

## Retraction of articles

This article reports the retraction of 39 articles published in *Acta Crystallographica Section E* between 2004 and 2009.

After thorough investigation (see Harrison *et al.*, 2010), 39 additional articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1

Details of articles to be retracted, in order of publication.

Title	Reference	Retracted by	DOI	Refcode
<i>trans</i> -Bis[1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato]copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
Bis(4-bromo-2-formylphenolato- $\kappa^2 O, O'$ )copper(II)	Sun & Gao (2005)	Author	10.1107/S160053680500187X	FEYSUY
Bis(salicylaldehyde)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
Bis(4-bromo-2-formylphenolato- $\kappa^2 O, O'$ )zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato- $\kappa^2 O, O'$ )nickel(II)	Li & Chen (2006)	Journal	10.1107/S1600536806012931	IDAZAP
Bis(2-formylphenolato)cobalt(II)	Qiu (2006)	Journal	10.1107/S1600536806015704	GEJDUV
Bis(2-formylphenolato- $\kappa^2 O, O'$ )manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline- $\kappa^2 N, N'$ )copper(II) naphthalene-1,5-disulfonate dihydrate	Liu <i>et al.</i> (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline- $\kappa^2 N, N'$ )nickel(II) naphthalene-1,5-disulfonate dihydrate	Liu & Fan (2006)	Author	10.1107/S1600536806035410	KERBEP
{6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratolutetium(III)copper(II)	Sui <i>et al.</i> (2006)	Journal	10.1107/S160053680604565X	HESPEP
Bis(2-formylphenolato- $\kappa^2 O, O'$ )iron(II)	Yang <i>et al.</i> (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer <i>et al.</i> (2007a)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanyl)acetohydrazide	Qadeer <i>et al.</i> (2007b)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)	Hu <i>et al.</i> (2007)	Author	10.1107/S1600536807031121	WIHKEE
{ $\mu$ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocerium(III)zinc(II)	Sui, Zhang, Hu & Yin (2007)	Author	10.1107/S1600536807032564	WIHREL
{ $\mu$ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)zinc(II)	Chen <i>et al.</i> (2007)	Author	10.1107/S1600536807032540	WIHRIP
{ $\mu$ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)	Sui, Li <i>et al.</i> (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1 $\kappa^4 O^1, O^2, O^3, O^4, O^5, O^6, O^7, O^8, O^9, O^{10}, O^{11}, O^{12}, O^{13}, O^{14}, O^{15}, O^{16}, O^{17}, O^{18}, O^{19}, O^{20}, O^{21}, O^{22}, O^{23}, O^{24}, O^{25}, O^{26}, O^{27}, O^{28}, O^{29}, O^{30}$ }(methanol-1 $\kappa O$ )- $\mu$ -nitrate-1:2 $\kappa^2 O: O'$ -dinitrate-1 $\kappa^4 O, O'$ -cerium(III)zinc(II)	Sui, Fang, Hu & Lin (2007)	Author	10.1107/S1600536807033314	UDUYIC
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol- $\mu$ -nitrate-dinitrosamarium(III)nickel(II)	Sui, Zhang, Hu & Jiang (2007)	Author	10.1107/S1600536807037130	AFECEU
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol- $\mu$ -nitrate-dinitratopraseodymium(III)zinc(II)	Sui, Fang & Yuan (2007)	Author	10.1107/S1600536807037488	AFICEY
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol- $\mu$ -nitrate-dinitratolutetium(III)zinc(II)	Sui, Sui <i>et al.</i> (2007)	Author	10.1107/S1600536807037737	AFEF0H
catena-Poly[[chloridonickel(II)]-di- $\mu$ -chlorido-[chloridonickel(II)]- $\mu$ -4,4'-methylenebis(3,5-dimethylpyrazole)- $\kappa^2 N^2, N^2$ ]	Huang & Chen (2007)	Author	10.1107/S1600536807039384	VIJYOD
{2,2'-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}zinc(II)	Liu <i>et al.</i> (2007a)	Author	10.1107/S1600536807040640	DIKYUS
<i>trans</i> -Bis(ethylenediamine- $\kappa^2 N, N'$ )bis(nitrate- $\kappa O$ )zinc(II)	Liu, Zeng & Chen (2007)	Author	10.1107/S1600536807042390	XIKYEW
[N,N'-(o-Phenylene)bis(picolinamido)- $\kappa^4 N, N', N'', N'''$ ]cobalt(II)	Liu & Zeng (2007a)	Author	10.1107/S1600536807044571	XILFII
[N,N'-(o-Phenylene)dipicolinamide- $\kappa^4 N$ ]nickel(II)	Liu & Zeng (2007b)	Author	10.1107/S1600536807048386	WINWEW
{2,2'-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}manganese(II)	Liu <i>et al.</i> (2007b)	Author	10.1107/S1600536807052993	VIQPIV
N-(2-Amino-3-pyridyl)urea monohydrate	Li <i>et al.</i> (2007)	Author	10.1107/S1600536807047526	SIMFEA
N-(2-Fluorophenyl)carbamic acid monohydrate	Yang (2007)	Author	10.1107/S1600536807052464	WINMOW
Aqua(dimethylglyoxime- $\kappa^2 N, N'$ )(3,5-dinitro-2-oxidobenzoato- $\kappa^2 O^1, O^2$ )-copper(II)	Liu & Wen (2007)	Author	10.1107/S1600536807054244	HIQCAM
$\mu$ -Acetato-tri- $\mu$ -ferrocenecarboxylatobis[(N,N-dimethylformamide)-copper(II)]	Liu, Lin <i>et al.</i> (2007)	Journal	10.1107/S1600536807059041	HIQQEE

**Table 1 (continued)**

Title	Reference	Retracted by	DOI	Refcode
{ $\mu$ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- $\mu$ -nitrate-dinitratoeuropium(III)zinc(II)	Hu <i>et al.</i> (2008)	Author	10.1107/S160053680706151X	MIRPAF
Bis(4-chloro-2-formylphenolato)nickel(II)	Li <i>et al.</i> (2008)	Author	10.1107/S1600536807056309	RISTET
{ $\mu$ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- $\mu$ -nitrate-dinitratoerbium(III)zinc(II)	Chen <i>et al.</i> (2008)	Author	10.1107/S1600536808006958	QIXHIP
Bis(2-ethoxy-6-formylphenolato- $\kappa^2 O^1, O^6$ )nickel(II)	Han (2008)	Journal	10.1107/S160053680800809X	QIXLIT
{ $\mu$ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- $\mu$ -nitrate-dinitratoholmium(III)zinc(II)	Xiao, Sui <i>et al.</i> (2008)	Author	10.1107/S1600536808013743	BIZTUA
{ $\mu$ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoholmium(III)nickel(II)	Xiao, Fu <i>et al.</i> (2008)	Author	10.1107/S1600536808013755	BIZVAI
Hydrogen-bonding patterns in the cocrystal terephthalic acid-4,4'-bipyridine (2I)	Wang <i>et al.</i> (2009)	Journal	10.1107/S160053680903236X	DUCZEH
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato- $1\kappa^4 O^1, O^1, O^6, O^6:2\kappa^4 O^1, N, N', O^1$ }(ethanol- $1\kappa O$ )- $\mu$ -nitrate- $1:2\kappa^2 O:O'$ -dinitrato- $1\kappa^2 O, O'$ -samarium(III)zinc(II)	Huang <i>et al.</i> (2009)	Journal	10.1107/S1600536809033558	YUCWAV

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## {2,2'-[*o*-Phenylenebis(nitrilomethylidyne)]diphenolato}zinc(II)

Yin-Qiu Liu,\* Xi-Rui Zeng, Qiu-Yan Luo and Ya-Ping Xu

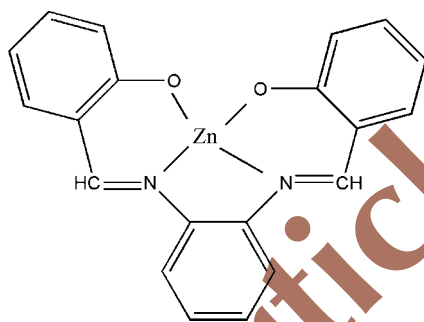
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.008$  Å;  $R$  factor = 0.045;  $wR$  factor = 0.118; data-to-parameter ratio = 14.3.

The title complex,  $[\text{Zn}(\text{C}_{20}\text{H}_{14}\text{N}_2\text{O}_2)]$ , is a mononuclear zinc(II) compound. The zinc(II) ion is four-coordinated in a square-planar geometry by two imine N and two phenolate O atoms from one 2,2'-[*o*-phenylenebis(nitrilomethylidyne)]-diphenolate Schiff base ligand. No strong hydrogen bonds were found in the crystal.



### Experimental

#### Crystal data

$[\text{Zn}(\text{C}_{20}\text{H}_{14}\text{N}_2\text{O}_2)]$   
 $M_r = 379.72$   
 Orthorhombic,  $P2_12_12_1$   
 $a = 5.5103$  (4) Å  
 $b = 16.5871$  (13) Å  
 $c = 17.3146$  (13) Å

$V = 1582.6$  (2) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.57$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 $0.16 \times 0.04 \times 0.02$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
 Absorption correction: none  
 10667 measured reflections  
 3235 independent reflections  
 1906 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.046$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.118$   
 $S = 0.97$   
 3235 reflections  
 226 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.28$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.33$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983), with 1327 Friedel pairs  
 Flack parameter: 0.05 (2)

Data collection: SMART (Bruker, 1997); cell refinement: SAINTE (Bruker, 1997); data reduction: SAINTE; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Siemens, 1996); 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: HG2281).

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**supplementary materials**

**Article retracted**

*Acta Cryst.* (2007). E63, m2396 [ doi:10.1107/S1600536807040640 ]

## {2,2'-[*o*-Phenylenebis(nitrilomethylidene)]diphenolato}zinc(II)

Y.-Q. Liu, X.-R. Zeng, Q.-Y. Luo and Y.-P. Xu

### Comment

In the title complex, each zinc(II) ion is four-coordinated in a square-planar geometry by two imine N and two phenolate O atoms from the Schiff base 1,2-bis{[(2-hydroxy-phenyl)-methyl]-imino}benzene (Fig. 1). The Zn—N and Zn—O bond lengths are Zn1—N1 1.859 (4) Å, Zn1—N2 1.852 (4) Å, Zn1—O1 1.839 (3) Å and Zn1—O2 1.831 (4) Å. Atoms O1, O2, N1 and N2 are approximately coplanar with the central Zn1 ion, the maximum deviation from the least-squares plane through all five atoms being 0.0140 Å for atom O1. No strong hydrogen bonds are found to exist in the crystal.

### Experimental

A mixture of 1,2-bis{[(2-hydroxy-phenyl)-methyl]-imino}benzene (0.341 g, 0.001 mol) and ZnSO<sub>4</sub> (0.161 g, 0.001 mol) was added to methanol. The mixture was heated for 5 h under reflux with stirring. The resulting solution was then filtered off. Single crystals suitable for X-ray diffraction analysis formed after a week by slow evaporation of the solvent.

### Refinement

All H atoms were located at calculated positions and refined as riding on their parent C atoms with the C—H bond length fixed to 0.93 Å with  $U_{\text{iso}}(\text{H}) = 1.2$  times  $U_{\text{eq}}(\text{C})$ .

### Figures

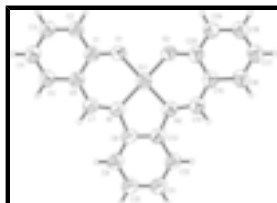


Fig. 1. The asymmetric unit of (I), showing 50% probability displacement ellipsoids.

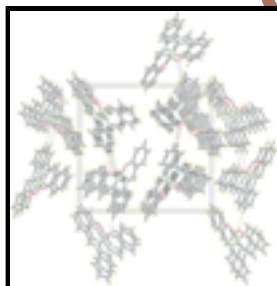


Fig. 2. The packing diagram of (I), viewed along the *a* axis.

{2,2'-[*o*-Phenylenebis(nitrilomethylidene)]diphenolato}zinc(II)

*Crystal data*

[Zn(C<sub>20</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>)]

*M<sub>r</sub>* = 379.72

Orthorhombic, *P*2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>

Hall symbol: P 2ac 2ab

*a* = 5.5103 (4) Å

*b* = 16.5871 (13) Å

*c* = 17.3146 (13) Å

*V* = 1582.6 (2) Å<sup>3</sup>

*Z* = 4

*F*<sub>000</sub> = 776.0

*D<sub>x</sub>* = 1.594 Mg m<sup>-3</sup>

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 2762 reflections

θ = 2.5–22.3°

μ = 1.57 mm<sup>-1</sup>

*T* = 293 (2) K

Block, colourless

0.16 × 0.04 × 0.02 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

*T* = 293(2) K

φ and ω scans

Absorption correction: none

10667 measured reflections

3235 independent reflections

1906 reflections with *I* > 2σ(*I*)

*R*<sub>int</sub> = 0.046

θ<sub>max</sub> = 26.5°

θ<sub>min</sub> = 2.4°

*h* = -6→6

*k* = -20→20

*l* = -21→21

*Refinement*

Refinement on *F*<sup>2</sup>

Least-squares matrix: full

*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.045

*wR*(*F*<sup>2</sup>) = 0.118

*S* = 0.97

3235 reflections

226 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

*w* = 1/[σ<sup>2</sup>(*F*<sub>o</sub><sup>2</sup>) + (0.0632*P*)<sup>2</sup>]

where *P* = (*F*<sub>o</sub><sup>2</sup> + 2*F*<sub>c</sub><sup>2</sup>)/3

(Δ/σ)<sub>max</sub> < 0.001

Δρ<sub>max</sub> = 0.29 e Å<sup>-3</sup>

Δρ<sub>min</sub> = -0.33 e Å<sup>-3</sup>

Extinction correction: none

Absolute structure: Flack (1983)

Flack parameter: 0.05 (2)

*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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	1.0111 (11)	0.0983 (3)	0.0897 (3)	0.0547 (13)
C2	0.9856 (10)	0.0192 (3)	0.0609 (3)	0.0574 (14)
H2	0.8507	-0.0111	0.0749	0.069*
C3	1.1570 (12)	-0.0140 (3)	0.0123 (3)	0.0603 (13)
H3	1.1355	-0.0662	-0.0060	0.072*
C4	1.3618 (12)	0.0294 (3)	-0.0097 (3)	0.0619 (14)
H4	1.4774	0.0061	-0.0418	0.074*
C5	1.3912 (11)	0.1057 (3)	0.0160 (3)	0.0587 (15)
H5	1.5264	0.1349	0.0003	0.070*
C6	1.2217 (10)	0.1421 (3)	0.0663 (3)	0.0537 (14)
C7	1.2639 (9)	0.2214 (3)	0.0924 (3)	0.0518 (12)
H7	1.4021	0.2472	0.0739	0.062*
C8	1.1889 (11)	0.3417 (3)	0.1633 (3)	0.0516 (13)
C9	1.3812 (11)	0.3882 (3)	0.1364 (3)	0.0565 (14)
H9	1.4856	0.3680	0.0989	0.068*
C10	1.4155 (11)	0.4645 (3)	0.1659 (3)	0.0599 (15)
H10	1.5444	0.4956	0.1482	0.072*
C11	1.2633 (11)	0.4950 (3)	0.2206 (3)	0.0602 (16)
H11	1.2920	0.5464	0.2399	0.072*
C12	1.0689 (11)	0.4519 (3)	0.2478 (3)	0.0570 (15)
H12	0.9626	0.4742	0.2837	0.068*
C13	1.0345 (10)	0.3726 (3)	0.2200 (3)	0.0524 (13)
C14	0.7065 (10)	0.3357 (3)	0.3027 (3)	0.0531 (13)
H14	0.7328	0.3841	0.3285	0.064*
C15	0.5211 (10)	0.2870 (3)	0.3292 (3)	0.0552 (13)
C16	0.3782 (11)	0.3131 (3)	0.3946 (3)	0.0609 (15)
H16	0.4175	0.3615	0.4187	0.073*
C17	0.1874 (10)	0.2691 (3)	0.4223 (3)	0.0639 (14)
H17	0.0991	0.2869	0.4647	0.077*
C18	0.1295 (12)	0.1991 (3)	0.3868 (3)	0.0626 (15)
H18	-0.0010	0.1694	0.4055	0.075*
C19	0.2578 (10)	0.1699 (3)	0.3234 (3)	0.0594 (15)
H19	0.2109	0.1219	0.3000	0.071*
C20	0.4579 (10)	0.2129 (3)	0.2946 (3)	0.0547 (13)
Zn1	0.84969 (12)	0.22299 (3)	0.18870 (3)	0.0573 (2)
N1	1.1265 (8)	0.2622 (2)	0.1402 (2)	0.0489 (10)
N2	0.8498 (9)	0.3188 (2)	0.2436 (2)	0.0498 (10)
O1	0.8500 (7)	0.12647 (18)	0.13644 (18)	0.0567 (9)

## supplementary materials

O2                    0.5762 (7)                    0.18339 (18)                    0.2353 (2)                    0.0543 (10)

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.062 (4)	0.052 (3)	0.050 (3)	0.000 (3)	0.001 (3)	-0.003 (2)
C2	0.067 (4)	0.053 (3)	0.053 (3)	0.000 (3)	0.002 (3)	-0.002 (3)
C3	0.070 (4)	0.056 (3)	0.055 (3)	0.004 (3)	0.000 (3)	-0.006 (2)
C4	0.068 (4)	0.061 (3)	0.057 (3)	0.006 (3)	0.002 (3)	-0.006 (2)
C5	0.064 (4)	0.059 (3)	0.053 (3)	0.004 (3)	0.002 (3)	-0.004 (3)
C6	0.061 (4)	0.052 (3)	0.049 (3)	0.001 (3)	0.001 (3)	-0.002 (2)
C7	0.061 (3)	0.049 (3)	0.046 (3)	0.000 (3)	-0.001 (2)	0.002 (3)
C8	0.064 (4)	0.046 (3)	0.044 (3)	0.001 (3)	-0.005 (3)	0.001 (2)
C9	0.069 (4)	0.051 (3)	0.049 (3)	-0.003 (3)	-0.003 (3)	0.000 (2)
C10	0.071 (4)	0.053 (3)	0.055 (3)	-0.006 (3)	-0.001 (3)	-0.001 (2)
C11	0.073 (4)	0.051 (3)	0.057 (3)	-0.005 (3)	-0.002 (3)	-0.002 (3)
C12	0.070 (5)	0.049 (3)	0.052 (3)	0.000 (3)	-0.002 (3)	0.000 (2)
C13	0.064 (4)	0.046 (3)	0.047 (3)	0.003 (3)	-0.004 (3)	0.003 (2)
C14	0.061 (4)	0.050 (3)	0.048 (3)	0.009 (2)	-0.003 (3)	0.004 (2)
C15	0.060 (4)	0.055 (3)	0.052 (3)	0.011 (3)	0.001 (3)	0.004 (2)
C16	0.065 (4)	0.064 (3)	0.055 (3)	0.011 (3)	0.003 (3)	0.002 (2)
C17	0.064 (4)	0.069 (4)	0.058 (3)	0.011 (4)	0.005 (3)	0.008 (3)
C18	0.061 (4)	0.065 (4)	0.062 (3)	0.010 (3)	0.005 (3)	0.013 (3)
C19	0.059 (4)	0.057 (3)	0.062 (4)	0.012 (3)	0.002 (3)	0.010 (3)
C20	0.057 (4)	0.051 (3)	0.057 (3)	0.012 (3)	0.002 (3)	0.007 (3)
Zn1	0.0659 (4)	0.0518 (3)	0.0543 (3)	0.0037 (3)	0.0003 (3)	0.0012 (3)
N1	0.061 (3)	0.044 (2)	0.041 (2)	0.000 (2)	-0.005 (2)	0.0025 (18)
N2	0.060 (3)	0.044 (2)	0.045 (2)	0.006 (2)	-0.005 (3)	0.0060 (18)
O1	0.060 (2)	0.0532 (19)	0.057 (2)	-0.004 (2)	0.004 (2)	-0.0051 (16)
O2	0.057 (3)	0.0471 (18)	0.058 (2)	0.0070 (16)	0.0021 (19)	0.0035 (16)

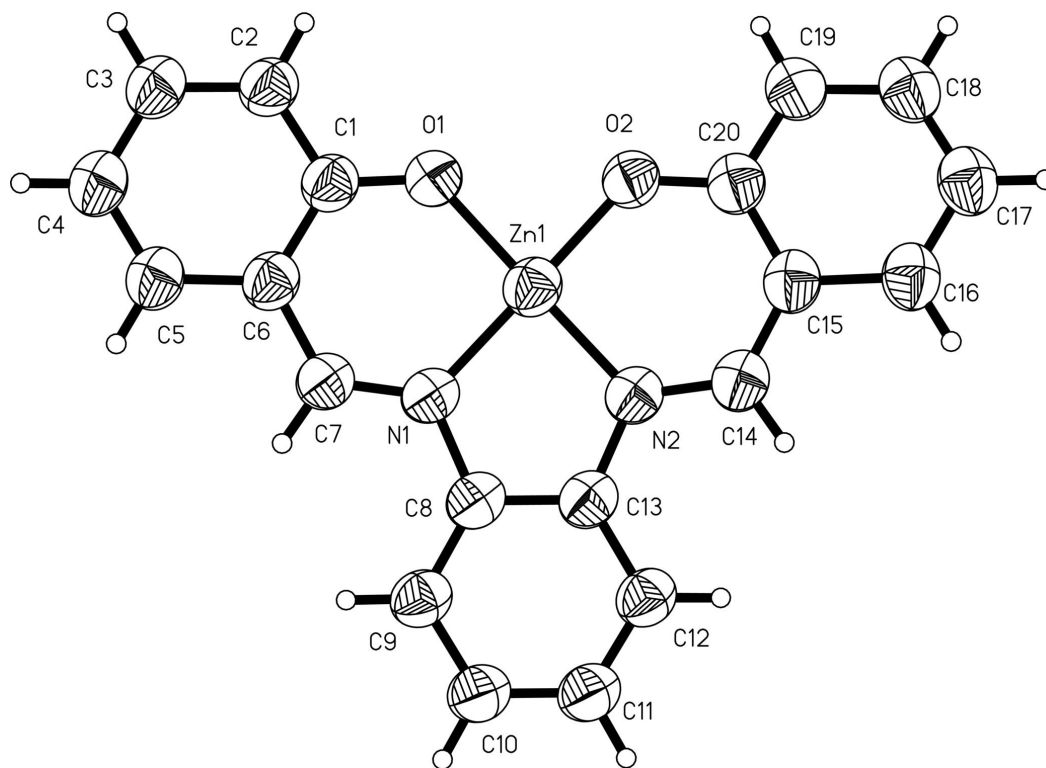
### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

C1—O1	1.289 (6)	C11—H11	0.9300
C1—C2	1.411 (7)	C12—C13	1.415 (6)
C1—C6	1.427 (7)	C12—H12	0.9300
C2—C3	1.379 (7)	C13—N2	1.414 (7)
C2—H2	0.9300	C14—N2	1.322 (6)
C3—C4	1.392 (7)	C14—C15	1.381 (7)
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.351 (6)	C15—C20	1.410 (7)
C4—H4	0.9300	C15—C16	1.446 (7)
C5—C6	1.412 (7)	C16—C17	1.367 (8)
C5—H5	0.9300	C16—H16	0.9300
C6—C7	1.411 (7)	C17—C18	1.350 (7)
C7—N1	1.309 (6)	C17—H17	0.9300
C7—H7	0.9300	C18—C19	1.394 (7)
C8—C9	1.391 (7)	C18—H18	0.9300
C8—C13	1.396 (7)	C19—C20	1.404 (7)



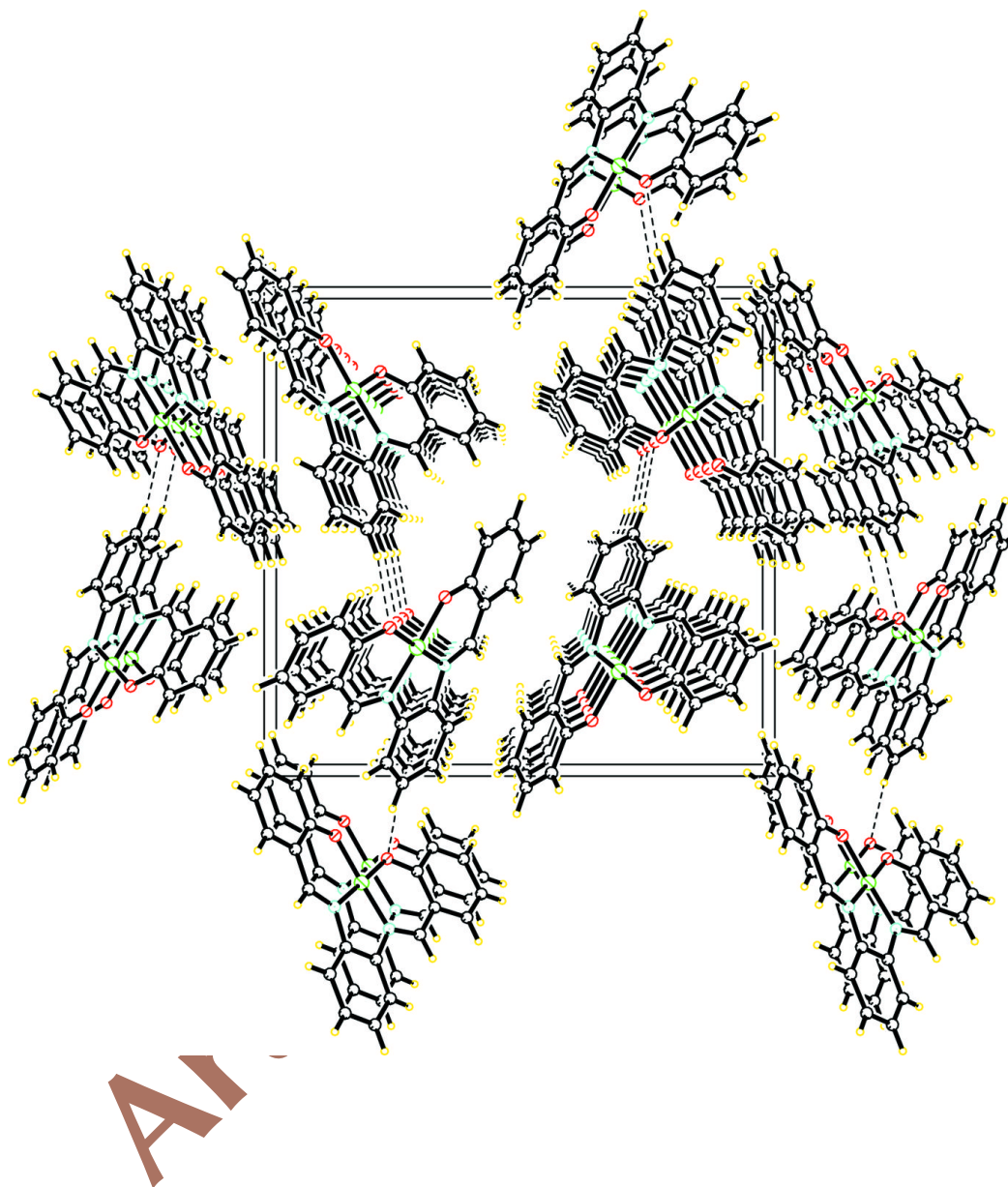
C8—N1	1.420 (6)	C19—H19	0.9300
C9—C10	1.377 (6)	C20—O2	1.311 (6)
C9—H9	0.9300	Zn1—O2	1.831 (4)
C10—C11	1.363 (7)	Zn1—O1	1.839 (3)
C10—H10	0.9300	Zn1—N2	1.852 (4)
C11—C12	1.372 (7)	Zn1—N1	1.858 (4)
O1—C1—C2	119.4 (5)	C8—C13—C12	120.0 (5)
O1—C1—C6	123.7 (4)	N2—C13—C12	125.7 (5)
C2—C1—C6	116.9 (5)	N2—C14—C15	125.1 (5)
C3—C2—C1	121.3 (5)	N2—C14—H14	117.4
C3—C2—H2	119.4	C15—C14—H14	117.4
C1—C2—H2	119.4	C14—C15—C20	123.5 (5)
C2—C3—C4	121.1 (5)	C14—C15—C16	119.2 (5)
C2—C3—H3	119.5	C20—C15—C16	117.3 (5)
C4—C3—H3	119.5	C17—C16—C15	122.2 (5)
C5—C4—C3	119.4 (5)	C17—C16—H16	118.9
C5—C4—H4	120.3	C15—C16—H16	118.9
C3—C4—H4	120.3	C18—C17—C16	118.8 (5)
C4—C5—C6	121.6 (5)	C18—C17—H17	120.6
C4—C5—H5	119.2	C16—C17—H17	120.6
C6—C5—H5	119.2	C17—C18—C19	122.5 (6)
C7—C6—C5	119.2 (5)	C17—C18—H18	118.8
C7—C6—C1	121.2 (5)	C19—C18—H18	118.8
C5—C6—C1	119.7 (5)	C18—C19—C20	120.1 (5)
N1—C7—C6	126.0 (5)	C18—C19—H19	120.0
N1—C7—H7	117.0	C20—C19—H19	120.0
C6—C7—H7	117.0	O2—C20—C19	118.6 (5)
C9—C8—C13	119.7 (5)	O2—C20—C15	122.4 (5)
C9—C8—N1	127.3 (5)	C19—C20—C15	119.0 (5)
C13—C8—N1	113.0 (5)	O2—Zn1—O1	84.56 (15)
C10—C9—C8	119.3 (5)	O2—Zn1—N2	94.70 (18)
C10—C9—H9	120.3	O1—Zn1—N2	178.58 (15)
C8—C9—H9	120.3	O2—Zn1—N1	179.15 (16)
C11—C10—C9	121.0 (5)	O1—Zn1—N1	94.66 (16)
C11—C10—H10	119.5	N2—Zn1—N1	86.09 (19)
C9—C10—H10	119.5	C7—N1—C8	121.1 (5)
C10—C11—C12	121.7 (5)	C7—N1—Zn1	125.4 (3)
C10—C11—H11	119.1	C8—N1—Zn1	113.3 (3)
C12—C11—H11	119.1	C14—N2—C13	121.4 (4)
C11—C12—C13	118.2 (5)	C14—N2—Zn1	125.3 (4)
C11—C12—H12	120.9	C13—N2—Zn1	113.1 (3)
C13—C12—H12	120.9	C1—O1—Zn1	128.7 (3)
C8—C13—N2	114.3 (4)	C20—O2—Zn1	128.3 (3)

Fig. 1



Article re

Fig. 2



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