

Retraction of articles by H. Zhong *et al.*

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A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *et al.* are retracted. 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	DOI	Refcode
<i>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate</i>	Zhong, Zeng, Liu & Luo (2006a)	10.1107/S1600536806041122	KERQEE
<i>cis-Dichlorobis(1,10-phenanthroline)cobalt(II)</i>	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
<i>Tris(quinolin-8-olato-κ<sup>2</sup>N,O)cobalt(III) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Liu & Luo (2006b)	10.1107/S1600536806050240	MEQHEW
<i>(8-Quinololinol-κ<sup>2</sup>N,O)bis(8-quinolinolato-κ<sup>2</sup>N,O)nickel(II) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
<i>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate</i>	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METQIM
<i>(8-Quinololinol-κ<sup>2</sup>N,O)-bis(8-quinolinolato-κ<sup>2</sup>N,O)zinc(II) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
<i>(Dimethylglyoxime-κ<sup>2</sup>N,N')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')nickel(II) dinitrate dihydrate</i>	Zhong, Zeng, Yang, Luo & Li (2007a)	10.1107/S1600536807004102	YEYGOZ
<i>(Dimethylglyoxime-κ<sup>2</sup>N,N')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')zinc(II) dinitrate dihydrate</i>	Zhong, Zeng, Yang, Luo & Li (2007b)	10.1107/S1600536807004096	YEYGUF
<i>Chloridobis(1,10-phenanthroline-κN,N')copper(I) hexahydrate</i>	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU1
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)</i>	Zhong, Zeng, Yang & Luo (2007a)	10.1107/S1600536807017461	ITPCOO1
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)</i>	Zhong, Zeng, Yang & Luo (2007b)	10.1107/S160053680701879X	AVUJEG02
<i>Tetrakis(nitrato-κ<sup>2</sup>O,O')bis(4-phenylpyridine-κN)cerium(IV)</i>	Zhong, Zeng, Yang & Luo (2007c)	10.1107/S1600536807018831	CICDOI
<i>Bis(4,4'-bipyridine-κ<sup>2</sup>N,N')tetrakis(nitrato-κ<sup>2</sup>O,O')cerium(IV)</i>	Zhong, Zeng, Yang & Luo (2007d)	10.1107/S1600536807021502	YIDNEF
<i>(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)</i>	Zhong, Zeng, Yang, Luo & Xu (2007)	10.1107/S1600536807027171	EDUROL
<i>(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)</i>	Zhong, Yang, Luo & Xu (2007a)	10.1107/S1600536807028061	EDUTUT
<i>(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)</i>	Zhong, Yang, Luo & Xu (2007b)	10.1107/S1600536807028693	RIGQEE
<i>(1,10-Phenanthroline-κ<sup>2</sup>N,N')tris(phenoxyacetato)-κO;κO;κO,O'-neodymium(III)</i>	Zhong, Yang, Luo & Xu (2007c)	10.1107/S1600536807030371	UDUMEM
<i>Bis(2,2'-bipyridyl-κ<sup>2</sup>N,N')bis(thiocyanato-κN)nickel(II)</i>	Zhong, Yang, Luo & Xu (2007d)	10.1107/S1600536807031613	YEJGOJ01
<i>Bis(2,2'-bipyridyl-κ<sup>2</sup>N,N')bis(isothiocyanato-κN)copper(II)</i>	Zhong, Yang, Luo & Xu (2007e)	10.1107/S1600536807033181	UFAPOH
<i>Bis(2,2'-bipyridyl-κ<sup>2</sup>N,N')bis(thiocyanato-κN)zinc(II)</i>	Zhong, Yang, Luo & Xu (2007f)	10.1107/S1600536807035337	TIGFAR
<i>(1,10-Phenanthroline-κ<sup>2</sup>N,N')tris(3-phenylpropanoato-κO)neodymium(III)</i>	Zhong, Yang, Luo & Xu (2007g)	10.1107/S1600536807035350	TIGFEV
<i>2-Fluoro-3,5-dinitrobenzamide monohydrate</i>	Zhong, Yang, Xie & Luo (2007j)	10.1107/S1600536807038676	VIKGAY
<i>2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)</i>	Zhong, Yang, Xie & Luo (2007k)	10.1107/S1600536807039724	KILKIA
<i>1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate</i>	Zhong, Yang, Xie & Luo (2007l)	10.1107/S1600536807040779	AFETAH
<i>N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)</i>	Zhong, Yang, Xie & Luo (2007m)	10.1107/S160053680704086X	AFINAF
<i>catena-Poly[[bis(μ-anilinoacetato-κ<sup>2</sup>O:O')bis(μ-anilinoacetato-κ<sup>2</sup>O:O')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')samarium(III)]-μ-anilinoacetato-κ<sup>2</sup>O:O']</i>	Zhong, Yang, Xie & Luo (2007a)	10.1107/S1600536807043528	PILDAQ
<i>2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate</i>	Zhong, Yang, Xie & Luo (2007n)	10.1107/S1600536807045199	XILWIZ
<i>catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]</i>	Zhong, Yang, Xie & Luo (2007b)	10.1107/S1600536807048489	WIMWEV
<i>Hexaaquacopper(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007c)	10.1107/S1600536807049525	TOLSCV01

**Table 1 (continued)**

Title	Reference	DOI	Refcode
<i>catena-Poly[[tetra-<math>\mu</math>-anilinoacetato-bis(1,10-phenanthroline)-dilanthanum(III)]-di-<math>\mu</math>-anilinoacetato]</i>	Zhong, Yang, Xie & Luo (2007d)	10.1107/S1600536807051240	GIMZEI
<i>Hexaaquachromium(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007e)	10.1107/S1600536807051227	GIMZIM
<i>Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007f)	10.1107/S1600536807052051	QUKQES01
<i>catena-Poly[(acetato-<math>\kappa</math>O)(1,10-phenanthroline-<math>\kappa^2</math>N,N')cobalt(II)]-<math>\mu</math>-acetato-<math>\kappa^2</math>O:O']</i>	Zhong, Yang, Xie & Luo (2007g)	10.1107/S1600536807053494	NIQLAB
<i>Hexaaquanickel(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Zhong, Xie & Luo (2007a)	10.1107/S1600536807054372	HIPZOW
<i>catena-Poly[(acetato-<math>\kappa</math>O)(1,10-phenanthroline-<math>\kappa^2</math>N,N')copper(II)]-<math>\mu</math>-acetato-<math>\kappa^2</math>O:O']</i>	Zhong, Yang, Xie & Luo (2007h)	10.1107/S160053680705622X	XIRGOV
<i>Hexaaquazinc(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Zhong, Xie & Luo (2007b)	10.1107/S1600536807056498	XIRJEO
<i>catena-Poly[(acetato-<math>\kappa</math>O)(1,10-phenanthroline-<math>\kappa^2</math>N,N')nickel(II)]-<math>\mu</math>-acetato-<math>\kappa^2</math>O:O']</i>	Zhong, Yang, Xie & Luo (2007i)	10.1107/S1600536807058540	HIQJOH
<i>Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Xie & Luo (2007)	10.1107/S1600536807058527	HIQJUN
<i>catena-Poly[[tetra-<math>\mu</math>-anilinoacetato-bis(1,10-phenanthroline)-dieuropium(III)]-di-<math>\mu</math>-anilinoacetato]</i>	Zhong, Yang, Duan & Hong (2007)	10.1107/S1600536807060643	YIQMAN
<i>(Dimethylglyoxime-<math>\kappa^2</math>N,N')bis(1,10-phenanthroline-<math>\kappa^2</math>N,N')copper(II) dinirate dihydrate</i>	Zhong, Yang, Luo & Li (2007)	10.1107/S1600536807061193	YIQNUI
<i>catena-Poly[(1,10-phenanthroline-<math>\kappa^2</math>N,N')praseodymium(III)]-di-<math>\mu</math>-phenoxyacetato-<math>\kappa^4</math>O:O'-[(1,10-phenanthroline-<math>\kappa^2</math>N,N')praseodymium(III)]-di-<math>\mu</math>-phenoxyacetato-<math>\kappa^4</math>O:O'-di-<math>\mu</math>-phenoxyacetato-<math>\kappa^3</math>O,O':<math>\kappa^3</math>O:O,O']</i>	Zhong, Yang, Luo & Xu (2008)	10.1107/S1600536807068614	GISJIC

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## Bis(2,2'-bipyridyl- $\kappa^2N,N'$ )bis(thiocyanato- $\kappa N$ )zinc(II)

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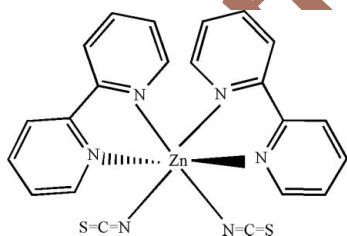
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Key indicators: single-crystal X-ray study;  $T = 273$  K; mean  $\sigma(C-C) = 0.005$  Å;  $R$  factor = 0.052;  $wR$  factor = 0.186; data-to-parameter ratio = 16.9.

In the molecule of the title compound,  $[Zn(NCS)_2(C_{10}H_8N_2)_2]$ , the  $Zn^{II}$  atom is six-coordinated by the four N atoms of two 2,2'-bipyridyl ligands and the two N atoms of two thiocyanate ligands, in a distorted octahedral arrangement. In the crystal structure, intramolecular  $C-H \cdots N$  and intermolecular  $C-H \cdots S$  hydrogen bonds and  $\pi-\pi$  stacking interactions, with a centroid-centroid distance of 3.569 (5) Å, lead to a supramolecular network structure.

### Related literature

For related structures, see: Zhong *et al.* (2007*a,b*). For bond-length data, see: Allen *et al.* (1987).



### Experimental

#### Crystal data

$[Zn(NCS)_2(C_{10}H_8N_2)_2]$   $V = 4327.3$  (6) Å<sup>3</sup>  
 $M_r = 493.90$   $Z = 8$   
 Orthorhombic,  $Pbca$   $Mo K\alpha$  radiation  
 $a = 15.8992$  (11) Å  $\mu = 1.35$  mm<sup>-1</sup>  
 $b = 16.0385$  (12) Å  $T = 273$  (2) K  
 $c = 16.9698$  (14) Å  $0.36 \times 0.34 \times 0.22$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{min} = 0.630$ ,  $T_{max} = 0.741$   
 28831 measured reflections

4738 independent reflections  
 3495 reflections with  $I > 2\sigma(I)$

 $R_{int} = 0.023$ 

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$  280 parameters  
 $wR(F^2) = 0.186$  H-atom parameters constrained  
 $S = 0.99$   $\Delta\rho_{max} = 0.60$  e Å<sup>-3</sup>  
 4738 reflections  $\Delta\rho_{min} = -1.09$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Zn1—N1	2.069 (3)	Zn1—N4	2.139 (2)
Zn1—N2	2.068 (3)	Zn1—N5	2.149 (2)
Zn1—N3	2.167 (2)	Zn1—N6	2.164 (2)
N1—Zn1—N2	99.63 (12)	N2—Zn1—N6	90.85 (10)
N1—Zn1—N3	90.94 (10)	N3—Zn1—N4	75.35 (9)
N1—Zn1—N4	94.45 (10)	N3—Zn1—N5	99.33 (9)
N1—Zn1—N5	90.69 (10)	N3—Zn1—N6	81.65 (9)
N1—Zn1—N6	163.34 (10)	N4—Zn1—N5	172.63 (8)
N2—Zn1—N3	164.48 (11)	N4—Zn1—N6	98.03 (9)
N2—Zn1—N4	92.42 (10)	N5—Zn1—N6	75.95 (9)
N2—Zn1—N5	91.92 (9)		

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C4—H4 $\cdots$ S1 <sup>i</sup>	0.93	2.82	3.702 (4)	159
C12—H12 $\cdots$ N2	0.93	2.61	3.153 (4)	118
C13—H13 $\cdots$ N1	0.93	2.59	3.140 (4)	118

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

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; 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: HK2297).

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**supplementary materials**

**Article retracted**

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## Bis(2,2'-bipyridyl- $\kappa^2N,N'$ )bis(thiocyanato- $\kappa N$ )zinc(II)

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### Comment

The crystal structure of bis[(2,2'-bipyridyl- $\kappa^2N,N'$ )bis(isothiocyanato- $\kappa N$ )] copper(II), (II) (Zhong *et al.*, 2007a) and bis[(2,2'-bipyridyl- $\kappa^2N,N'$ )- bis(thiocyanato- $\kappa N$ )]nickel(II), (III) (Zhong *et al.*, 2007b) have previously been reported. The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation and to compare it with those of (II) and (III).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The six-coordinate environment of the Zn atom is completed by the four N atoms of two 2,2'-bipyridyl ligands and two N atoms of two SCN<sup>-</sup> ligands, in a distorted octahedral arrangement (Table 1). The Zn—N bonds [average 2.155 (4) Å] of the 2,2'-bipyridyl ligands are somewhat longer than the Zn—N bonds [average 2.068 (2) Å] of the SCN<sup>-</sup> ligands. The two 2,2'-bipyridyl ligands are nearly perpendicular to each other, with a dihedral angle of 104.9 (8)°, as in (II) and (III).

In the crystal structure, intramolecular C—H $\cdots$ N and intermolecular C—H $\cdots$ S hydrogen bonds (Table 2) and  $\pi$ - $\pi$  stacking interactions, with a centroid-centroid distance of 3.569 (5) Å [symmetry code: 2 - x, 1 - y, -z] lead to a supramolecular network structure (Fig. 2), as in (II) and (III).

The compounds, (I), (II) and (III), are isostructural.

### Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb. Zinc dinitrate hexahydrate (89.2 mg, 0.3 mmol), 2,2'-bipyridyl (93.6 mg, 0.6 mmol), potassium thiocyanate (58.4 mg, 0.6 mmol) and distilled water (4 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 423 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small colorless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

### Refinement

H atoms were positioned geometrically, with C—H = 0.93 Å, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Figures

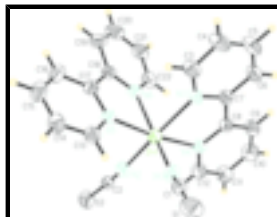


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

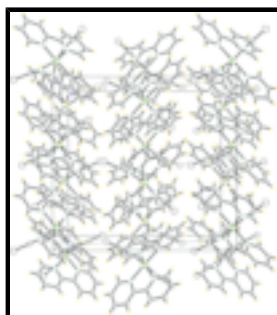


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

**Bis(2,2'-bipyridyl- $\kappa^2N,N'$ )bis(isothiocyanato- $\kappa N$ )zinc(II)**

*Crystal data*

[Zn(NCS)<sub>2</sub>(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>]

$M_r = 493.90$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 15.8992$  (11) Å

$b = 16.0385$  (12) Å

$c = 16.9698$  (14) Å

$V = 4327.3$  (6) Å<sup>3</sup>

$Z = 8$

$F_{000} = 2016$

$D_x = 1.516$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 11498 reflections

$\theta = 2.4$ – $27.0^\circ$

$\mu = 1.35$  mm<sup>-1</sup>

$T = 273$  (2) K

Block, colourless

$0.36 \times 0.34 \times 0.22$  mm

*Data collection*

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 273$ (2) K

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.630$ ,  $T_{\max} = 0.741$

28831 measured reflections

4738 independent reflections

3495 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

$\theta_{\text{max}} = 27.1^\circ$

$\theta_{\text{min}} = 2.2^\circ$

$h = -20 \rightarrow 20$

$k = -20 \rightarrow 20$

$l = -21 \rightarrow 21$

Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	H-atom parameters constrained
$wR(F^2) = 0.186$	$w = 1/[\sigma^2(F_o^2) + (0.1398P)^2 + 0.816P]$
$S = 0.99$	where $P = (F_o^2 + 2F_c^2)/3$
4738 reflections	$(\Delta/\sigma)_{\max} = 0.001$
280 parameters	$\Delta\rho_{\max} = 0.60 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -1.09 \text{ e } \text{\AA}^{-3}$
	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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.70225 (2)	0.38401 (2)	-0.000708 (18)	0.05079 (19)
S1	0.57515 (6)	0.51150 (7)	-0.22514 (6)	0.0801 (3)
S2	0.51121 (6)	0.22556 (6)	0.15952 (6)	0.0719 (3)
N1	0.62893 (17)	0.44603 (16)	-0.08262 (17)	0.0628 (7)
N2	0.60960 (16)	0.31786 (16)	0.05769 (17)	0.0589 (6)
N3	0.80968 (14)	0.46132 (15)	-0.02969 (15)	0.0467 (5)
N4	0.69877 (14)	0.48309 (15)	0.08361 (15)	0.0466 (5)
N5	0.72279 (14)	0.28369 (14)	-0.08243 (14)	0.0446 (5)
N6	0.79902 (13)	0.30932 (15)	0.05457 (15)	0.0470 (5)
C1	0.60601 (17)	0.47314 (17)	-0.14212 (19)	0.0511 (7)
C2	0.56803 (16)	0.28030 (16)	0.09987 (17)	0.0463 (6)
C3	0.8634 (2)	0.4455 (2)	-0.08795 (18)	0.0623 (8)
H3	0.8549	0.3983	-0.1187	0.075*
C4	0.9306 (2)	0.4958 (3)	-0.1045 (2)	0.0773 (11)
H4	0.9668	0.4838	-0.1460	0.093*
C5	0.9426 (2)	0.5644 (3)	-0.0580 (2)	0.0792 (11)
H5	0.9874	0.6002	-0.0680	0.095*
C6	0.8892 (2)	0.5805 (2)	0.00312 (19)	0.0658 (9)

## supplementary materials

H6	0.8972	0.6271	0.0349	0.079*
C7	0.82337 (19)	0.52679 (18)	0.01688 (18)	0.0481 (6)
C8	0.76314 (17)	0.53797 (16)	0.08206 (16)	0.0461 (6)
C9	0.7705 (2)	0.5996 (2)	0.1391 (2)	0.0626 (8)
H9	0.8160	0.6360	0.1381	0.075*
C10	0.7113 (2)	0.6068 (2)	0.1962 (2)	0.0742 (10)
H10	0.7167	0.6471	0.2353	0.089*
C11	0.6435 (2)	0.5541 (2)	0.1957 (2)	0.0704 (9)
H11	0.6005	0.5598	0.2325	0.084*
C12	0.6404 (2)	0.4920 (2)	0.13901 (18)	0.0573 (7)
H12	0.5955	0.4548	0.1398	0.069*
C13	0.67720 (19)	0.26889 (19)	-0.14711 (18)	0.0536 (7)
H13	0.6372	0.3081	-0.1620	0.064*
C14	0.6864 (2)	0.1988 (2)	-0.1926 (2)	0.0657 (9)
H14	0.6531	0.1903	-0.2369	0.079*
C15	0.7460 (3)	0.1416 (2)	-0.1711 (2)	0.0718 (10)
H15	0.7536	0.0933	-0.2006	0.086*
C16	0.7945 (2)	0.1560 (2)	-0.1056 (2)	0.0658 (9)
H16	0.8358	0.1180	-0.0911	0.079*
C17	0.78161 (17)	0.22704 (18)	-0.06150 (18)	0.0484 (6)
C18	0.82905 (18)	0.2460 (2)	0.01152 (17)	0.0492 (7)
C19	0.8998 (2)	0.2013 (2)	0.0338 (3)	0.0693 (9)
H19	0.9205	0.1585	0.0024	0.083*
C20	0.9385 (2)	0.2220 (3)	0.1037 (3)	0.0837 (12)
H20	0.9860	0.1929	0.1200	0.100*
C21	0.9068 (2)	0.2863 (2)	0.1500 (2)	0.0746 (11)
H21	0.9316	0.3003	0.1979	0.089*
C22	0.8381 (2)	0.3279 (2)	0.12271 (19)	0.0604 (8)
H22	0.8170	0.3716	0.1528	0.072*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Zn1	0.0503 (3)	0.0504 (3)	0.0517 (3)	-0.00322 (14)	0.00050 (13)	-0.00129 (13)
S1	0.0713 (6)	0.1006 (7)	0.0684 (6)	-0.0091 (5)	-0.0228 (4)	0.0129 (5)
S2	0.0773 (6)	0.0678 (5)	0.0706 (6)	-0.0117 (4)	0.0250 (4)	0.0009 (4)
N1	0.0687 (16)	0.0501 (14)	0.0696 (18)	0.0037 (12)	-0.0176 (14)	0.0021 (13)
N2	0.0523 (13)	0.0545 (14)	0.0700 (17)	-0.0059 (11)	0.0085 (13)	-0.0045 (12)
N3	0.0489 (12)	0.0489 (13)	0.0423 (12)	-0.0080 (10)	0.0022 (10)	0.0014 (10)
N4	0.0466 (12)	0.0460 (12)	0.0473 (13)	-0.0040 (9)	0.0015 (9)	-0.0045 (10)
N5	0.0447 (11)	0.0434 (12)	0.0456 (13)	-0.0002 (9)	0.0016 (9)	-0.0010 (9)
N6	0.0444 (12)	0.0516 (13)	0.0449 (13)	-0.0044 (9)	-0.0009 (9)	0.0044 (10)
C1	0.0442 (13)	0.0449 (14)	0.0642 (19)	0.0010 (11)	-0.0071 (13)	-0.0088 (13)
C2	0.0404 (12)	0.0443 (13)	0.0543 (16)	-0.0005 (11)	0.0037 (12)	-0.0086 (12)
C3	0.0622 (17)	0.073 (2)	0.0514 (17)	-0.0135 (16)	0.0121 (14)	-0.0048 (15)
C4	0.063 (2)	0.107 (3)	0.061 (2)	-0.0242 (19)	0.0213 (17)	-0.001 (2)
C5	0.064 (2)	0.089 (3)	0.085 (3)	-0.0305 (19)	0.0116 (18)	0.005 (2)
C6	0.0594 (19)	0.062 (2)	0.075 (3)	-0.0191 (17)	-0.0004 (15)	-0.0054 (15)



C7	0.0456 (14)	0.0473 (15)	0.0513 (15)	-0.0038 (12)	-0.0052 (12)	0.0037 (12)
C8	0.0464 (14)	0.0448 (14)	0.0469 (15)	-0.0010 (11)	-0.0081 (11)	-0.0009 (11)
C9	0.0620 (18)	0.0639 (19)	0.062 (2)	-0.0090 (15)	-0.0087 (16)	-0.0127 (16)
C10	0.087 (3)	0.078 (2)	0.058 (2)	-0.0030 (19)	-0.0023 (18)	-0.0273 (18)
C11	0.075 (2)	0.081 (2)	0.0545 (19)	-0.0046 (18)	0.0123 (16)	-0.0174 (17)
C12	0.0606 (17)	0.0583 (17)	0.0530 (17)	-0.0033 (14)	0.0103 (14)	-0.0063 (13)
C13	0.0536 (15)	0.0550 (17)	0.0522 (17)	-0.0034 (13)	-0.0017 (13)	-0.0042 (13)
C14	0.079 (2)	0.065 (2)	0.0534 (18)	-0.0079 (17)	0.0004 (16)	-0.0127 (15)
C15	0.089 (3)	0.0593 (19)	0.067 (2)	0.0046 (19)	0.0144 (19)	-0.0180 (16)
C16	0.073 (2)	0.0520 (17)	0.073 (2)	0.0136 (15)	0.0085 (16)	-0.0066 (16)
C17	0.0472 (13)	0.0497 (15)	0.0484 (16)	0.0000 (11)	0.0089 (12)	0.0004 (12)
C18	0.0373 (13)	0.0525 (15)	0.0577 (17)	-0.0021 (12)	0.0051 (11)	0.0106 (13)
C19	0.0467 (16)	0.073 (2)	0.088 (3)	0.0120 (15)	0.0032 (17)	0.0173 (19)
C20	0.0481 (17)	0.094 (3)	0.109 (3)	0.0044 (17)	-0.020 (2)	0.028 (3)
C21	0.065 (2)	0.082 (3)	0.076 (2)	-0.0155 (18)	-0.0257 (18)	0.017 (2)
C22	0.0668 (18)	0.0608 (18)	0.0536 (17)	-0.0100 (15)	-0.0101 (15)	0.0090 (14)

*Geometric parameters (Å, °)*

Zn1—N1	2.069 (3)	C7—C8	1.474 (4)
Zn1—N2	2.068 (3)	C8—C9	1.388 (4)
Zn1—N3	2.167 (2)	C9—C10	1.356 (5)
Zn1—N4	2.139 (2)	C9—H9	0.9300
Zn1—N5	2.149 (2)	C10—C11	1.371 (5)
Zn1—N6	2.164 (2)	C10—H10	0.9300
S1—C1	1.614 (3)	C11—C12	1.386 (4)
S2—C2	1.616 (3)	C11—H11	0.9300
N1—C1	1.158 (4)	C12—H12	0.9300
N2—C2	1.145 (4)	C13—C14	1.372 (5)
N3—C3	1.331 (4)	C13—H13	0.9300
N3—C7	1.332 (4)	C14—C15	1.368 (5)
N4—C12	1.328 (4)	C14—H14	0.9300
N4—C8	1.350 (3)	C15—C16	1.372 (5)
N5—C13	1.337 (4)	C15—H15	0.9300
N5—C17	1.351 (4)	C16—C17	1.379 (4)
N6—C18	1.338 (4)	C16—H16	0.9300
N6—C22	1.346 (4)	C17—C18	1.482 (4)
C3—C4	1.367 (4)	C18—C19	1.386 (4)
C3—H3	0.9300	C19—C20	1.377 (6)
C4—C5	1.368 (6)	C19—H19	0.9300
C4—H4	0.9300	C20—C21	1.391 (6)
C5—C6	1.364 (5)	C20—H20	0.9300
C5—H5	0.9300	C21—C22	1.361 (5)
C6—C7	1.376 (4)	C21—H21	0.9300
C6—H6	0.9300	C22—H22	0.9300
N1—Zn1—N2	99.63 (12)	N4—C8—C9	120.9 (3)
N1—Zn1—N3	90.94 (10)	N4—C8—C7	115.3 (2)
N1—Zn1—N4	94.45 (10)	C9—C8—C7	123.7 (3)
N1—Zn1—N5	90.69 (10)	C10—C9—C8	120.1 (3)

## supplementary materials

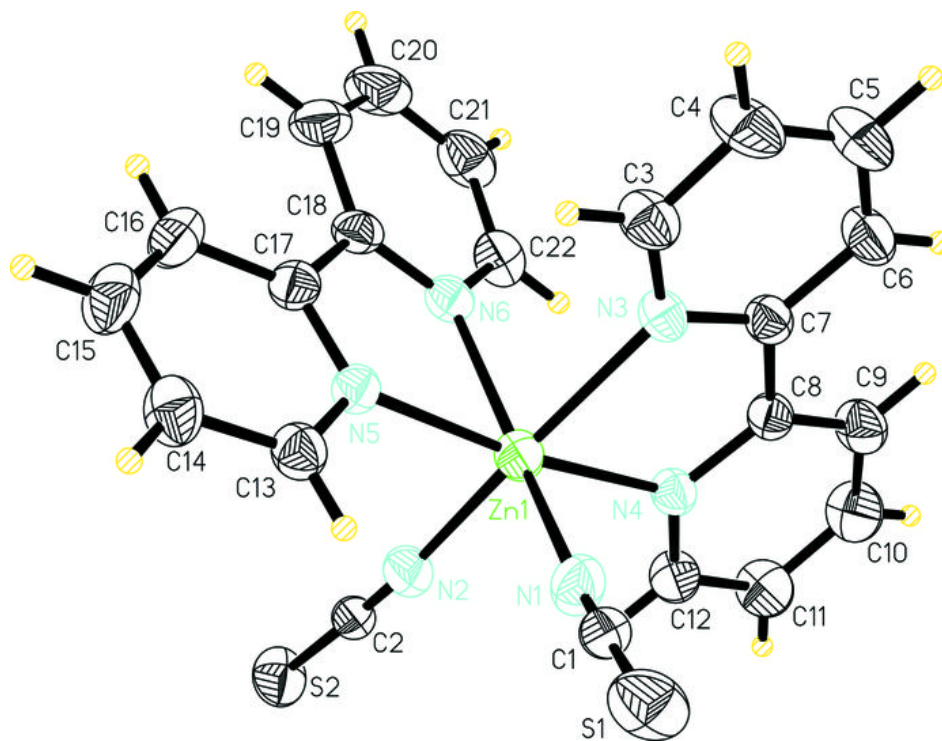
N1—Zn1—N6	163.34 (10)	C10—C9—H9	120.0
N2—Zn1—N3	164.48 (11)	C8—C9—H9	120.0
N2—Zn1—N4	92.42 (10)	C9—C10—C11	119.3 (3)
N2—Zn1—N5	91.92 (9)	C9—C10—H10	120.4
N2—Zn1—N6	90.85 (10)	C11—C10—H10	120.4
N3—Zn1—N4	75.35 (9)	C10—C11—C12	118.4 (3)
N3—Zn1—N5	99.33 (9)	C10—C11—H11	120.8
N3—Zn1—N6	81.65 (9)	C12—C11—H11	120.8
N4—Zn1—N5	172.63 (8)	N4—C12—C11	123.0 (3)
N4—Zn1—N6	98.03 (9)	N4—C12—H12	118.5
N5—Zn1—N6	75.95 (9)	C11—C12—H12	118.5
C1—N1—Zn1	160.7 (3)	N5—C13—C14	123.3 (3)
C2—N2—Zn1	168.6 (3)	N5—C13—H13	118.3
C3—N3—C7	119.1 (3)	C14—C13—H13	118.3
C3—N3—Zn1	124.4 (2)	C15—C14—C13	118.3 (3)
C7—N3—Zn1	116.4 (2)	C15—C14—H14	120.9
C12—N4—C8	118.2 (2)	C13—C14—H14	120.9
C12—N4—Zn1	124.83 (19)	C14—C15—C16	119.5 (3)
C8—N4—Zn1	116.85 (18)	C14—C15—H15	120.3
C13—N5—C17	118.1 (2)	C16—C15—H15	120.3
C13—N5—Zn1	125.48 (19)	C15—C16—C17	119.7 (3)
C17—N5—Zn1	116.04 (19)	C15—C16—H16	120.1
C18—N6—C22	118.2 (3)	C17—C16—H16	120.1
C18—N6—Zn1	115.90 (19)	N5—C17—C16	121.0 (3)
C22—N6—Zn1	125.3 (2)	N5—C17—C18	115.7 (3)
N1—C1—S1	179.3 (3)	C16—C17—C18	123.3 (3)
N2—C2—S2	178.6 (3)	N6—C18—C19	122.2 (3)
N3—C3—C4	122.8 (3)	N6—C18—C17	115.5 (3)
N3—C3—H3	118.6	C19—C18—C17	122.3 (3)
C4—C3—H3	118.6	C20—C19—C18	118.3 (4)
C3—C4—C5	117.7 (3)	C20—C19—H19	120.9
C3—C4—H4	121.1	C18—C19—H19	120.9
C5—C4—H4	121.1	C19—C20—C21	120.2 (3)
C6—C5—C4	120.3 (3)	C19—C20—H20	119.9
C6—C5—H5	119.9	C21—C20—H20	119.9
C4—C5—H5	119.9	C22—C21—C20	117.5 (3)
C5—C6—C7	118.9 (3)	C22—C21—H21	121.2
C5—C6—H6	120.5	C20—C21—H21	121.2
C7—C6—H6	120.5	N6—C22—C21	123.7 (4)
N3—C7—C6	121.2 (3)	N6—C22—H22	118.2
N3—C7—C8	115.8 (2)	C21—C22—H22	118.2
C6—C7—C8	123.1 (3)		

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4—H4 $\cdots$ S1 <sup>i</sup>	0.93	2.82	3.702 (4)	159
C12—H12 $\cdots$ N2	0.93	2.61	3.153 (4)	118
C13—H13 $\cdots$ N1	0.93	2.59	3.140 (4)	118

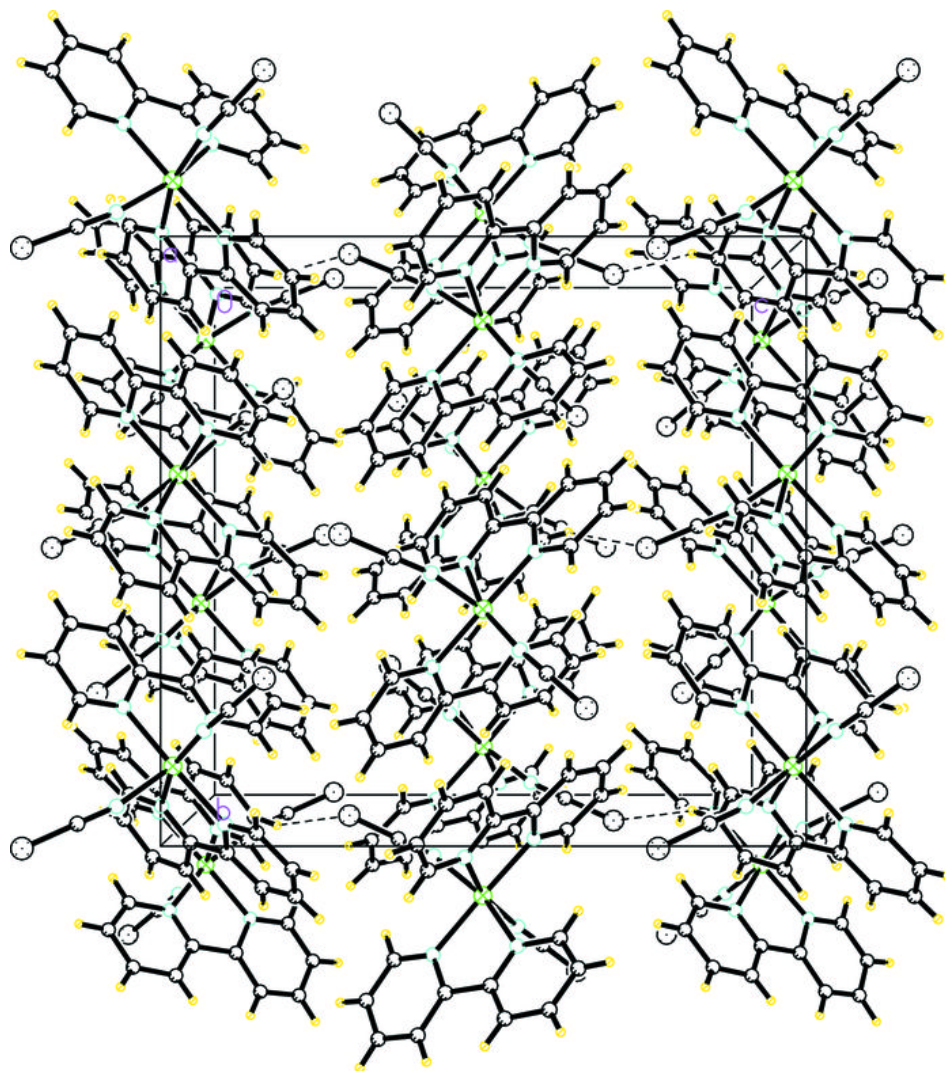
Symmetry codes: (i)  $x+1/2, y, -z-1/2$ .

Fig. 1



Article re

Fig. 2



Ar