Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[[bis(thiocyanato-κ*N*)-zinc(II)]-μ-1,2-bis{[2-(2-pyridyl)-1*H*-imidazol-1-yl]methyl}benzene] 0.28-hydrate]

Fei Han, Haochen Shi,* Yunfeng Gao and Hongjun Ma

Department of Physics Education, Changchun Normal University, 667 Changji Highway (North), Erdao District, Jilin Province 130032, People's Republic of China
Correspondence e-mail: shi19781980@yahoo.cn

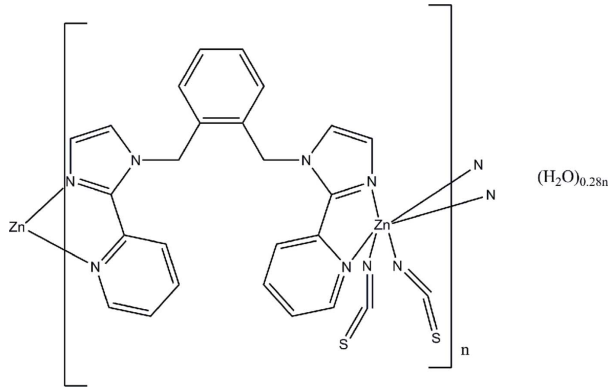
Received 20 June 2010; accepted 12 July 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.038; wR factor = 0.102; data-to-parameter ratio = 13.0.

The title one-dimensional coordination polymer, $\{[Zn(NCS)_2(C_{24}H_{20}N_6)_2]\cdot 0.28H_2O\}_n$, was obtained by the reaction of $Zn(OAc)_2\cdot 2H_2O$, KSCN and 1,2-bis{[2-(2-pyridyl)-1*H*-imidazol-1-yl]methyl}benzene (hereafter *L*). The Zn^{II} ion shows a distorted octahedral coordination geometry and is coordinated by two N atoms from two SCN^- anions and four N atoms from two organic ligands. The *L* ligands act as bridging bis-chelating ligands with *cis* coordination modes at the Zn^{II} ion. One-dimensional coordination polymers are arranged into layers by π–π stacking interactions between the imidazole rings of adjacent chains, with an interplanar distance of 3.46 (1) Å and centroid–centroid distances of 3.8775 (16) Å. One of the thiocyanate ligands is disordered over two positions with an occupancy factor of 0.564 (3) for the major component. The partially occupied water molecule forms an O—H···S hydrogen bond with the disordered thiocyanate group.

Related literature

For backgroud to the topologies, supramolecular structures and applications of metal-organic frameworks (MOFs), see: Dybtsev *et al.* (2004); Evans & Lin (2002); Moulton & Zaworotko (2001). For coordination modes of organic ligands, see: Janiak (2003). For similar structures, see: Dai *et al.* (2002); Luan *et al.* (2006). For the synthesis of 1,2-bis{[2-(2-pyridyl)-1*H*-imidazol-1-yl]methyl}benzene, see: Li *et al.* (2008).



Experimental

Crystal data

$[Zn(NCS)_2(C_{24}H_{20}N_6)_2]\cdot 0.28H_2O$
M_r = 579.03
Monoclinic, $P2_1/c$
a = 7.8780 (4) Å
b = 13.1770 (7) Å
c = 25.9620 (14) Å
β = 98.462 (1)°
V = 2665.7 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.11 mm^{-1}
T = 293 K
0.26 × 0.22 × 0.21 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.750, T_{max} = 0.792
13328 measured reflections
4707 independent reflections
3127 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.102
S = 1.04
4707 reflections
362 parameters
30 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H2W···S1^{i}	0.85	2.68	3.30 (2)	132

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2008); software used to prepare material for publication: *SHELXL97*.

We greatly acknowledge the financial support of this work by the Department of Education of Jilin Province.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2287).

References

Brandenburg, K. & Putz, H. (2008). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (1997). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dai, J.-C., Wu, X.-T., Fu, Z.-Y., Cui, C.-P., Hu, S.-M., Du, W.-X., Wu, L.-M., Zhang, H.-H. & Sun, R.-Q. (2002). *Inorg. Chem.* **41**, 1391–1396.
Dybtsev, D. N., Chun, H., Yoon, S. H., Kim, D. & Kim, K. (2004). *J. Am. Chem. Soc.* **126**, 32–33.
Evans, O. R. & Lin, W. (2002). *Acc. Chem. Res.* **35**, 511–522.
Janiak, C. (2003). *Dalton Trans.* pp. 2781–2804.
Li, S.-L., Lan, Y.-Q., Ma, J.-F., Fu, Y.-M., Yang, J., Ping, G.-J., Liu, J. & Su, Z.-M. (2008). *Cryst. Growth Des.* **8**, 1610–1616.
Luan, X.-J., Cai, X.-H., Wang, Y.-Y., Li, D.-S., Wang, C.-J., Liu, P., Hu, H.-M., Shi, Q.-Z. & Peng, S.-M. (2006). *Chem. Eur. J.* **12**, 6281–6289.
Moulton, B. & Zaworotko, M. (2001). *Chem. Rev.* **101**, 1629–1658.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2010). E**66**, m943-m944 [**doi:10.1107/S1600536810027571**]

catena-Poly[[[bis(thiocyanato-κ*N*)zinc(II)]-μ-1,2-bis{[2-(2-pyridyl)-1*H*-imidazol-1-yl]methyl}benzene] 0.28-hydrate]

F. Han, H. Shi, Y. Gao and H. Ma

Comment

In recent years, there is an increasing interest in metal-organic frameworks (MOFs) for the versatile architectures and intriguing topologies as well as their wide potential applications (Dybtsev *et al.* 2004; Evans & Lin, 2002). A universal strategy for the construction of MOFs is dependent primarily on the appropriate choice of inorganic building blocks and different organic ligands. Among them, N-donor organic ligands are important because of their divers coordination modes to metal ions resulting in different structures (Janiak, 2003) and the ability to form of weak interactions to assemble supramolecular structures (Moulton & Zaworotko, 2001). In this case, 1,2-bis{[2-(2-pyridyl)-1*H*-imidazol-1-yl]methyl}benzene (hereafter *L*) is selected as organic ligand and reacted with $Zn(OAc)_2.2H_2O$ and KSCN to obtain the title compound.

In the title compound, there is one kind of *L* ligand, Zn^{II} ion and two kinds of SCN^- anions in the unit cell (Fig. 1). Each Zn^{II} ion is coordinated by two nitrogen atoms from two SCN^- anions and four aromatic N atoms from two different *L* molecules with normal Zn—N distances (Dai *et al.* 2002; Luan *et al.* 2006), showing a distorted octahedral coordination geometry. Each *L* molecule is acting as a bridging bis-bidentate ligand coordinated to two Zn^{II} ions to form polymeric one-dimensional chain (Fig. 2). Moreover, a two-dimensional supramolecular layer is finally formed by linking these chains through the π–π stacking interactions between imidazole rings from adjacent chains, with the plane to plane distance of 3.46 (1) Å and the centroid-centroid distances of 3.87 (8) Å. (Fig. 3).

Experimental

A mixture of $Zn(OAc)_2.2H_2O$ (1 mmol), *L* (1 mmol) (Li *et al.* 2008), KSCN (0.10 g, 2 mmol) and H_2O (8 ml) was sealed in a 18 ml Teflon- lined stainless steel container which was heated to 120 °C for 50 h, and cooled to room temperature. Colorless polyhedron crystals were collected in 85% yield.

Refinement

The disordered SCN^- anion was refined with S and C atoms split over two sites, with the sum of the occupancy factors equal to 1.00. In this anion restraints were imposed on the anion geometry (DFIX instructions of SHELXL-97) and anisotropic displacement parameter of C and S atoms (ISOR instruction). The occupancy factor of the water molecule was initially refined but it was fixed in the final refinement cycles. Positions of H atoms from water molecules were calculated assuming interactions with the anion S atoms and these atoms were refined as riding with O-H = 0.85 Å and U_{iso}=1.5U_{eq} (O). All H atoms bound to C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 and 0.97 Å, and U_{iso}=1.2U_{eq} (C).

Figures

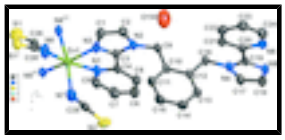


Fig. 1. A displacement ellipsoids view of the title compound with the displacement ellipsoids drawn at the 30% probability level. Symmetry code #2: x, -y+1/2, z-1/2.

Fig. 2. View of the one-dimensional chain.

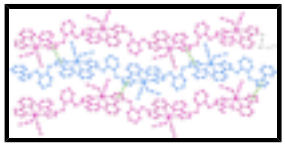


Fig. 3. View of the two-dimensional supramolecular structure formed by π–π stacking interactions.

catena-Poly[[[bis(thiocyanato-κ*N*)zinc(II)]- μ-1,2-bis{[2-(2-pyridyl)-1*H*-imidazol-1-yl]methyl}benzene] 0.28-hydrate]

Crystal data

$[Zn(NCS)_2(C_{24}H_{20}N_6)_2]\cdot 0.28H_2O$	$F(000) = 1187$
$M_r = 579.03$	$D_x = 1.443$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Hall symbol: -P 2ybc	Cell parameters from 2199 reflections
$a = 7.8780$ (4) Å	$\theta = 1.6$–$26.4°$
$b = 13.1770$ (7) Å	$\mu = 1.11$ mm^{-1}
$c = 25.9620$ (14) Å	$T = 293$ K
$\beta = 98.462$ (1)°	Block, colorless
$V = 2665.7$ (2) Å^3	0.26 × 0.22 × 0.21 mm
$Z = 4$	

Data collection

Bruker APEX CCD area-detector diffractometer	4707 independent reflections
Radiation source: fine-focus sealed tube	3127 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.036$
ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 1.6°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -9\rightarrow9$
$T_{min} = 0.750$, $T_{max} = 0.792$	$k = -13\rightarrow15$
13328 measured reflections	$l = -28\rightarrow30$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.038$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.102$	H-atom parameters constrained
$S = 1.04$	$w = 1/[\sigma^2(F_o^2) + (0.0472P)^2 + 0.0052P]$ where $P = (F_o^2 + 2F_c^2)/3$
4707 reflections	$(\Delta/\sigma)_{max} = 0.001$
362 parameters	$\Delta\rho_{max} = 0.38$ e Å^{-3}
30 restraints	$\Delta\rho_{min} = -0.33$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.1405 (4)	0.0988 (2)	0.23131 (12)	0.0627 (9)	
H1	0.0560	0.0583	0.2128	0.075*	
C2	0.1380 (4)	0.1355 (2)	0.27956 (12)	0.0628 (9)	
H2	0.0527	0.1253	0.3003	0.075*	
C3	0.3735 (4)	0.1861 (2)	0.25115 (10)	0.0498 (7)	
C4	0.5346 (4)	0.2347 (2)	0.24331 (11)	0.0488 (7)	
C5	0.6518 (4)	0.2810 (2)	0.28088 (12)	0.0652 (9)	
H5	0.6360	0.2801	0.3157	0.078*	
C6	0.7924 (5)	0.3283 (3)	0.26590 (14)	0.0787 (10)	
H6	0.8719	0.3607	0.2905	0.094*	
C7	0.8146 (4)	0.3274 (3)	0.21460 (15)	0.0797 (11)	
H7	0.9059	0.3615	0.2034	0.096*	
C8	0.6981 (4)	0.2748 (3)	0.18015 (13)	0.0715 (10)	
H8	0.7162	0.2710	0.1456	0.086*	
C9	0.3326 (4)	0.2402 (2)	0.34290 (10)	0.0562 (8)	
H9A	0.2287	0.2595	0.3564	0.067*	
H9B	0.3960	0.3018	0.3382	0.067*	
C10	0.4402 (4)	0.1734 (2)	0.38252 (10)	0.0493 (7)	
C11	0.4785 (4)	0.0736 (2)	0.37134 (12)	0.0633 (9)	
H11	0.4402	0.0475	0.3384	0.076*	
C12	0.4998 (3)	0.2120 (2)	0.43188 (10)	0.0464 (7)	
C13	0.5948 (4)	0.1497 (2)	0.46849 (11)	0.0574 (8)	
H13	0.6355	0.1751	0.5014	0.069*	
C14	0.6294 (4)	0.0511 (3)	0.45663 (13)	0.0699 (9)	

H14	0.6921	0.0100	0.4816	0.084*	
C15	0.5719 (4)	0.0128 (3)	0.40811 (14)	0.0747 (10)	
H15	0.5961	−0.0539	0.4001	0.090*	
C16	0.4598 (4)	0.3198 (2)	0.44434 (10)	0.0514 (7)	
H16A	0.5126	0.3644	0.4215	0.062*	
H16B	0.3366	0.3297	0.4368	0.062*	
C17	0.6633 (4)	0.4061 (2)	0.51368 (11)	0.0594 (8)	
H17	0.7419	0.4278	0.4926	0.071*	
C18	0.6701 (4)	0.4240 (2)	0.56517 (12)	0.0610 (8)	
H18	0.7552	0.4611	0.5857	0.073*	
C19	0.4434 (4)	0.3341 (2)	0.54193 (10)	0.0460 (7)	
C20	0.2902 (4)	0.2752 (2)	0.54843 (10)	0.0480 (7)	
C21	0.1991 (4)	0.2117 (2)	0.51218 (11)	0.0554 (8)	
H21	0.2308	0.2040	0.4793	0.066*	
C22	0.0594 (4)	0.1596 (3)	0.52576 (13)	0.0691 (9)	
H22	−0.0047	0.1173	0.5017	0.083*	
C23	0.0159 (4)	0.1703 (3)	0.57424 (14)	0.0728 (10)	
H23	−0.0774	0.1357	0.5839	0.087*	
C24	0.1140 (4)	0.2337 (3)	0.60837 (13)	0.0715 (10)	
H24	0.0857	0.2404	0.6417	0.086*	
N1	0.5617 (3)	0.22928 (18)	0.19344 (9)	0.0557 (6)	
N2	0.2857 (3)	0.19105 (18)	0.29238 (8)	0.0531 (6)	
N3	0.2880 (3)	0.13082 (18)	0.21386 (9)	0.0556 (6)	
N4	0.5181 (3)	0.34985 (17)	0.49856 (8)	0.0490 (6)	
N5	0.5331 (3)	0.37948 (18)	0.58233 (9)	0.0525 (6)	
N6	0.2472 (3)	0.28627 (19)	0.59660 (9)	0.0566 (7)	
N7	0.6024 (4)	0.0045 (2)	0.18550 (12)	0.0833 (9)	
C25	0.6692 (4)	−0.0180 (2)	0.22631 (14)	0.0603 (8)	
S2	0.75961 (13)	−0.04934 (9)	0.28408 (4)	0.0927 (3)	
N8	0.2453 (4)	−0.0111 (2)	0.11975 (10)	0.0852 (10)	
C26	0.1381 (15)	−0.0639 (10)	0.1031 (6)	0.052 (3)	0.56 (3)
S1	0.0107 (12)	−0.1515 (10)	0.0796 (4)	0.1109 (18)	0.56 (3)
C26'	0.1698 (19)	−0.0857 (8)	0.1087 (8)	0.042 (3)	0.44 (3)
S1'	0.0605 (18)	−0.1874 (10)	0.0912 (4)	0.091 (3)	0.44 (3)
Zn1	0.41177 (5)	0.10351 (3)	0.149130 (12)	0.05821 (16)	
O1W	−0.0298 (16)	0.1050 (10)	0.3898 (4)	0.154 (5)	0.28
H1W	−0.1226	0.0745	0.3782	0.231*	0.28
H2W	−0.0408	0.1642	0.3768	0.231*	0.28

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.070 (2)	0.072 (2)	0.0484 (19)	−0.0175 (18)	0.0148 (17)	−0.0006 (16)
C2	0.063 (2)	0.080 (2)	0.050 (2)	−0.0060 (18)	0.0228 (17)	0.0030 (16)
C3	0.0625 (19)	0.0526 (18)	0.0363 (16)	−0.0014 (15)	0.0143 (15)	−0.0020 (13)
C4	0.0609 (19)	0.0455 (17)	0.0416 (17)	0.0010 (15)	0.0127 (15)	−0.0043 (13)
C5	0.072 (2)	0.069 (2)	0.055 (2)	−0.0104 (19)	0.0133 (18)	−0.0107 (17)
C6	0.076 (2)	0.085 (3)	0.075 (3)	−0.014 (2)	0.010 (2)	−0.024 (2)

C7	0.072 (2)	0.087 (3)	0.087 (3)	−0.027 (2)	0.034 (2)	−0.018 (2)
C8	0.081 (2)	0.077 (2)	0.064 (2)	−0.015 (2)	0.037 (2)	−0.0131 (18)
C9	0.077 (2)	0.0581 (19)	0.0361 (16)	0.0103 (17)	0.0170 (15)	−0.0024 (14)
C10	0.0592 (18)	0.0525 (19)	0.0394 (17)	0.0047 (15)	0.0185 (14)	0.0039 (13)
C11	0.083 (2)	0.056 (2)	0.0514 (19)	0.0117 (18)	0.0113 (17)	−0.0073 (15)
C12	0.0553 (17)	0.0495 (18)	0.0379 (16)	0.0036 (14)	0.0185 (14)	0.0064 (13)
C13	0.069 (2)	0.058 (2)	0.0458 (18)	0.0074 (17)	0.0093 (16)	0.0041 (15)
C14	0.078 (2)	0.062 (2)	0.068 (2)	0.0175 (19)	0.0052 (19)	0.0107 (18)
C15	0.094 (3)	0.054 (2)	0.077 (2)	0.023 (2)	0.013 (2)	−0.0041 (19)
C16	0.073 (2)	0.0531 (18)	0.0303 (15)	−0.0011 (16)	0.0139 (14)	0.0033 (13)
C17	0.075 (2)	0.061 (2)	0.0472 (19)	−0.0101 (17)	0.0248 (17)	−0.0008 (15)
C18	0.078 (2)	0.059 (2)	0.0481 (19)	−0.0122 (17)	0.0143 (17)	−0.0020 (15)
C19	0.0625 (19)	0.0425 (17)	0.0356 (16)	0.0050 (15)	0.0156 (15)	0.0051 (13)
C20	0.0558 (18)	0.0485 (17)	0.0406 (17)	0.0087 (15)	0.0102 (14)	0.0085 (13)
C21	0.0595 (19)	0.063 (2)	0.0448 (18)	0.0008 (17)	0.0104 (15)	0.0038 (15)
C22	0.059 (2)	0.078 (2)	0.069 (2)	−0.0022 (19)	0.0041 (18)	−0.0009 (19)
C23	0.063 (2)	0.089 (3)	0.071 (2)	−0.008 (2)	0.0235 (19)	0.009 (2)
C24	0.074 (2)	0.088 (3)	0.057 (2)	−0.002 (2)	0.0279 (19)	0.0067 (19)
N1	0.0656 (16)	0.0576 (16)	0.0482 (15)	−0.0092 (13)	0.0228 (13)	−0.0068 (12)
N2	0.0680 (17)	0.0611 (16)	0.0325 (13)	0.0014 (14)	0.0155 (12)	−0.0008 (11)
N3	0.0691 (16)	0.0614 (16)	0.0382 (14)	−0.0151 (14)	0.0142 (13)	−0.0044 (12)
N4	0.0662 (16)	0.0491 (14)	0.0336 (13)	−0.0013 (13)	0.0140 (12)	0.0002 (11)
N5	0.0698 (16)	0.0537 (15)	0.0357 (14)	−0.0045 (13)	0.0136 (13)	0.0005 (11)
N6	0.0664 (17)	0.0643 (17)	0.0419 (14)	0.0053 (14)	0.0180 (13)	0.0081 (12)
N7	0.124 (3)	0.0640 (19)	0.0637 (19)	0.0083 (18)	0.0209 (18)	0.0063 (16)
C25	0.067 (2)	0.0435 (18)	0.075 (2)	0.0036 (16)	0.0286 (19)	−0.0005 (17)
S2	0.0803 (7)	0.1023 (8)	0.0907 (8)	0.0078 (6)	−0.0037 (6)	0.0145 (6)
N8	0.125 (3)	0.077 (2)	0.0556 (19)	−0.029 (2)	0.0210 (18)	−0.0141 (15)
C26	0.049 (5)	0.060 (5)	0.046 (5)	0.014 (4)	0.006 (4)	0.001 (4)
S1	0.065 (2)	0.129 (4)	0.137 (3)	−0.031 (3)	0.007 (2)	−0.033 (3)
C26'	0.038 (5)	0.053 (5)	0.034 (5)	0.020 (5)	0.006 (4)	0.001 (4)
S1'	0.072 (3)	0.113 (4)	0.089 (3)	−0.031 (3)	0.019 (2)	−0.043 (2)
Zn1	0.0859 (3)	0.0552 (2)	0.0370 (2)	−0.00799 (19)	0.02056 (19)	−0.00498 (16)
O1W	0.159 (11)	0.198 (14)	0.117 (10)	−0.065 (9)	0.058 (8)	−0.028 (8)

Geometric parameters (Å, °)

C1—C2	1.346 (4)	C16—H16A	0.9700
C1—N3	1.374 (4)	C16—H16B	0.9700
C1—H1	0.9300	C17—C18	1.351 (4)
C2—N2	1.373 (4)	C17—N4	1.371 (4)
C2—H2	0.9300	C17—H17	0.9300
C3—N3	1.315 (3)	C18—N5	1.360 (4)
C3—N2	1.359 (3)	C18—H18	0.9300
C3—C4	1.463 (4)	C19—N5	1.319 (3)
C4—N1	1.345 (3)	C19—N4	1.361 (3)
C4—C5	1.382 (4)	C19—C20	1.465 (4)
C5—C6	1.376 (4)	C20—N6	1.351 (3)
C5—H5	0.9300	C20—C21	1.379 (4)

C6—C7	1.369 (4)	C21—C22	1.386 (4)
C6—H6	0.9300	C21—H21	0.9300
C7—C8	1.372 (4)	C22—C23	1.360 (4)
C7—H7	0.9300	C22—H22	0.9300
C8—N1	1.321 (4)	C23—C24	1.371 (4)
C8—H8	0.9300	C23—H23	0.9300
C9—N2	1.461 (3)	C24—N6	1.330 (4)
C9—C10	1.515 (4)	C24—H24	0.9300
C9—H9A	0.9700	N1—Zn1	2.250 (2)
C9—H9B	0.9700	N3—Zn1	2.095 (2)
C10—C11	1.390 (4)	N5—Zn1^{i}	2.112 (2)
C10—C12	1.394 (4)	N6—Zn1^{i}	2.265 (2)
C11—C15	1.374 (4)	N7—C25	1.151 (4)
C11—H11	0.9300	N7—Zn1	2.105 (3)
C12—C13	1.389 (4)	C25—S2	1.616 (4)
C12—C16	1.501 (4)	N8—C26	1.130 (4)
C13—C14	1.371 (4)	N8—Zn1	2.071 (3)
C13—H13	0.9300	C26—S1	1.591 (4)
C14—C15	1.371 (4)	C26'—S1'	1.621 (4)
C14—H14	0.9300	O1W—H1W	0.8500
C15—H15	0.9300	O1W—H2W	0.8500
C16—N4	1.469 (3)		
C2—C1—N3	109.0 (3)	C17—C18—H18	125.3
C2—C1—H1	125.5	N5—C18—H18	125.3
N3—C1—H1	125.5	N5—C19—N4	110.0 (2)
C1—C2—N2	106.8 (3)	N5—C19—C20	120.2 (2)
C1—C2—H2	126.6	N4—C19—C20	129.8 (3)
N2—C2—H2	126.6	N6—C20—C21	121.4 (3)
N3—C3—N2	110.0 (3)	N6—C20—C19	111.8 (2)
N3—C3—C4	120.1 (2)	C21—C20—C19	126.7 (3)
N2—C3—C4	129.9 (3)	C20—C21—C22	118.7 (3)
N1—C4—C5	121.3 (3)	C20—C21—H21	120.7
N1—C4—C3	112.0 (2)	C22—C21—H21	120.7
C5—C4—C3	126.8 (3)	C23—C22—C21	120.1 (3)
C6—C5—C4	118.8 (3)	C23—C22—H22	119.9
C6—C5—H5	120.6	C21—C22—H22	119.9
C4—C5—H5	120.6	C22—C23—C24	117.8 (3)
C7—C6—C5	119.7 (3)	C22—C23—H23	121.1
C7—C6—H6	120.2	C24—C23—H23	121.1
C5—C6—H6	120.2	N6—C24—C23	123.9 (3)
C6—C7—C8	118.0 (3)	N6—C24—H24	118.0
C6—C7—H7	121.0	C23—C24—H24	118.0
C8—C7—H7	121.0	C8—N1—C4	118.5 (3)
N1—C8—C7	123.5 (3)	C8—N1—Zn1	126.0 (2)
N1—C8—H8	118.3	C4—N1—Zn1	112.71 (18)
C7—C8—H8	118.3	C3—N2—C2	107.1 (2)
N2—C9—C10	113.2 (2)	C3—N2—C9	129.6 (3)
N2—C9—H9A	108.9	C2—N2—C9	123.2 (2)

C10—C9—H9A	108.9	C3—N3—C1	107.1 (2)
N2—C9—H9B	108.9	C3—N3—Zn1	115.93 (19)
C10—C9—H9B	108.9	C1—N3—Zn1	136.7 (2)
H9A—C9—H9B	107.7	C19—N4—C17	106.9 (2)
C11—C10—C12	118.9 (3)	C19—N4—C16	129.7 (2)
C11—C10—C9	121.7 (3)	C17—N4—C16	123.4 (2)
C12—C10—C9	119.4 (3)	C19—N5—C18	107.1 (2)
C15—C11—C10	121.1 (3)	C19—N5—Zn1^{i}	116.53 (19)
C15—C11—H11	119.4	C18—N5—Zn1^{i}	134.4 (2)
C10—C11—H11	119.4	C24—N6—C20	118.0 (3)
C13—C12—C10	119.3 (3)	C24—N6—Zn1^{i}	126.6 (2)
C13—C12—C16	121.4 (3)	C20—N6—Zn1^{i}	115.3 (2)
C10—C12—C16	119.3 (2)	C25—N7—Zn1	140.6 (3)
C14—C13—C12	120.7 (3)	N7—C25—S2	178.9 (3)
C14—C13—H13	119.6	C26—N8—Zn1	170.9 (9)
C12—C13—H13	119.6	N8—C26—S1	170.8 (12)
C15—C14—C13	120.4 (3)	N8—Zn1—N3	94.38 (10)
C15—C14—H14	119.8	N8—Zn1—N7	94.87 (13)
C13—C14—H14	119.8	N3—Zn1—N7	97.60 (11)
C14—C15—C11	119.7 (3)	N8—Zn1—N5^{ii}	96.53 (10)
C14—C15—H15	120.2	N3—Zn1—N5^{ii}	163.98 (9)
C11—C15—H15	120.2	N7—Zn1—N5^{ii}	93.14 (11)
N4—C16—C12	114.5 (2)	N8—Zn1—N1	168.99 (10)
N4—C16—H16A	108.6	N3—Zn1—N1	74.61 (9)
C12—C16—H16A	108.6	N7—Zn1—N1	86.62 (11)
N4—C16—H16B	108.6	N5^{ii}—Zn1—N1	94.28 (9)
C12—C16—H16B	108.6	N8—Zn1—N6^{ii}	88.30 (11)
H16A—C16—H16B	107.6	N3—Zn1—N6^{ii}	94.60 (9)
C18—C17—N4	106.7 (3)	N7—Zn1—N6^{ii}	167.12 (10)
C18—C17—H17	126.6	N5^{ii}—Zn1—N6^{ii}	74.07 (9)
N4—C17—H17	126.6	N1—Zn1—N6^{ii}	92.65 (9)
C17—C18—N5	109.3 (3)	H1W—O1W—H2W	105.1

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H2W···S1^{iii}	0.85	2.68	3.30 (2)	132

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

Fig. 1

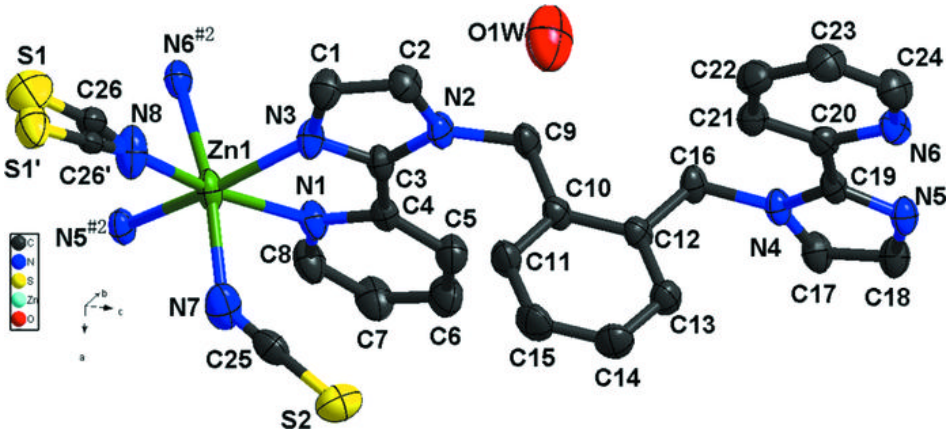

S1
N6#2
C1
C2
O1W
C23
C24
C26
N8
N3
N2
C22
C21
C20
N6
S1'
C26'
Zn1
C9
C16
C19
N5
N1
C3
C10
C4
C5
N5#2
C12
N4
C8
C11
C17
C18
N7
C13
C7
C6
C15
C14
C25
S2

Fig. 2

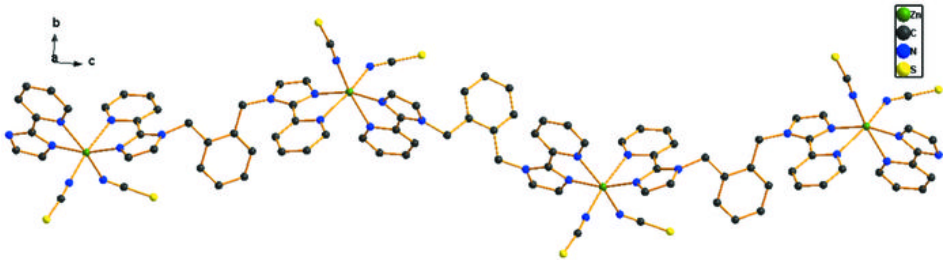


Fig. 3