

## Bis(2-amino-1,3-thiazole- $\kappa N^3$ )diazido-zinc

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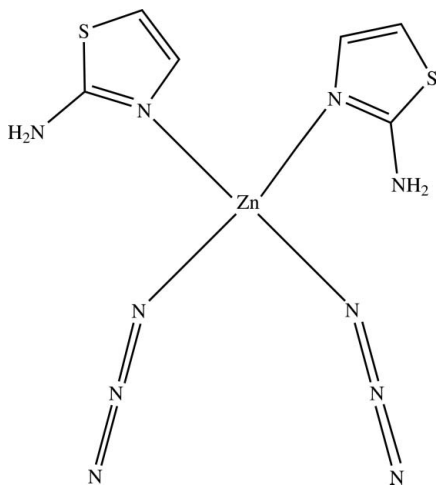
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Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(C-C) = 0.004$  Å;  $R$  factor = 0.025;  $wR$  factor = 0.068; data-to-parameter ratio = 15.9.

In the title complex,  $[Zn(N_3)_2(C_3H_4N_2S)_2]$ , the  $Zn^{II}$  atom is tetrahedrally coordinated by two terminal azide ligands and by the ring N atoms of two different 2-aminothiazole ligands. Intramolecular  $N-H \cdots N$  hydrogen bonds between the amino groups of both 2-aminothiazole ligands and the N atom of one of the azide ligands ensure that the heterocyclic rings are oriented in the same direction. Intermolecular  $N-H \cdots N$  hydrogen bonds link the molecules into zigzag sheets in the  $ac$  plane.

### Related literature

For multi-dimensional supramolecular complexes with organic-inorganic hybrids, see: Iwamoto (1996); Batten & Robson (1998); Braga *et al.* (1998). For the use of pseudo-halides in the construction of supramolecular assemblies, see: Vrieze & Koten (1987); Cortes *et al.* (1997); Yun *et al.* (2004); Kim *et al.* (2008). For the coordination chemistry of imidazole and thiazole derivatives, see: Costes *et al.* (1991); Balch *et al.* (1993); Suh *et al.* (2005, 2007, 2009); Kim & Kim (2010).



### Experimental

#### Crystal data

$[Zn(N_3)_2(C_3H_4N_2S)_2]$   
 $M_r = 349.71$   
 Triclinic,  $P\bar{1}$   
 $a = 8.096$  (1) Å  
 $b = 8.4004$  (8) Å  
 $c = 10.066$  (1) Å  
 $\alpha = 96.489$  (9)°  
 $\beta = 100.66$  (1)°

$\gamma = 96.885$  (9)°  
 $V = 661.5$  (1) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 2.18$  mm<sup>-1</sup>  
 $T = 295$  K  
 $0.42 \times 0.38 \times 0.24$  mm

#### Data collection

Bruker P4 diffractometer  
 Absorption correction:  $\psi$  scan  
 (North *et al.*, 1968)  
 $T_{min} = 0.462$ ,  $T_{max} = 0.623$   
 3352 measured reflections  
 2747 independent reflections

2544 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.013$   
 3 standard reflections every 97 reflections  
 intensity decay: none

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$   
 $wR(F^2) = 0.068$   
 $S = 1.09$   
 2747 reflections

173 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{max} = 0.29$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.28$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N16-H16A \cdots N4$	0.86	2.30	3.080 (3)	151
$N16-H16A \cdots N6^i$	0.86	2.57	3.033 (3)	115
$N16-H16B \cdots N3^{ii}$	0.86	2.34	3.102 (3)	148
$N26-H26A \cdots N4$	0.86	2.24	3.005 (3)	148
$N26-H26B \cdots N3^{iii}$	0.86	2.28	3.071 (3)	153

Symmetry codes: (i)  $-x + 1, -y, -z + 1$ ; (ii)  $x, y, z + 1$ ; (iii)  $-x, -y, -z$ .

Data collection: XSCANS (Bruker, 1996); cell refinement: XSCANS; data reduction: SHELXTL (Sheldrick, 2008); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

This work was supported by Konyang University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2293).

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**supplementary materials**

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## Bis(2-amino-1,3-thiazole- $\kappa N^3$ )diazidozinc

S. W. Suh, C.-H. Kim and I. H. Kim

### Comment

Multi-dimensional supramolecular complexes with both organic and inorganic ligands have become of great interest recently (Iwamoto, 1996; Batten & Robson, 1998). They have been shown to have useful electronic, magnetic, optical, catalytic, *etc.* properties (Braga *et al.*, 1998). For designing novel 1-, 2- and 3-D frameworks, we (Kim *et al.*, 2008) and others (Cortes *et al.*, 1997; Yun *et al.*, 2004) have used the coordination properties of pseudohalide ions and complementary organic ligands. Pseudo-halide ions are known to build up 1-, 2- and 3-D structures by bridging metal centers (Vrieze & Korten, 1987). The use of complementary organic ligands, such as aliphatic and aromatic amines is known to play an important role in stabilizing multi-dimensional structures. In particular, aromatic heterocycles such as imidazole and thiazole derivatives represent an important class of ligands in coordination chemistry (Balch *et al.*, 1993; Costes *et al.*, 1991). However, the frameworks of metal complexes with thiazole derivatives have been considerably less investigated. Our research is focused on the development of novel supramolecular structures utilizing the terminal and bridging properties of pseudo-halide ions, and the coordination behaviour of thiazole derivatives as complementary organic ligands (Suh *et al.*, 2005, 2007, 2009; Kim & Kim, 2010). Herein, we present the synthesis and structure determination of the title complex,  $Zn(N_3)_2(C_3H_4N_2S)_2$ , with 2-aminothiazole as shown in Fig. 1. In the title complex, the  $Zn^{II}$  atom is tetrahedrally coordinated by two terminal azido ligands, and by the N atoms of two different 2-aminothiazole ligands. Intramolecular N—H $\cdots$ N hydrogen bonds between the amino groups of both 2-aminothiazole ligands and the nitrogen atom of one of the azido ligands ensure that the heterocyclic rings are oriented in the same direction. Intermolecular N—H $\cdots$ N hydrogen bonds form the molecules into zig-zag sheets in the *ac* plane (Fig. 2).

### Experimental

A water-methanolic (2:1) solution (60 ml) of sodium azide (9 mmol, 0.59 g) was added to a water-methanolic (2:1) solution (50 ml) of  $ZnSO_4 \cdot 7H_2O$  (3 mmol, 0.87 g). To this mixture, a water-methanolic (2:1) solution (80 ml) of 2-aminobenzothiazole (10 mmol, 1.00 g) was introduced, with stirring for 1 h. The small amount of precipitates formed from the resulting solution were filtered off. The filtered solution was allowed to stand at room temperature. After a 1 week dark-yellow block crystals suitable for X-ray analysis were obtained. Elemental analysis found: C 20.73, H 2.25, N 40.22, S 18.50, Zn 18.70%;  $C_6H_8N_{10}S_2Zn$  requires: C 20.61, H 2.31, N 40.05, S 18.34, Zn 18.76%.

### Refinement

All H atoms were placed in calculated positions using a riding model, with C—H = 0.93 Å and  $U_{iso}(H) = 1.2 U_{eq}(C)$  for heterocyclic H atoms and N—H = 0.86 Å and  $U_{iso}(H) = 1.2 U_{eq}(N)$  for amino H atom.

## Figures

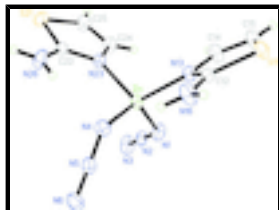


Fig. 1. The molecular structure of the title complex with the atomic numbering and 30% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radius.

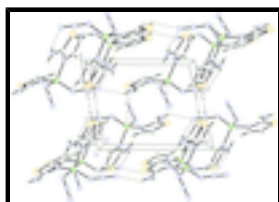


Fig. 2. The crystal packing diagram of the title complex, viewed down the *b* axis showing the N—H...N(dashed lines) hydrogen bonds.

## Bis(2-amino-1,3-thiazole- $\kappa N^3$ )diazidozinc

### Crystal data

[Zn(N<sub>3</sub>)<sub>2</sub>(C<sub>3</sub>H<sub>4</sub>N<sub>2</sub>S)<sub>2</sub>]

*M<sub>r</sub>* = 349.71

Triclinic, *P* $\bar{1}$

Hall symbol: -P 1

*a* = 8.096 (1) Å

*b* = 8.4004 (8) Å

*c* = 10.066 (1) Å

$\alpha$  = 96.489 (9)°

$\beta$  = 100.66 (1)°

$\gamma$  = 96.885 (9)°

*V* = 661.5 (1) Å<sup>3</sup>

*Z* = 2

*F*(000) = 352

*D<sub>x</sub>* = 1.756 Mg m<sup>-3</sup>

*D<sub>m</sub>* = 1.76 Mg m<sup>-3</sup>

*D<sub>m</sub>* measured by flotation method

Mo *K*α radiation,  $\lambda$  = 0.71073 Å

Cell parameters from 39 reflections

$\theta$  = 4.7–14.6°

$\mu$  = 2.18 mm<sup>-1</sup>

*T* = 295 K

Block, dark yellow

0.42 × 0.38 × 0.24 mm

### Data collection

Bruker P4  
diffractometer

Radiation source: fine-focus sealed tube

graphite

2 $\theta$ / $\omega$  scans

Absorption correction:  $\psi$  scan  
(North *et al.*, 1968)

*T<sub>min</sub>* = 0.462, *T<sub>max</sub>* = 0.623

3352 measured reflections

2747 independent reflections

2544 reflections with *I* > 2 $\sigma$ (*I*)

*R<sub>int</sub>* = 0.013

$\theta_{\max}$  = 26.5°,  $\theta_{\min}$  = 2.1°

*h* = -1 → 10

*k* = -10 → 10

*l* = -12 → 12

3 standard reflections every 97 reflections

intensity decay: none

Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.025$	H-atom parameters constrained
$wR(F^2) = 0.068$	$w = 1/[\sigma^2(F_o^2) + (0.0243P)^2 + 0.3124P]$
$S = 1.09$	where $P = (F_o^2 + 2F_c^2)/3$
2747 reflections	$(\Delta/\sigma)_{\max} < 0.001$
173 parameters	$\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\min} = -0.28 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.0118 (11)

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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn	0.22961 (3)	0.28874 (3)	0.27010 (2)	0.03913 (10)
N1	0.3512 (3)	0.4038 (3)	0.1481 (2)	0.0578 (5)
N2	0.3327 (3)	0.3684 (2)	0.0289 (2)	0.0479 (4)
N3	0.3184 (4)	0.3406 (3)	-0.0866 (2)	0.0758 (8)
N4	0.3014 (3)	0.1005 (2)	0.3536 (2)	0.0496 (5)
N5	0.4122 (3)	0.0255 (2)	0.32922 (19)	0.0475 (5)
N6	0.5156 (3)	-0.0496 (3)	0.3098 (3)	0.0689 (6)
S11	0.28221 (10)	0.65810 (8)	0.64496 (7)	0.05854 (18)
C12	0.2849 (3)	0.4728 (3)	0.5514 (2)	0.0407 (4)
N13	0.2265 (3)	0.4669 (2)	0.41986 (18)	0.0434 (4)
C14	0.1766 (4)	0.6139 (3)	0.3920 (3)	0.0646 (7)
H14A	0.1319	0.6314	0.3038	0.077*
C15	0.1962 (4)	0.7276 (3)	0.4978 (3)	0.0655 (7)
H15	0.1674	0.8310	0.4931	0.079*
N16	0.3412 (3)	0.3506 (3)	0.6102 (2)	0.0649 (6)
H16A	0.3410	0.2596	0.5614	0.078*

## supplementary materials

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H16B	0.3779	0.3623	0.6970	0.078*
S21	-0.28571 (8)	0.04332 (9)	0.02647 (7)	0.05992 (18)
C22	-0.0995 (3)	0.0694 (3)	0.1466 (2)	0.0424 (5)
N23	-0.0062 (2)	0.2108 (2)	0.15549 (18)	0.0408 (4)
C24	-0.0868 (3)	0.3032 (3)	0.0654 (3)	0.0561 (6)
H24A	-0.0395	0.4079	0.0589	0.067*
C25	-0.2352 (4)	0.2348 (3)	-0.0113 (3)	0.0616 (7)
H25	-0.3018	0.2835	-0.0760	0.074*
N26	-0.0579 (3)	-0.0446 (3)	0.2244 (3)	0.0672 (7)
H26A	0.0349	-0.0273	0.2847	0.081*
H26B	-0.1241	-0.1351	0.2141	0.081*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Zn	0.04775 (16)	0.03781 (14)	0.03000 (14)	0.00320 (10)	0.00434 (10)	0.00587 (9)
N1	0.0701 (14)	0.0594 (12)	0.0389 (10)	-0.0144 (11)	0.0145 (10)	0.0049 (9)
N2	0.0579 (12)	0.0396 (9)	0.0457 (11)	-0.0058 (8)	0.0160 (9)	0.0081 (8)
N3	0.117 (2)	0.0644 (14)	0.0413 (12)	-0.0165 (14)	0.0270 (13)	0.0021 (10)
N4	0.0558 (12)	0.0490 (11)	0.0446 (10)	0.0134 (9)	0.0044 (9)	0.0130 (8)
N5	0.0559 (12)	0.0406 (10)	0.0401 (10)	0.0058 (9)	-0.0050 (8)	0.0070 (8)
N6	0.0728 (16)	0.0597 (14)	0.0763 (16)	0.0273 (12)	0.0086 (13)	0.0100 (12)
S11	0.0711 (4)	0.0552 (3)	0.0448 (3)	0.0152 (3)	0.0066 (3)	-0.0102 (3)
C12	0.0433 (11)	0.0447 (11)	0.0333 (10)	0.0047 (9)	0.0090 (8)	0.0020 (8)
N13	0.0566 (11)	0.0393 (9)	0.0330 (8)	0.0074 (8)	0.0056 (8)	0.0050 (7)
C14	0.096 (2)	0.0496 (14)	0.0472 (13)	0.0235 (14)	0.0030 (14)	0.0101 (11)
C15	0.085 (2)	0.0483 (14)	0.0629 (16)	0.0222 (14)	0.0088 (15)	0.0033 (12)
N16	0.1032 (19)	0.0590 (13)	0.0313 (10)	0.0276 (13)	0.0015 (11)	0.0047 (9)
S21	0.0440 (3)	0.0662 (4)	0.0607 (4)	0.0020 (3)	-0.0054 (3)	0.0040 (3)
C22	0.0405 (11)	0.0445 (11)	0.0406 (11)	0.0059 (9)	0.0053 (9)	0.0037 (9)
N23	0.0439 (10)	0.0395 (9)	0.0381 (9)	0.0061 (7)	0.0035 (7)	0.0088 (7)
C24	0.0614 (15)	0.0534 (14)	0.0525 (14)	0.0089 (12)	0.0011 (12)	0.0201 (11)
C25	0.0622 (16)	0.0697 (17)	0.0516 (14)	0.0199 (13)	-0.0030 (12)	0.0163 (12)
N26	0.0603 (14)	0.0470 (11)	0.0853 (17)	-0.0080 (10)	-0.0084 (12)	0.0262 (11)

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

Zn—N4	1.9711 (19)	C14—H14A	0.9300
Zn—N1	1.974 (2)	C15—H15	0.9300
Zn—N13	2.0066 (18)	N16—H16A	0.8600
Zn—N23	2.0292 (18)	N16—H16B	0.8600
N1—N2	1.181 (3)	S21—C25	1.714 (3)
N2—N3	1.140 (3)	S21—C22	1.723 (2)
N4—N5	1.202 (3)	C22—N23	1.313 (3)
N5—N6	1.138 (3)	C22—N26	1.339 (3)
S11—C15	1.712 (3)	N23—C24	1.384 (3)
S11—C12	1.730 (2)	C24—C25	1.326 (4)
C12—N13	1.314 (3)	C24—H24A	0.9300
C12—N16	1.327 (3)	C25—H25	0.9300

N13—C14	1.386 (3)	N26—H26A	0.8600
C14—C15	1.320 (4)	N26—H26B	0.8600
N4—Zn—N1	124.47 (10)	C14—C15—H15	124.8
N4—Zn—N13	108.49 (8)	S11—C15—H15	124.8
N1—Zn—N13	102.24 (8)	C12—N16—H16A	120.0
N4—Zn—N23	105.71 (8)	C12—N16—H16B	120.0
N1—Zn—N23	104.23 (8)	H16A—N16—H16B	120.0
N13—Zn—N23	111.56 (8)	C25—S21—C22	89.76 (12)
N2—N1—Zn	125.88 (17)	N23—C22—N26	124.1 (2)
N3—N2—N1	177.1 (2)	N23—C22—S21	113.83 (17)
N5—N4—Zn	127.06 (17)	N26—C22—S21	122.09 (18)
N6—N5—N4	177.2 (3)	C22—N23—C24	110.0 (2)
C15—S11—C12	89.52 (12)	C22—N23—Zn	127.90 (15)
N13—C12—N16	124.6 (2)	C24—N23—Zn	121.96 (16)
N13—C12—S11	113.59 (17)	C25—C24—N23	116.5 (2)
N16—C12—S11	121.83 (17)	C25—C24—H24A	121.7
C12—N13—C14	110.16 (19)	N23—C24—H24A	121.7
C12—N13—Zn	127.78 (16)	C24—C25—S21	109.9 (2)
C14—N13—Zn	121.67 (16)	C24—C25—H25	125.1
C15—C14—N13	116.3 (2)	S21—C25—H25	125.1
C15—C14—H14A	121.9	C22—N26—H26A	120.0
N13—C14—H14A	121.9	C22—N26—H26B	120.0
C14—C15—S11	110.5 (2)	H26A—N26—H26B	120.0
N4—Zn—N1—N2	86.1 (3)	C12—N13—C14—C15	0.0 (4)
N13—Zn—N1—N2	-151.0 (2)	Zn—N13—C14—C15	-173.3 (2)
N23—Zn—N1—N2	-34.7 (3)	N13—C14—C15—S11	0.3 (4)
Zn—N1—N2—N3	164 (6)	C12—S11—C15—C14	-0.4 (3)
N1—Zn—N4—N5	-8.6 (2)	C25—S21—C22—N23	-0.86 (19)
N13—Zn—N4—N5	-128.7 (2)	C25—S21—C22—N26	178.0 (2)
N23—Zn—N4—N5	111.6 (2)	N26—C22—N23—C24	-177.6 (2)
Zn—N4—N5—N6	-177 (100)	S21—C22—N23—C24	1.2 (3)
C15—S11—C12—N13	0.5 (2)	N26—C22—N23—Zn	6.5 (3)
C15—S11—C12—N16	-179.4 (2)	S21—C22—N23—Zn	-174.66 (10)
N16—C12—N13—C14	179.5 (3)	N4—Zn—N23—C22	5.3 (2)
S11—C12—N13—C14	-0.4 (3)	N1—Zn—N23—C22	138.0 (2)
N16—C12—N13—Zn	-7.8 (4)	N13—Zn—N23—C22	-112.44 (19)
S11—C12—N13—Zn	172.39 (11)	N4—Zn—N23—C24	-170.06 (19)
N4—Zn—N13—C12	9.6 (2)	N1—Zn—N23—C24	-37.4 (2)
N1—Zn—N13—C12	-123.5 (2)	N13—Zn—N23—C24	72.2 (2)
N23—Zn—N13—C12	125.6 (2)	C22—N23—C24—C25	-1.0 (3)
N4—Zn—N13—C14	-178.4 (2)	Zn—N23—C24—C25	175.2 (2)
N1—Zn—N13—C14	48.5 (2)	N23—C24—C25—S21	0.3 (3)
N23—Zn—N13—C14	-62.3 (2)	C22—S21—C25—C24	0.3 (2)

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

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N16—H16A $\cdots$ N4	0.86	2.30	3.080 (3)	151



## supplementary materials

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N16—H16A···N6 <sup>i</sup>	0.86	2.57	3.033 (3)	115
N16—H16B···N3 <sup>ii</sup>	0.86	2.34	3.102 (3)	148
N26—H26A···N4	0.86	2.24	3.005 (3)	148
N26—H26B···N3 <sup>iii</sup>	0.86	2.28	3.071 (3)	153

Symmetry codes: (i)  $-x+1, -y, -z+1$ ; (ii)  $x, y, z+1$ ; (iii)  $-x, -y, -z$ .

Fig. 1

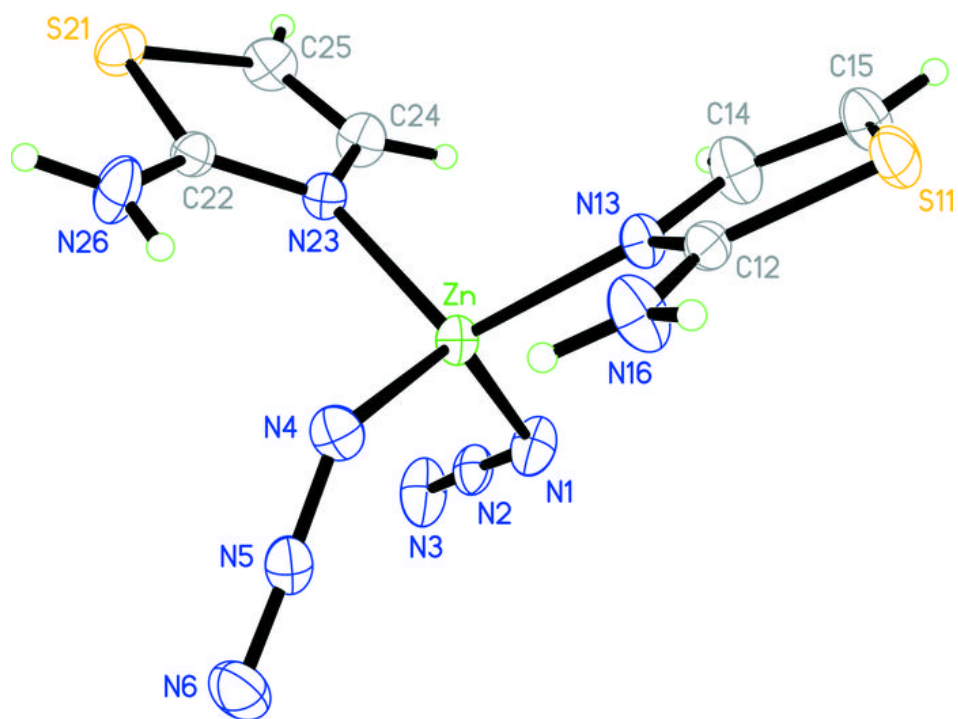


Fig. 2

