33$ (11) Å ³
$M_r = 391.66$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 10.9266$ (5) Å	$\mu = 1.62$ mm ⁻¹
$b = 8.5717$ (3) Å	$T = 120$ K
$c = 16.8073$ (7) Å	$0.5 \times 0.4 \times 0.31$ mm
$\beta = 97.873$ (4)°	

Data collection

Bruker APEXII CCD area-detector diffractometer	16739 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2001)	4193 independent reflections
$T_{min} = 0.460$, $T_{max} = 0.596$	3596 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.054$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.084$	$\Delta\rho_{max} = 0.50$ e Å ⁻³
$S = 1.08$	$\Delta\rho_{min} = -0.65$ e Å ⁻³
4193 reflections	
227 parameters	

Table 1

Selected bond lengths (Å).

Zn1—N1	2.1157 (16)	Zn1—O2	2.5143 (16)
Zn1—N2	2.0727 (17)	Zn1—O4	2.0340 (15)
Zn1—O1	2.0965 (15)	Zn1—O7	2.0752 (15)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O7—H7A \cdots O4 ⁱ	0.85 (3)	1.90 (3)	2.724 (2)	163 (3)
O7—H7B \cdots O3 ⁱⁱ	0.87 (4)	1.94 (4)	2.799 (2)	174 (3)
C5—H5 \cdots O2 ⁱⁱⁱ	0.93	2.53	3.420 (2)	161
C8—H8 \cdots O2 ⁱⁱⁱ	0.93	2.36	3.230 (2)	156
C11—H11 \cdots O6 ^{iv}	0.93	2.44	3.284 (3)	151

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5709).

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supplementary materials

Acta Cryst. (2011). E67, m1866-m1867 [doi:10.1107/S1600536811050227]

Aqua(4,4'-dimethyl-2,2'-bipyridine- κ^2N,N')(nitrate- κO)(nitrate- κ^2O,O')zinc

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Comment

4,4'-Dimethyl-2,2'-bipyridine (4,4'-dmbipy), is a good bidentate ligand, and numerous complexes with 4,4'-dmbipy have been prepared, such as that of mercury (Kalateh *et al.*, 2008; Yousefi *et al.*, 2008), indium (Ahmadi *et al.*, 2008), iron (Amani *et al.*, 2009), platinum (Hojjat Kashani *et al.*, 2008), manganese (Sakamoto *et al.*, 2004), silver (Bellusci *et al.*, 2008), gallium (Sofetis *et al.*, 2006), copper (Willett *et al.*, 2001), iridium (Yoshikawa *et al.*, 2003), cadmium (Kalateh *et al.*, 2010) and zinc (Alizadeh *et al.*, 2010). Here, we report the synthesis and structure of the title compound.

In the molecule of the title compound, (Fig. 1), the Zn^{II} atom is six-coordinated in a distorted octahedral configuration by two N atoms from the chelating 4,4'-dimethyl-2,2'-bipyridine, one O atom from water, one O atom from monodentate nitrate anion and two O atoms from the chelating nitrate anion. The Zn—O and Zn—N bond lengths and angles are collected in Table 1.

In the crystal structure, intermolecular O—H \cdots O and C—H \cdots O hydrogen bonds (Table 2 & Fig. 2) link the molecules, in which they may be effective in the stabilization of the structure. There are also aromatic π - π contacts between the pyridine rings, Cg3 \cdots Cg4ⁱ [symmetry cods: (i) 1-*X*,*-Y*,*-Z*, where Cg3 and Cg4 are centroids of the rings (N1/C1—C3/C5—C6) and (N2/C7—C9/C11—C12), respectively] further stabilize the structure, with centroid-centroid distances of 3.9577 (13) Å.

Experimental

For the preparation of the title compound, a solution of 4,4'-dimethyl-2,2'-bipyridine (0.20 g, 1.10 mmol) in methanol (10 ml) was added to a solution of Zn(NO₃)₂·6H₂O (0.33 g, 1.10 mmol) in acetonitrile (10 ml) and the resulting colorless solution was stirred for 20 min at 313 K. This solution was left to evaporate slowly at room temperature. After one week, colorless prismatic crystals of the title compound were isolated (yield 0.33 g, 76.6%).

Refinement

H atoms bonded to C were positioned geometrically, with C—H=0.93 Å for aromatics H and constrained to ride on their parent atoms, with $U_{iso}(H)=1.2U_{eq}$. H atoms bonded to O were freely refined.

Figures

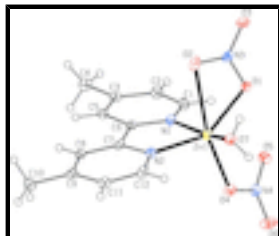


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

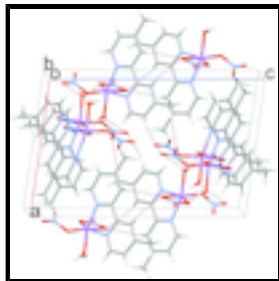


Fig. 2. Unit-cell packing diagram for title compound.

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Crystal data

[Zn(NO₃)₂(C₁₂H₁₂N₂)(H₂O)]

$M_r = 391.66$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 10.9266$ (5) Å

$b = 8.5717$ (3) Å

$c = 16.8073$ (7) Å

$\beta = 97.873$ (4)°

$V = 1559.33$ (11) Å³

$Z = 4$

$F(000) = 800$

$D_x = 1.668$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 16739 reflections

$\theta = 2.1$ – 29.2 °

$\mu = 1.62$ mm⁻¹

$T = 120$ K

Prism, colorless

$0.5 \times 0.4 \times 0.31$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer

graphite

ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2001)

$T_{\min} = 0.460$, $T_{\max} = 0.596$

16739 measured reflections

4193 independent reflections

3596 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.054$

$\theta_{\text{max}} = 29.2$ °, $\theta_{\text{min}} = 2.1$ °

$h = -14 \rightarrow 14$

$k = -11 \rightarrow 11$

$l = -20 \rightarrow 23$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.037$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.084$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.08$	$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2 + 0.5925P]$
4193 reflections	where $P = (F_o^2 + 2F_c^2)/3$
227 parameters	$(\Delta/\sigma)_{\max} = 0.011$
0 restraints	$\Delta\rho_{\max} = 0.50 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -0.65 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.66295 (19)	0.0759 (2)	0.21188 (13)	0.0223 (4)
H1	0.6598	0.1397	0.2563	0.027*
C2	0.77558 (18)	0.0545 (3)	0.18405 (13)	0.0235 (4)
H2	0.8465	0.1018	0.2102	0.028*
C3	0.78166 (17)	-0.0388 (2)	0.11638 (12)	0.0193 (4)
C4	0.90160 (18)	-0.0652 (3)	0.08374 (15)	0.0266 (4)
H4A	0.9514	-0.1379	0.1175	0.032*
H4B	0.945	0.0319	0.0826	0.032*
H4C	0.8849	-0.1066	0.0303	0.032*
C5	0.67277 (17)	-0.1087 (2)	0.08084 (12)	0.0180 (4)
H5	0.6732	-0.1716	0.0358	0.022*
C6	0.56307 (16)	-0.0844 (2)	0.11273 (11)	0.0154 (3)
C7	0.44364 (16)	-0.1594 (2)	0.07909 (11)	0.0157 (3)
C8	0.43269 (17)	-0.2639 (2)	0.01571 (11)	0.0178 (4)
H8	0.5013	-0.2879	-0.0092	0.021*
C9	0.31873 (18)	-0.3335 (2)	-0.01087 (12)	0.0188 (4)
C10	0.3034 (2)	-0.4469 (3)	-0.07953 (14)	0.0275 (4)

supplementary materials

H10C	0.2531	-0.5329	-0.0668	0.033*
H10B	0.383	-0.4849	-0.0886	0.033*
H10A	0.2643	-0.3956	-0.1271	0.033*
C11	0.21939 (18)	-0.2944 (3)	0.02924 (12)	0.0220 (4)
H11	0.1423	-0.3396	0.0142	0.026*
C12	0.23656 (17)	-0.1886 (3)	0.09121 (12)	0.0227 (4)
H12	0.1693	-0.163	0.1171	0.027*
N1	0.55839 (15)	0.0081 (2)	0.17723 (10)	0.0179 (3)
N2	0.34579 (14)	-0.1203 (2)	0.11628 (10)	0.0180 (3)
N3	0.39927 (16)	0.3475 (2)	0.16842 (11)	0.0222 (3)
N4	0.44300 (15)	-0.0611 (2)	0.36776 (10)	0.0202 (3)
O1	0.41779 (13)	0.27826 (17)	0.23681 (8)	0.0216 (3)
O2	0.36572 (15)	0.2656 (2)	0.10800 (9)	0.0288 (3)
O3	0.41477 (16)	0.4902 (2)	0.16496 (11)	0.0316 (4)
O4	0.37061 (13)	-0.10009 (18)	0.30217 (9)	0.0224 (3)
O5	0.50246 (15)	0.06073 (19)	0.36678 (10)	0.0287 (3)
O6	0.44574 (16)	-0.1479 (2)	0.42578 (10)	0.0360 (4)
O7	0.19144 (14)	0.0920 (2)	0.20178 (10)	0.0242 (3)
H7A	0.169 (3)	0.185 (4)	0.1905 (18)	0.036 (8)*
H7B	0.156 (4)	0.067 (4)	0.243 (2)	0.058 (11)*
Zn1	0.37859 (2)	0.04435 (3)	0.207009 (13)	0.01710 (7)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0188 (9)	0.0263 (11)	0.0217 (10)	-0.0027 (7)	0.0022 (7)	-0.0054 (8)
C2	0.0149 (8)	0.0291 (11)	0.0259 (10)	-0.0042 (8)	0.0002 (7)	-0.0003 (8)
C3	0.0117 (8)	0.0217 (9)	0.0246 (9)	0.0021 (7)	0.0031 (7)	0.0059 (8)
C4	0.0132 (8)	0.0314 (12)	0.0360 (12)	0.0009 (8)	0.0064 (8)	0.0022 (9)
C5	0.0152 (8)	0.0191 (9)	0.0203 (9)	0.0015 (7)	0.0046 (7)	0.0011 (7)
C6	0.0133 (8)	0.0175 (9)	0.0157 (8)	0.0017 (6)	0.0025 (6)	0.0032 (6)
C7	0.0106 (8)	0.0210 (9)	0.0158 (8)	-0.0002 (6)	0.0024 (6)	0.0025 (7)
C8	0.0152 (8)	0.0207 (9)	0.0182 (9)	0.0006 (7)	0.0047 (6)	0.0011 (7)
C9	0.0185 (9)	0.0212 (10)	0.0164 (9)	-0.0008 (7)	0.0009 (7)	0.0019 (7)
C10	0.0268 (10)	0.0263 (11)	0.0283 (11)	-0.0032 (9)	0.0003 (8)	-0.0058 (9)
C11	0.0142 (8)	0.0295 (11)	0.0215 (9)	-0.0022 (8)	-0.0006 (7)	0.0022 (8)
C12	0.0106 (8)	0.0368 (12)	0.0209 (9)	-0.0003 (8)	0.0026 (7)	0.0007 (8)
N1	0.0139 (7)	0.0210 (8)	0.0189 (8)	0.0010 (6)	0.0026 (6)	-0.0005 (6)
N2	0.0112 (7)	0.0250 (9)	0.0178 (8)	0.0015 (6)	0.0024 (5)	-0.0008 (6)
N3	0.0190 (8)	0.0264 (9)	0.0232 (9)	0.0038 (7)	0.0099 (6)	0.0031 (7)
N4	0.0160 (7)	0.0248 (9)	0.0189 (8)	0.0005 (6)	-0.0006 (6)	-0.0003 (6)
O1	0.0255 (7)	0.0218 (7)	0.0182 (7)	0.0021 (6)	0.0055 (5)	0.0024 (5)
O2	0.0269 (8)	0.0409 (10)	0.0195 (7)	0.0022 (7)	0.0063 (6)	-0.0033 (6)
O3	0.0360 (9)	0.0257 (8)	0.0370 (9)	0.0029 (7)	0.0185 (7)	0.0095 (7)
O4	0.0209 (7)	0.0262 (7)	0.0185 (7)	-0.0056 (6)	-0.0029 (5)	0.0013 (6)
O5	0.0281 (8)	0.0273 (8)	0.0299 (8)	-0.0102 (6)	0.0011 (6)	-0.0023 (6)
O6	0.0388 (9)	0.0395 (10)	0.0257 (8)	-0.0091 (8)	-0.0103 (7)	0.0133 (7)
O7	0.0182 (7)	0.0229 (8)	0.0333 (9)	0.0056 (6)	0.0102 (6)	0.0052 (6)

Zn1 0.01435 (11) 0.02035 (12) 0.01732 (12) 0.00208 (9) 0.00476 (7) -0.00014 (9)

Geometric parameters (Å, °)

C1—N1	1.342 (3)	C10—H10B	0.96
C1—C2	1.387 (3)	C10—H10A	0.96
C1—H1	0.93	C11—C12	1.374 (3)
C2—C3	1.399 (3)	C11—H11	0.93
C2—H2	0.93	C12—N2	1.344 (2)
C3—C5	1.392 (3)	C12—H12	0.93
C3—C4	1.506 (3)	Zn1—N1	2.1157 (16)
C4—H4A	0.96	Zn1—N2	2.0727 (17)
C4—H4B	0.96	N3—O3	1.238 (3)
C4—H4C	0.96	N3—O2	1.248 (2)
C5—C6	1.394 (3)	N3—O1	1.285 (2)
C5—H5	0.93	N4—O6	1.223 (2)
C6—N1	1.350 (3)	N4—O5	1.231 (2)
C6—C7	1.494 (2)	N4—O4	1.309 (2)
C7—N2	1.352 (2)	Zn1—O1	2.0965 (15)
C7—C8	1.385 (3)	Zn1—O2	2.5143 (16)
C8—C9	1.397 (3)	Zn1—O4	2.0340 (15)
C8—H8	0.93	Zn1—O7	2.0752 (15)
C9—C11	1.395 (3)	O7—H7A	0.84 (3)
C9—C10	1.501 (3)	O7—H7B	0.87 (4)
C10—H10C	0.96		
N1—C1—C2	122.57 (19)	H10B—C10—H10A	109.5
N1—C1—H1	118.7	C12—C11—C9	119.35 (18)
C2—C1—H1	118.7	C12—C11—H11	120.3
C1—C2—C3	119.52 (18)	C9—C11—H11	120.3
C1—C2—H2	120.2	N2—C12—C11	123.24 (18)
C3—C2—H2	120.2	N2—C12—H12	118.4
C5—C3—C2	117.51 (17)	C11—C12—H12	118.4
C5—C3—C4	120.95 (19)	C1—N1—C6	118.65 (17)
C2—C3—C4	121.53 (18)	C1—N1—Zn1	126.65 (14)
C3—C4—H4A	109.5	C6—N1—Zn1	114.51 (12)
C3—C4—H4B	109.5	C12—N2—C7	118.13 (18)
H4A—C4—H4B	109.5	C12—N2—Zn1	125.71 (14)
C3—C4—H4C	109.5	C7—N2—Zn1	116.15 (13)
H4A—C4—H4C	109.5	O3—N3—O2	123.01 (19)
H4B—C4—H4C	109.5	O3—N3—O1	119.53 (18)
C3—C5—C6	120.01 (18)	O2—N3—O1	117.46 (18)
C3—C5—H5	120	O6—N4—O5	124.81 (17)
C6—C5—H5	120	O6—N4—O4	117.51 (17)
N1—C6—C5	121.72 (17)	O5—N4—O4	117.68 (17)
N1—C6—C7	115.43 (16)	N3—O1—Zn1	103.06 (12)
C5—C6—C7	122.85 (18)	N4—O4—Zn1	114.88 (12)
N2—C7—C8	121.69 (17)	Zn1—O7—H7A	116 (2)
N2—C7—C6	115.03 (17)	Zn1—O7—H7B	118 (2)
C8—C7—C6	123.26 (17)	H7A—O7—H7B	105 (3)

supplementary materials

C7—C8—C9	120.09 (17)	O4—Zn1—N2	98.18 (7)
C7—C8—H8	120	O4—Zn1—O7	90.28 (6)
C9—C8—H8	120	N2—Zn1—O7	91.88 (6)
C11—C9—C8	117.48 (18)	O4—Zn1—O1	115.06 (6)
C11—C9—C10	120.98 (18)	N2—Zn1—O1	146.72 (6)
C8—C9—C10	121.54 (18)	O7—Zn1—O1	89.42 (6)
C9—C10—H10C	109.5	O4—Zn1—N1	103.76 (6)
C9—C10—H10B	109.5	N2—Zn1—N1	78.38 (6)
H10C—C10—H10B	109.5	O7—Zn1—N1	163.82 (7)
C9—C10—H10A	109.5	O1—Zn1—N1	91.77 (6)
H10C—C10—H10A	109.5		
N1—C1—C2—C3	1.2 (3)	C6—C7—N2—Zn1	3.6 (2)
C1—C2—C3—C5	-1.2 (3)	O3—N3—O1—Zn1	-179.98 (15)
C1—C2—C3—C4	179.8 (2)	O2—N3—O1—Zn1	0.18 (19)
C2—C3—C5—C6	0.1 (3)	O6—N4—O4—Zn1	-176.91 (15)
C4—C3—C5—C6	179.08 (19)	O5—N4—O4—Zn1	3.7 (2)
C3—C5—C6—N1	1.1 (3)	N4—O4—Zn1—N2	147.48 (13)
C3—C5—C6—C7	-178.21 (18)	N4—O4—Zn1—O7	-120.58 (14)
N1—C6—C7—N2	2.1 (2)	N4—O4—Zn1—O1	-31.09 (15)
C5—C6—C7—N2	-178.61 (18)	N4—O4—Zn1—N1	67.52 (14)
N1—C6—C7—C8	-176.59 (18)	C12—N2—Zn1—O4	73.10 (18)
C5—C6—C7—C8	2.7 (3)	C7—N2—Zn1—O4	-107.81 (14)
N2—C7—C8—C9	-0.7 (3)	C12—N2—Zn1—O7	-17.46 (18)
C6—C7—C8—C9	177.87 (18)	C7—N2—Zn1—O7	161.64 (15)
C7—C8—C9—C11	-0.7 (3)	C12—N2—Zn1—O1	-109.26 (19)
C7—C8—C9—C10	179.82 (19)	C7—N2—Zn1—O1	69.83 (18)
C8—C9—C11—C12	1.3 (3)	C12—N2—Zn1—N1	175.56 (18)
C10—C9—C11—C12	-179.2 (2)	C7—N2—Zn1—N1	-5.34 (14)
C9—C11—C12—N2	-0.6 (3)	N3—O1—Zn1—O4	-170.58 (10)
C2—C1—N1—C6	0.0 (3)	N3—O1—Zn1—N2	12.00 (17)
C2—C1—N1—Zn1	-174.67 (16)	N3—O1—Zn1—O7	-80.55 (12)
C5—C6—N1—C1	-1.1 (3)	N3—O1—Zn1—N1	83.32 (12)
C7—C6—N1—C1	178.23 (17)	C1—N1—Zn1—O4	-83.06 (18)
C5—C6—N1—Zn1	174.17 (14)	C6—N1—Zn1—O4	102.12 (14)
C7—C6—N1—Zn1	-6.5 (2)	C1—N1—Zn1—N2	-178.76 (19)
C11—C12—N2—C7	-0.8 (3)	C6—N1—Zn1—N2	6.43 (14)
C11—C12—N2—Zn1	178.30 (16)	C1—N1—Zn1—O7	127.3 (2)
C8—C7—N2—C12	1.4 (3)	C6—N1—Zn1—O7	-47.5 (3)
C6—C7—N2—C12	-177.27 (17)	C1—N1—Zn1—O1	33.29 (18)
C8—C7—N2—Zn1	-177.75 (14)	C6—N1—Zn1—O1	-141.52 (14)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O7—H7A \cdots O4 ⁱ	0.85 (3)	1.90 (3)	2.724 (2)	163 (3)
O7—H7B \cdots O3 ⁱⁱ	0.87 (4)	1.94 (4)	2.799 (2)	174 (3)
C5—H5 \cdots O2 ⁱⁱⁱ	0.93	2.53	3.420 (2)	161
C8—H8 \cdots O2 ⁱⁱⁱ	0.93	2.36	3.230 (2)	156

C11—H11...O6^{iv} 0.93 2.44 3.284 (3) 151
Symmetry codes: (i) $-x+1/2, y+1/2, -z+1/2$; (ii) $-x+1/2, y-1/2, -z+1/2$; (iii) $-x+1, -y, -z$; (iv) $x-1/2, -y-1/2, z-1/2$.

Fig. 1

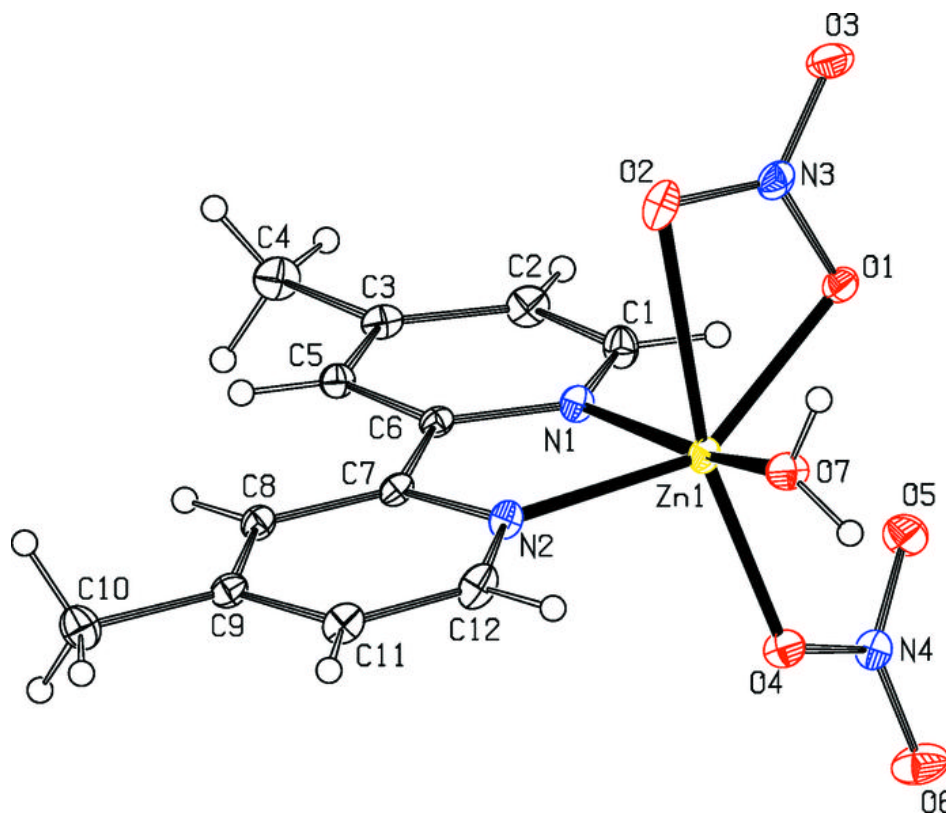


Fig. 2

