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(2,2′-Bipyridine-κ^2N,N')dichlorido-(dimethyl sulfoxide-κO)zinc(II)

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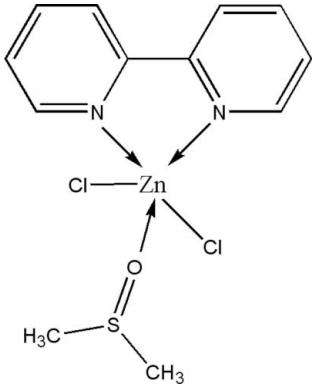
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.079; data-to-parameter ratio = 19.5.

In the title compound, $[ZnCl_2(C_{10}H_8N_2)(C_2H_6OS)]$, the Zn atom is five-coordinate, forming a distorted trigonal–bipyramidal geometry involving one Cl atom, one dimethyl sulfoxide O atom and one 2,2′-bipyridine N atom in equatorial positions, with distances Zn—Cl = 2.2863 (7) Å, Zn—O = 2.1024 (15) Å and Zn—N = 2.1546 (16) Å. The axial positions are occupied by the other 2,2′-bipyridine N atom and a Cl atom, with distances N—Zn = 2.1604 (16) Å and Zn—Cl = 2.3123 (7) Å.

Related literature

For related literature, see: Lemoine *et al.* (2003); Marjani *et al.* (2005).



Experimental

Crystal data

$[ZnCl_2(C_{10}H_8N_2)(C_2H_6OS)]$
M_r = 370.61
Triclinic, $P\overline{1}$
a = 7.9553 (17) Å
b = 9.5504 (19) Å
c = 10.003 (2) Å
α = 84.042 (16)°
β = 86.787 (17)°
γ = 83.798 (17)°
V = 750.7 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.12 mm^{-1}
T = 293 (2) K
0.5 × 0.5 × 0.45 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: numerical (*X-RED32*; Stoe & Cie, 2005)
T_{min} = 0.360, T_{max} = 0.380
7002 measured reflections
3420 independent reflections
3325 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.080
S = 1.07
3420 reflections
175 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2047).

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supplementary materials

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(2,2'-Bipyridine-κ^2N,N')dichlorido(dimethyl sulfoxide-κO)zinc(II)

K. Marjani, M. Mousavi, H. R. Khavasi, M. Ansari and H. R. Qumi

Comment

The title compound, [$ZnCl_2$(*Bipy*)(*DMSO*)] (I), has triclinic ($P\bar{1}$) symmetry. The asymetric unit of (I) contains one monomeric five–coordinate zinc complex. The Zn atom is coordinated by one 2,2'–bipyridine ligand *via* both N atoms, two Cl^- anions and one *DMSO* molecule *via* O atom. The complex exhibits a distorted trigonal bipyramidal geometry about the zinc atom, with atoms N2 and Cl2 in axial positions (Cl2—Zn1—N2 158.40 (5)°) and N1, Cl1 and O1 in equitorial positions. The Zn atom is 0.256 Å out of the equaitorial plane. The axial Zn—N and Zn—Cl bond lenghts are slightly longer than related equatorial bond lenghts. The *Bipy* ligand is slightly twisted, making an angle of 4.66° between the planes of two pyridine rings. The solid state of the molecule has a layer structure with the avrage distance of 3.397Å between 2,2'–bipyridins in closest layers. For related literature, see Lemoine *et al.* (2003) and Marjani *et al.* (2005).

Experimental

To a solution of $ZnCl_2$ (0.136 g, 1 mmol) in freshly distilled ethanol (10 ml), was aded 2,2'–bipyridine (0.156 g, 1 mmol) and 2–mercaptopyridine (0.223 g, 2 mmol). The mixture was stirred under dinitrogen atmosphere for 4 h. Then resulted yellow suspension was filtered, washed with ethanol and dried in *vacuo*. The crude product was recrystalized from *DMSO*, yeild crystals of [$ZnCl_2(C_{10}H_8N_2)$(*DMSO*)], (0.28 g, 75.68%). *M*.p. = 593–598 K (decompose). Found: C, 38.66; H, 3.81; N, 6.75%. Calculated for $C_{12}H_{14}Cl_2N_2OSZn$: C, 38.89; H, 3.81; N, 7.56%.

Figures

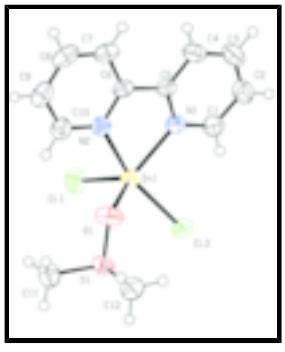

Fig. 1. The molecular structure of (I) with the numbering scheme. Displacement ellipsoids drawn at the 50% probability level. H atoms are presented as a spheres of arbitrary radius.

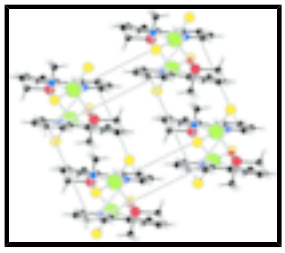

Fig. 2. The crystal packing of (I), showing its layer structure.

(2,2'-Bipyridine-κ^2*N*,*N*')dichlorido(dimethyl sulfoxide-κ*O*)zinc(II)

Crystal data

$[ZnCl_2(C_{10}H_8N_2)(C_2H_6OS)]$	V = 750.7 (3) Å^3
M_r = 370.61	Z = 2
Triclinic, $P\overline{1}$	F_{000} = 376
Hall symbol: -P 1	D_x = 1.640 Mg m^{-3}
a = 7.9553 (17) Å	Melting point: 593 K
b = 9.5504 (19) Å	Mo $K\alpha$ radiation λ = 0.71073 Å
c = 10.003 (2) Å	μ = 2.12 mm^{-1}
α = 84.042 (16)º	T = 293 (2) K
β = 86.787 (17)º	Block, colourless
γ = 83.798 (17)º	0.5 × 0.5 × 0.45 mm

Data collection

Stoe IPDSII diffractometer	3420 independent reflections
Radiation source: fine–focus sealed tube	3325 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.046
Detector resolution: 0.15 pixels mm^{-1}	θ_{max} = 27.9º
T = 293(2) K	θ_{min} = 2.1º
ω scans	h = −10→8
Absorption correction: numerical (X-RED32; Stoe & Cie, 2005)	k = −12→12
T_{min} = 0.360, T_{max} = 0.380	l = −13→13
7002 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.030	$w = 1/[\sigma^2(F_o^2) + (0.0362P)^2 + 0.2984P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.080	$(\Delta/\sigma)_{max}$ = 0.013
S = 1.07	$\Delta\rho_{max}$ = 0.54 e Å^{-3}
3420 reflections	$\Delta\rho_{min}$ = −0.48 e Å^{-3}
175 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.127 (11)
Secondary atom site location: difference Fourier map	

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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4259 (3)	−0.0788 (2)	0.2605 (2)	0.0447 (4)
H1	0.4517	−0.0535	0.1699	0.054*
C2	0.4984 (3)	−0.2067 (2)	0.3198 (3)	0.0540 (5)
H2	0.5710	−0.2666	0.2700	0.065*
C3	0.4610 (3)	−0.2435 (2)	0.4539 (3)	0.0557 (6)
H3	0.5084	−0.3289	0.4960	0.067*
C4	0.3527 (3)	−0.1527 (2)	0.5255 (2)	0.0473 (5)
H4	0.3259	−0.1761	0.6162	0.057*
C5	0.2844 (2)	−0.02600 (18)	0.45973 (18)	0.0342 (3)
C6	0.1691 (2)	0.07944 (19)	0.52816 (17)	0.0338 (3)
C7	0.1270 (3)	0.0653 (2)	0.6656 (2)	0.0471 (5)
H7	0.1680	−0.0149	0.7197	0.057*
C8	0.0234 (3)	0.1726 (3)	0.7201 (2)	0.0545 (6)
H8	−0.0066	0.1650	0.8116	0.065*
C9	−0.0351 (3)	0.2901 (3)	0.6387 (2)	0.0528 (5)
H9	−0.1031	0.3641	0.6741	0.063*
C10	0.0094 (3)	0.2960 (2)	0.5028 (2)	0.0466 (4)
H10	−0.0317	0.3748	0.4470	0.056*
C11	−0.2481 (3)	0.5039 (2)	0.1321 (3)	0.0540 (5)
H11A	−0.1767	0.5631	0.1698	0.065*
H11B	−0.3323	0.4750	0.1988	0.065*
H11C	−0.3026	0.5557	0.0562	0.065*
C12	−0.2877 (3)	0.2621 (3)	0.0277 (3)	0.0559 (5)
H12A	−0.3768	0.2600	0.0965	0.067*
H12B	−0.2441	0.1670	0.0127	0.067*
H12C	−0.3313	0.3103	−0.0541	0.067*
N1	0.32037 (19)	0.00978 (16)	0.32836 (16)	0.0354 (3)
N2	0.1092 (2)	0.19316 (16)	0.44821 (15)	0.0362 (3)
O1	−0.06662 (18)	0.26907 (18)	0.21056 (15)	0.0500 (4)
Zn1	0.19104 (2)	0.20350 (2)	0.238136 (19)	0.03318 (11)
S1	−0.12365 (6)	0.35232 (5)	0.07942 (5)	0.03847 (13)
Cl1	0.32074 (7)	0.40566 (5)	0.23911 (6)	0.04915 (15)
Cl2	0.23552 (10)	0.13441 (6)	0.02310 (5)	0.06124 (18)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0436 (10)	0.0488 (10)	0.0407 (10)	0.0033 (8)	−0.0032 (8)	−0.0069 (8)
C2	0.0479 (11)	0.0471 (11)	0.0662 (14)	0.0107 (9)	−0.0106 (10)	−0.0135 (10)
C3	0.0575 (13)	0.0400 (10)	0.0673 (15)	0.0045 (9)	−0.0174 (11)	0.0032 (10)
C4	0.0534 (11)	0.0442 (10)	0.0432 (11)	−0.0069 (8)	−0.0113 (9)	0.0085 (8)
C5	0.0352 (8)	0.0365 (8)	0.0317 (8)	−0.0088 (6)	−0.0070 (6)	0.0004 (6)
C6	0.0350 (8)	0.0402 (8)	0.0280 (8)	−0.0122 (6)	−0.0032 (6)	−0.0016 (6)
C7	0.0514 (11)	0.0603 (12)	0.0302 (9)	−0.0148 (9)	−0.0026 (8)	0.0026 (8)
C8	0.0534 (12)	0.0832 (16)	0.0305 (9)	−0.0173 (11)	0.0039 (8)	−0.0144 (10)
C9	0.0498 (11)	0.0642 (13)	0.0477 (12)	−0.0071 (10)	0.0060 (9)	−0.0247 (10)
C10	0.0523 (11)	0.0443 (10)	0.0431 (10)	−0.0017 (8)	0.0016 (8)	−0.0094 (8)
C11	0.0581 (13)	0.0422 (10)	0.0605 (14)	−0.0043 (9)	0.0048 (10)	−0.0049 (9)
C12	0.0603 (13)	0.0563 (12)	0.0531 (13)	−0.0065 (10)	−0.0126 (10)	−0.0101 (10)
N1	0.0369 (7)	0.0368 (7)	0.0319 (7)	−0.0023 (6)	−0.0035 (6)	−0.0020 (6)
N2	0.0406 (8)	0.0377 (7)	0.0303 (7)	−0.0055 (6)	0.0006 (6)	−0.0033 (6)
O1	0.0365 (7)	0.0688 (10)	0.0399 (8)	−0.0023 (6)	−0.0026 (6)	0.0141 (7)
Zn1	0.03600 (14)	0.03394 (14)	0.02856 (14)	−0.00156 (8)	−0.00143 (8)	−0.00035 (8)
S1	0.0346 (2)	0.0440 (2)	0.0339 (2)	−0.00181 (17)	0.00193 (16)	0.00573 (17)
Cl1	0.0550 (3)	0.0430 (3)	0.0505 (3)	−0.0150 (2)	0.0055 (2)	−0.0035 (2)
Cl2	0.0945 (5)	0.0534 (3)	0.0326 (3)	0.0171 (3)	−0.0126 (3)	−0.0099 (2)

Geometric parameters (Å, °)

C1—N1	1.335 (3)	C9—H9	0.9300
C1—C2	1.383 (3)	C10—N2	1.337 (3)
C1—H1	0.9300	C10—H10	0.9300
C2—C3	1.375 (4)	C11—S1	1.773 (2)
C2—H2	0.9300	C11—H11A	0.9600
C3—C4	1.380 (3)	C11—H11B	0.9600
C3—H3	0.9300	C11—H11C	0.9600
C4—C5	1.388 (3)	C12—S1	1.768 (2)
C4—H4	0.9300	C12—H12A	0.9600
C5—N1	1.346 (2)	C12—H12B	0.9600
C5—C6	1.482 (3)	C12—H12C	0.9600
C6—N2	1.341 (2)	N1—Zn1	2.1546 (16)
C6—C7	1.393 (3)	N2—Zn1	2.1604 (16)
C7—C8	1.382 (3)	O1—S1	1.5268 (15)
C7—H7	0.9300	O1—Zn1	2.1024 (15)
C8—C9	1.371 (4)	Zn1—Cl1	2.2863 (7)
C8—H8	0.9300	Zn1—Cl2	2.3123 (7)
C9—C10	1.383 (3)		
N1—C1—C2	122.4 (2)	S1—C11—H11B	109.5
N1—C1—H1	118.8	H11A—C11—H11B	109.5
C2—C1—H1	118.8	S1—C11—H11C	109.5
C3—C2—C1	118.7 (2)	H11A—C11—H11C	109.5

C3—C2—H2	120.7	H11B—C11—H11C	109.5
C1—C2—H2	120.7	S1—C12—H12A	109.5
C2—C3—C4	119.53 (19)	S1—C12—H12B	109.5
C2—C3—H3	120.2	H12A—C12—H12B	109.5
C4—C3—H3	120.2	S1—C12—H12C	109.5
C3—C4—C5	118.8 (2)	H12A—C12—H12C	109.5
C3—C4—H4	120.6	H12B—C12—H12C	109.5
C5—C4—H4	120.6	C1—N1—C5	118.86 (16)
N1—C5—C4	121.69 (18)	C1—N1—Zn1	123.98 (13)
N1—C5—C6	115.39 (15)	C5—N1—Zn1	117.07 (12)
C4—C5—C6	122.92 (17)	C10—N2—C6	118.90 (17)
N2—C6—C7	121.45 (18)	C10—N2—Zn1	123.67 (14)
N2—C6—C5	115.02 (15)	C6—N2—Zn1	117.35 (12)
C7—C6—C5	123.51 (17)	S1—O1—Zn1	120.57 (8)
C8—C7—C6	118.8 (2)	O1—Zn1—N1	132.24 (6)
C8—C7—H7	120.6	O1—Zn1—N2	82.67 (6)
C6—C7—H7	120.6	N1—Zn1—N2	75.01 (6)
C9—C8—C7	119.7 (2)	O1—Zn1—Cl1	106.16 (5)
C9—C8—H8	120.2	N1—Zn1—Cl1	117.33 (5)
C7—C8—H8	120.2	N2—Zn1—Cl1	95.19 (5)
C8—C9—C10	118.4 (2)	O1—Zn1—Cl2	93.00 (5)
C8—C9—H9	120.8	N1—Zn1—Cl2	92.94 (5)
C10—C9—H9	120.8	N2—Zn1—Cl2	158.40 (5)
N2—C10—C9	122.7 (2)	Cl1—Zn1—Cl2	106.32 (3)
N2—C10—H10	118.6	O1—S1—C12	105.02 (11)
C9—C10—H10	118.6	O1—S1—C11	104.08 (11)
S1—C11—H11A	109.5	C12—S1—C11	98.71 (12)
N1—C1—C2—C3	−0.4 (3)	C7—C6—N2—Zn1	178.26 (14)
C1—C2—C3—C4	0.1 (4)	C5—C6—N2—Zn1	−0.48 (19)
C2—C3—C4—C5	−0.1 (3)	S1—O1—Zn1—N1	−139.32 (10)
C3—C4—C5—N1	0.4 (3)	S1—O1—Zn1—N2	158.65 (12)
C3—C4—C5—C6	−179.00 (19)	S1—O1—Zn1—Cl1	65.35 (12)
N1—C5—C6—N2	3.3 (2)	S1—O1—Zn1—Cl2	−42.60 (11)
C4—C5—C6—N2	−177.26 (17)	C1—N1—Zn1—O1	114.68 (16)
N1—C5—C6—C7	−175.40 (17)	C5—N1—Zn1—O1	−61.81 (15)
C4—C5—C6—C7	4.0 (3)	C1—N1—Zn1—N2	179.75 (17)
N2—C6—C7—C8	−1.1 (3)	C5—N1—Zn1—N2	3.26 (12)
C5—C6—C7—C8	177.55 (18)	C1—N1—Zn1—Cl1	−92.14 (16)
C6—C7—C8—C9	−0.2 (3)	C5—N1—Zn1—Cl1	91.37 (13)
C7—C8—C9—C10	1.3 (3)	C1—N1—Zn1—Cl2	17.94 (16)
C8—C9—C10—N2	−1.2 (3)	C5—N1—Zn1—Cl2	−158.55 (12)
C2—C1—N1—C5	0.7 (3)	C10—N2—Zn1—O1	−47.13 (17)
C2—C1—N1—Zn1	−175.75 (16)	C6—N2—Zn1—O1	136.01 (13)
C4—C5—N1—C1	−0.7 (3)	C10—N2—Zn1—N1	175.47 (17)
C6—C5—N1—C1	178.77 (16)	C6—N2—Zn1—N1	−1.38 (12)
C4—C5—N1—Zn1	175.99 (14)	C10—N2—Zn1—Cl1	58.54 (16)
C6—C5—N1—Zn1	−4.56 (19)	C6—N2—Zn1—Cl1	−118.31 (12)
C9—C10—N2—C6	−0.1 (3)	C10—N2—Zn1—Cl2	−126.67 (16)
C9—C10—N2—Zn1	−176.92 (17)	C6—N2—Zn1—Cl2	56.5 (2)

C7—C6—N2—C10	1.2 (3)	Zn1—O1—S1—C12	129.40 (13)
C5—C6—N2—C10	−177.49 (17)	Zn1—O1—S1—C11	−127.36 (12)

Fig. 1

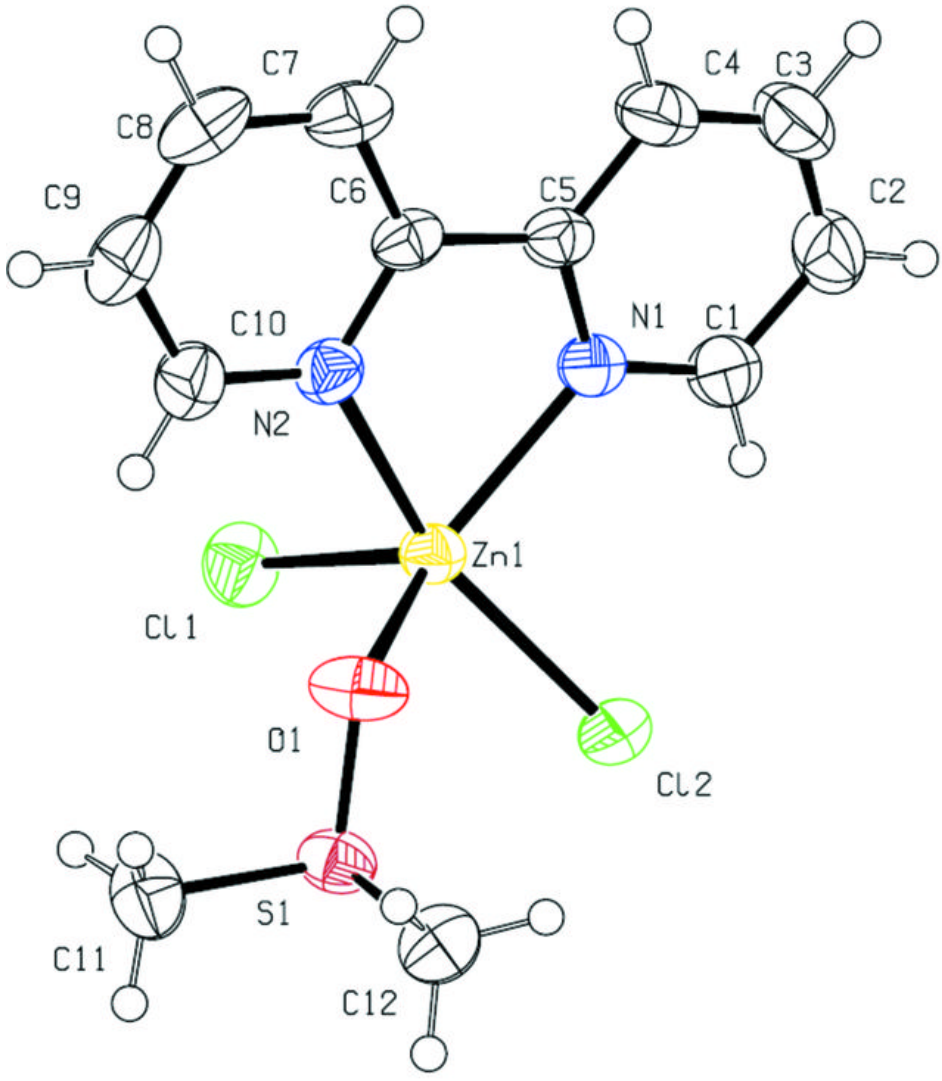

Fig. 2