Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Bis[2-(2-pyridylmethyleneamino)-benzenesulfonato-$\kappa^3N,N',O$]zinc(II) dihydrate

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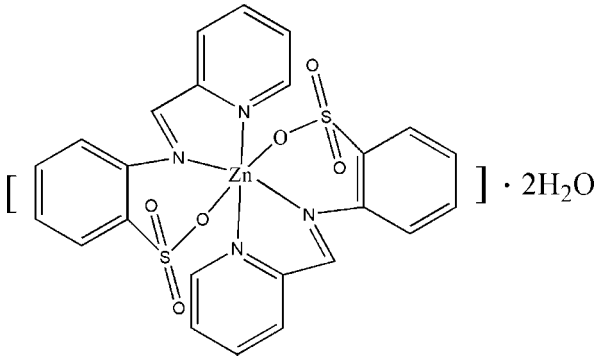
Received 26 July 2008; accepted 14 August 2008

Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.027; $wR$ factor = 0.075; data-to-parameter ratio = 13.6.

In the title complex, $[Zn(C_{12}H_9N_2O_3S)_2]\cdot 2H_2O$, the $Zn^{II}$ ion lies on a crystallographic inversion center and is coordinated by four N atoms and two O atoms from two tridentate 2-(2-pyridylmethyleneamino)benzenesulfonate ligands in a slightly distorted octahedral environment. In the crystal structure, the complex forms a two-dimensional network through intermolecular O—H···O and C—H···O hydrogen bonds.

## Related literature

For related literature, see: Casella & Gullotti (1981, 1986); Jiang *et al.* (2006); Li *et al.* (2006, 2007); Wang *et al.* (1994); Zhang *et al.* (2004, 2007, 2008); Correia *et al.* (2003); Zheng *et al.* (2001); Zhou *et al.* (2004).




## Experimental

### Crystal data

$[Zn(C_{12}H_9N_2O_3S)_2]\cdot 2H_2O$
$M_r$ = 623.95
Orthorhombic, *Pbcn*
$a$ = 19.7090 (15) Å
$b$ = 8.0722 (6) Å
$c$ = 16.3390 (13) Å
$V$ = 2599.5 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.16 mm$^{-1}$
$T$ = 295 (2) K
0.49 × 0.45 × 0.37 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.600, $T_{max}$ = 0.673
17894 measured reflections
2412 independent reflections
2100 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.074
$S$ = 1.04
2412 reflections
177 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O4—H1$W$···O3$^{i}$ | 0.83 | 2.21 | 3.014 (3) | 162 |
| O4—H2$W$···O2 | 0.83 | 2.06 | 2.877 (3) | 166 |
| C4—H4···O3$^{ii}$ | 0.93 | 2.48 | 3.407 (3) | 175 |
| C6—H6···O4$^{iii}$ | 0.93 | 2.57 | 3.436 (3) | 155 |

Symmetry codes: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, z$; (ii) $-x+1, y+1, -z+\frac{1}{2}$; (iii) $x, -y+2, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was funded by Guangxi Science Foundation, Guangxi Zhuang Autonomous Region of the People's Republic of China (grant No. 0731053).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2112).

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# supplementary materials

*Acta Cryst.* (2008). E**64**, m1195 [ **doi:10.1107/S1600536808026342** ]

# Bis[2-(2-pyridylmethyleneamino)benzenesulfonato-$\kappa^3N,N',O$]zinc(II) dihydrate

**C.-X. Cai, M. Ou-Yang, Z.-Y. Zhao and Y.-M. Jiang**

## Comment

The design and control of supermolecular coordination complex networks in which both coordination bonds and hydrogen bonds take part in the self-assembly chemistry (Zheng, *et al.*, 2001; Zhou, *et al.*, 2004) have recently garnered increasing interest. Schiff base complexes that contain both sulfur and amino acid functionalities have received much attention owing to their potential applications in pharmacy. (Casella & Gullotti, 1981, 1986; Wang *et al.*, 1994; Li *et al.*, 2006; Zhang *et al.*, 2007, 2008).

Our group has focused on the exploration of the coordination chemistry of the sulfonate ligands for years (Zhang *et al.* 2004; Jiang *et al.* 2006; Li *et al.* 2007). We report here the synthesis and the structure of the mononuclear $Zn^{II}$ Paba complex (Fig. 1). The structure is composed of one $Zn^{II}$, two deprotonated $Paba^-$ ligands and two guest water molecules. The six-coordinated $Zn^{II}$ atom has a distorted octahedral geometry, being coordinated by pyridine N, imine N and sulfonate O atoms from two deprotonated $Paba^-$ ligands in a tridentate facial arrangement. This structure is similar to those reported for complexes with N,N',O-tridentate donor ligands (Li *et al.*, 2006; Correia *et al.*, 2003).

There are extensive hydrogen bonds (O4-H2W···O2 and O4-H1W···O3), in which the donor is O-H of the guest water and S=O acts as acceptor, which forms a two-dimension sheet structure (Fig. 2).

## Experimental

The potassium salt of 2-(pyridylmethyl)imine-2-benzenesulfonic acid (PabaK) was synthesized according to the literature method (Casella & Gullotti, 1986).

To prepare the title complex, the ligand PabaK (1 mmol, 0.30 g) was dissolved in methanol (10 mL) at 333 K and an aqueous solution (10 mL) containing $ZnCl_2$(0.5 mmol, 0.068 g) was added. The resulting solution was stirred at 333 K for 4 h, then cooled to room temperature and filtered. Yellow crystals suitable for X-ray diffraction were obtained by slow evaporation over several days, with a yield of 55%. Elemental analysis, found (%): C, 46.05; H, 3.55; N, 8.95; S, 10.42; calc (%): C, 46.16; H, 3.53; N, 8.98; S, 10.26.

## Refinement

H atoms bonded to C atoms were positioned geometrically with the C-H distance of 0.93 Å, and treated as riding atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$. Water hydrogens were placed in fixed positions and assigned $U_{iso}$ values of $1.5U_{eq}$ of the water oxygen atom.

**Figures**

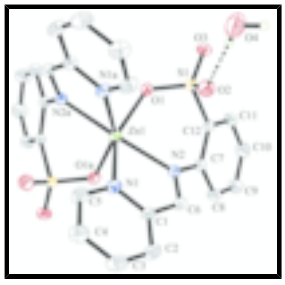

Fig. 1. An ellipsoid plot (30% probability) showing the numbering scheme. Dashed lines indicate hydrogen bonds. Symmetry code: (a) -x+1, y, -z+1/2.

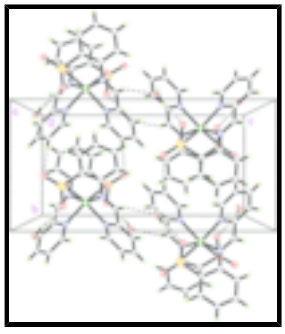

Fig. 2. 2-D structure, as viewed down the a axis. Dashed lines indicate hydrogen bonds.

**Bis[2-(2-pyridylmethyleneamino)benzenesulfonato- $\kappa^3N,N',O$]zinc(II) dihydrate**

*Crystal data*

| | |
|---|---|
| $[Zn(C_{12}H_9N_2O_3S_1)_2]\cdot 2H_2O$ | $F_{000}$ = 1280 |
| $M_r$ = 623.95 | $D_x$ = 1.594 Mg m$^{-3}$ |
| Orthorhombic, *Pbcn* | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2n 2ab | Cell parameters from 7323 reflections |
| *a* = 19.7090 (15) Å | θ = 2.5–28.2º |
| *b* = 8.0722 (6) Å | μ = 1.16 mm$^{-1}$ |
| *c* = 16.3390 (13) Å | *T* = 295 (2) K |
| *V* = 2599.5 (3) Å$^3$ | Block, yellow |
| *Z* = 4 | 0.49 × 0.45 × 0.37 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 2412 independent reflections |
| Radiation source: fine-focus sealed tube | 2100 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.024 |
| *T* = 295(2) K | $\theta_{max}$ = 25.5º |
| φ and ω scans | $\theta_{min}$ = 2.5º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | *h* = −23→23 |
| $T_{min}$ = 0.600, $T_{max}$ = 0.673 | *k* = −9→9 |
| 17894 measured reflections | *l* = −19→19 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.026$ | H-atom parameters constrained |
| $wR(F^2) = 0.074$ | $w = 1/[\sigma^2(F_o^2) + (0.0373P)^2 + 1.7627P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.04$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 2412 reflections | $\Delta\rho_{max} = 0.46$ e Å$^{-3}$ |
| 177 parameters | $\Delta\rho_{min} = -0.42$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Zn1 | 0.5000 | 0.82446 (4) | 0.2500 | 0.02769 (11) |
| S1 | 0.37616 (2) | 0.67719 (6) | 0.34320 (3) | 0.03070 (14) |
| O1 | 0.45098 (7) | 0.67650 (18) | 0.33822 (8) | 0.0344 (3) |
| O2 | 0.34865 (8) | 0.84229 (19) | 0.33446 (10) | 0.0456 (4) |
| O3 | 0.35256 (7) | 0.5876 (2) | 0.41443 (8) | 0.0431 (4) |
| N1 | 0.49613 (8) | 1.0216 (2) | 0.16032 (10) | 0.0341 (4) |
| N2 | 0.40820 (8) | 0.7687 (2) | 0.17245 (9) | 0.0297 (4) |
| C1 | 0.44459 (10) | 1.0145 (3) | 0.10605 (12) | 0.0332 (4) |
| C2 | 0.43673 (13) | 1.1301 (3) | 0.04460 (14) | 0.0452 (6) |
| H2 | 0.4007 | 1.1223 | 0.0081 | 0.054* |
| C3 | 0.48322 (13) | 1.2579 (3) | 0.03809 (15) | 0.0506 (6) |
| H3 | 0.4786 | 1.3380 | −0.0025 | 0.061* |
| C4 | 0.53638 (13) | 1.2645 (3) | 0.09261 (15) | 0.0483 (6) |
| H4 | 0.5688 | 1.3480 | 0.0890 | 0.058* |
| C5 | 0.54084 (12) | 1.1447 (3) | 0.15295 (14) | 0.0420 (5) |
| H5 | 0.5766 | 1.1503 | 0.1900 | 0.050* |
| C6 | 0.39854 (10) | 0.8728 (3) | 0.11481 (12) | 0.0354 (5) |
| H6 | 0.3626 | 0.8590 | 0.0786 | 0.042* |

| | | | | |
|---|---|---|---|---|
| C7 | 0.36755 (9) | 0.6238 (3) | 0.17777 (12) | 0.0313 (4) |
| C8 | 0.34696 (11) | 0.5353 (3) | 0.10925 (13) | 0.0437 (5) |
| H8 | 0.3579 | 0.5736 | 0.0572 | 0.052* |
| C9 | 0.31015 (12) | 0.3900 (3) | 0.11817 (15) | 0.0524 (6) |
| H9 | 0.2962 | 0.3320 | 0.0720 | 0.063* |
| C10 | 0.29391 (13) | 0.3306 (3) | 0.19512 (16) | 0.0516 (6) |
| H10 | 0.2698 | 0.2322 | 0.2005 | 0.062* |
| C11 | 0.31364 (11) | 0.4180 (3) | 0.26416 (13) | 0.0403 (5) |
| H11 | 0.3022 | 0.3792 | 0.3160 | 0.048* |
| C12 | 0.35039 (10) | 0.5632 (3) | 0.25581 (11) | 0.0300 (4) |
| O4 | 0.29845 (11) | 1.0939 (4) | 0.44343 (14) | 0.1079 (10) |
| H1W | 0.2572 | 1.1144 | 0.4394 | 0.162* |
| H2W | 0.3083 | 1.0105 | 0.4158 | 0.162* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.02732 (18) | 0.03263 (19) | 0.02311 (18) | 0.000 | −0.00389 (11) | 0.000 |
| S1 | 0.0291 (3) | 0.0396 (3) | 0.0234 (2) | −0.0001 (2) | 0.00018 (18) | −0.0016 (2) |
| O1 | 0.0287 (7) | 0.0462 (9) | 0.0285 (7) | −0.0028 (6) | −0.0034 (6) | 0.0038 (6) |
| O2 | 0.0482 (9) | 0.0452 (9) | 0.0436 (9) | 0.0102 (7) | −0.0018 (7) | −0.0079 (7) |
| O3 | 0.0416 (8) | 0.0620 (10) | 0.0257 (7) | −0.0062 (8) | 0.0039 (6) | 0.0035 (7) |
| N1 | 0.0400 (9) | 0.0346 (9) | 0.0278 (9) | −0.0007 (7) | −0.0057 (7) | 0.0011 (7) |
| N2 | 0.0278 (8) | 0.0375 (9) | 0.0238 (8) | −0.0006 (7) | 0.0004 (6) | 0.0004 (7) |
| C1 | 0.0343 (10) | 0.0377 (11) | 0.0275 (10) | 0.0035 (9) | −0.0036 (8) | 0.0023 (8) |
| C2 | 0.0519 (14) | 0.0471 (13) | 0.0367 (12) | 0.0017 (11) | −0.0113 (10) | 0.0096 (10) |
| C3 | 0.0728 (17) | 0.0386 (13) | 0.0403 (13) | −0.0023 (12) | −0.0064 (12) | 0.0105 (11) |
| C4 | 0.0628 (15) | 0.0363 (12) | 0.0458 (13) | −0.0117 (11) | −0.0019 (11) | 0.0022 (10) |
| C5 | 0.0490 (13) | 0.0391 (12) | 0.0380 (12) | −0.0084 (10) | −0.0102 (10) | 0.0012 (9) |
| C6 | 0.0310 (11) | 0.0475 (12) | 0.0276 (10) | 0.0001 (9) | −0.0057 (8) | 0.0034 (9) |
| C7 | 0.0245 (10) | 0.0410 (11) | 0.0284 (10) | −0.0009 (8) | −0.0004 (8) | −0.0015 (9) |
| C8 | 0.0417 (12) | 0.0609 (15) | 0.0286 (11) | −0.0085 (11) | 0.0014 (9) | −0.0050 (10) |
| C9 | 0.0505 (14) | 0.0679 (16) | 0.0389 (13) | −0.0180 (13) | −0.0001 (11) | −0.0169 (12) |
| C10 | 0.0464 (14) | 0.0552 (15) | 0.0530 (15) | −0.0211 (12) | 0.0021 (11) | −0.0085 (12) |
| C11 | 0.0363 (12) | 0.0495 (13) | 0.0351 (11) | −0.0088 (10) | 0.0038 (9) | 0.0017 (10) |
| C12 | 0.0232 (9) | 0.0399 (11) | 0.0270 (10) | −0.0007 (8) | −0.0001 (7) | −0.0023 (8) |
| O4 | 0.0592 (13) | 0.168 (3) | 0.0964 (18) | 0.0323 (15) | −0.0209 (12) | −0.0725 (19) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Zn1—O1 | 2.1065 (14) | C3—C4 | 1.376 (3) |
| Zn1—O1$^{i}$ | 2.1065 (14) | C3—H3 | 0.9300 |
| Zn1—N1$^{i}$ | 2.1643 (18) | C4—C5 | 1.384 (3) |
| Zn1—N1 | 2.1643 (18) | C4—H4 | 0.9300 |
| Zn1—N2 | 2.2544 (16) | C5—H5 | 0.9300 |
| Zn1—N2$^{i}$ | 2.2544 (16) | C6—H6 | 0.9300 |
| S1—O2 | 1.4459 (16) | C7—C8 | 1.389 (3) |
| S1—O3 | 1.4470 (15) | C7—C12 | 1.407 (3) |

| | | | |
|---|---|---|---|
| S1—O1 | 1.4769 (14) | C8—C9 | 1.387 (3) |
| S1—C12 | 1.7730 (19) | C8—H8 | 0.9300 |
| N1—C5 | 1.334 (3) | C9—C10 | 1.383 (3) |
| N1—C1 | 1.350 (2) | C9—H9 | 0.9300 |
| N2—C6 | 1.277 (3) | C10—C11 | 1.386 (3) |
| N2—C7 | 1.421 (3) | C10—H10 | 0.9300 |
| C1—C2 | 1.380 (3) | C11—C12 | 1.384 (3) |
| C1—C6 | 1.467 (3) | C11—H11 | 0.9300 |
| C2—C3 | 1.384 (3) | O4—H1W | 0.8332 |
| C2—H2 | 0.9300 | O4—H2W | 0.8339 |
| O1—Zn1—O1$^{i}$ | 110.92 (8) | C3—C2—H2 | 120.5 |
| O1—Zn1—N1$^{i}$ | 88.27 (6) | C4—C3—C2 | 118.9 (2) |
| O1$^{i}$—Zn1—N1$^{i}$ | 149.76 (6) | C4—C3—H3 | 120.6 |
| O1—Zn1—N1 | 149.76 (6) | C2—C3—H3 | 120.6 |
| O1$^{i}$—Zn1—N1 | 88.27 (6) | C3—C4—C5 | 118.9 (2) |
| N1$^{i}$—Zn1—N1 | 85.36 (9) | C3—C4—H4 | 120.6 |
| O1—Zn1—N2 | 84.45 (5) | C5—C4—H4 | 120.6 |
| O1$^{i}$—Zn1—N2 | 82.55 (5) | N1—C5—C4 | 122.9 (2) |
| N1$^{i}$—Zn1—N2 | 123.75 (6) | N1—C5—H5 | 118.5 |
| N1—Zn1—N2 | 74.81 (6) | C4—C5—H5 | 118.5 |
| O1—Zn1—N2$^{i}$ | 82.55 (5) | N2—C6—C1 | 119.53 (18) |
| O1$^{i}$—Zn1—N2$^{i}$ | 84.45 (5) | N2—C6—H6 | 120.2 |
| N1$^{i}$—Zn1—N2$^{i}$ | 74.81 (6) | C1—C6—H6 | 120.2 |
| N1—Zn1—N2$^{i}$ | 123.75 (6) | C8—C7—C12 | 118.80 (19) |
| N2—Zn1—N2$^{i}$ | 156.97 (9) | C8—C7—N2 | 122.62 (18) |
| O2—S1—O3 | 114.81 (10) | C12—C7—N2 | 118.51 (17) |
| O2—S1—O1 | 111.87 (9) | C9—C8—C7 | 120.2 (2) |
| O3—S1—O1 | 111.31 (9) | C9—C8—H8 | 119.9 |
| O2—S1—C12 | 106.94 (9) | C7—C8—H8 | 119.9 |
| O3—S1—C12 | 107.23 (9) | C10—C9—C8 | 120.7 (2) |
| O1—S1—C12 | 103.86 (9) | C10—C9—H9 | 119.7 |
| S1—O1—Zn1 | 119.57 (8) | C8—C9—H9 | 119.7 |
| C5—N1—C1 | 118.00 (18) | C9—C10—C11 | 119.9 (2) |
| C5—N1—Zn1 | 125.86 (14) | C9—C10—H10 | 120.1 |
| C1—N1—Zn1 | 116.11 (14) | C11—C10—H10 | 120.1 |
| C6—N2—C7 | 120.22 (17) | C12—C11—C10 | 119.8 (2) |
| C6—N2—Zn1 | 113.76 (14) | C12—C11—H11 | 120.1 |
| C7—N2—Zn1 | 125.63 (12) | C10—C11—H11 | 120.1 |
| N1—C1—C2 | 122.3 (2) | C11—C12—C7 | 120.62 (18) |
| N1—C1—C6 | 115.76 (17) | C11—C12—S1 | 120.65 (15) |
| C2—C1—C6 | 121.93 (19) | C7—C12—S1 | 118.73 (15) |
| C1—C2—C3 | 119.1 (2) | H1W—O4—H2W | 110.2 |
| C1—C2—H2 | 120.5 | | |

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

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4—H1W···O3$^{ii}$ | 0.83 | 2.21 | 3.014 (3) | 162 |
| O4—H2W···O2 | 0.83 | 2.06 | 2.877 (3) | 166 |
| C4—H4···O3$^{iii}$ | 0.93 | 2.48 | 3.407 (3) | 175 |
| C6—H6···O4$^{iv}$ | 0.93 | 2.57 | 3.436 (3) | 155 |

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

**Fig. 1**

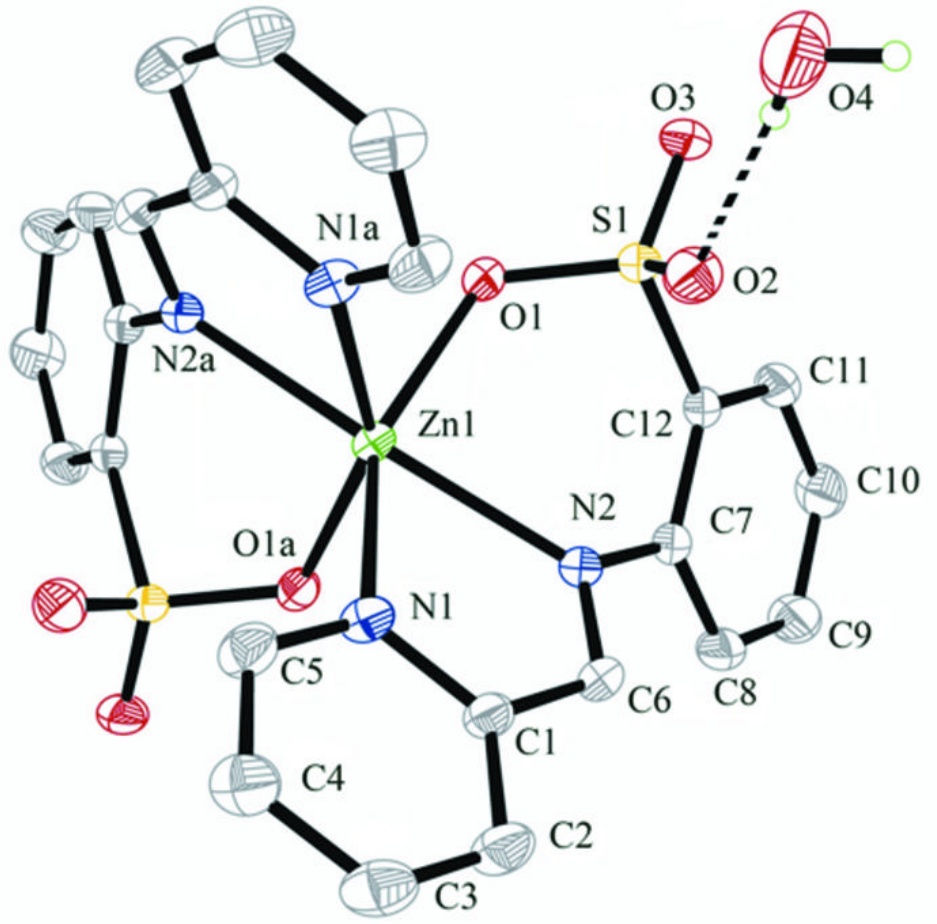
O3
O4
S1
N1a
O2
O1
N2a
C11
Zn1
C12
C10
N2
C7
O1a
N1
C9
C5
C6
C8
C1
C4
C2
C3

**Fig. 2**