

catena-Poly[[dichloridozinc(II)]- μ -1,4-bis(pyridin-2-ylmethoxy)benzene- κ^2 N:N']

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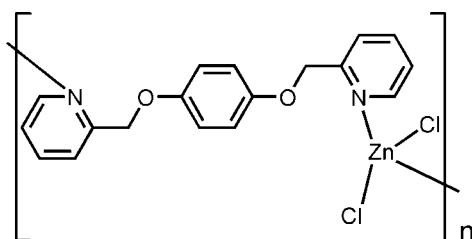
Received 14 July 2011; accepted 3 September 2011

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.032; wR factor = 0.073; data-to-parameter ratio = 17.8.

In the title compound, $[\text{ZnCl}_2(\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_2)]_n$, the Zn^{II} ion is tetrahedrally coordinated by two Cl atoms and by two N atoms from different 1,4-bis(pyridin-2-ylmethoxy)benzene ligands. The ligand shows a non-planar configuration, in which the dihedral angles between the two terminal pyridine rings and the linking benzene ring are 7.86 (12) and 70.74 (11)°. The flexible ligand coordinates to the Zn^{II} ions, generating an infinite chain propagating along [001].

Related literature

For the synthesis and general background to flexible pyridyl-based ligands, see: Wang *et al.* (2007); Liu *et al.* (2010a,b)



Experimental

Crystal data

| | |
|---|-----------------------------------|
| $[\text{ZnCl}_2(\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_2)]$ | $\gamma = 72.31$ (3)° |
| $M_r = 428.62$ | $V = 894.9$ (3) Å ³ |
| Triclinic, $P\bar{1}$ | $Z = 2$ |
| $a = 8.8797$ (18) Å | Mo $K\alpha$ radiation |
| $b = 10.458$ (2) Å | $\mu = 1.69$ mm ⁻¹ |
| $c = 10.561$ (2) Å | $T = 293$ K |
| $\alpha = 87.55$ (3)° | $0.21 \times 0.19 \times 0.17$ mm |
| $\beta = 73.50$ (3)° | |

Data collection

| | |
|---|--|
| Rigaku R-AXIS RAPID diffractometer | 8755 measured reflections |
| Absorption correction: multi-scan (ABSCOR; Higashi, 1995) | 4028 independent reflections |
| $T_{\text{min}} = 0.719$, $T_{\text{max}} = 0.760$ | 3222 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.028$ |

Refinement

| | |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.032$ | 226 parameters |
| $wR(F^2) = 0.073$ | H-atom parameters constrained |
| $S = 1.05$ | $\Delta\rho_{\text{max}} = 0.32$ e Å ⁻³ |
| 4028 reflections | $\Delta\rho_{\text{min}} = -0.29$ e Å ⁻³ |

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSK, 2002); 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: *SHELXL97*.

The authors thank the Educational Commission of Heilongjiang Province of China (project No. 12511472), Heilongjiang Institute of Technology and Heilongjiang University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2447).

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supplementary materials

Acta Cryst. (2011). E67, m1373 [doi:10.1107/S1600536811035963]

***catena*-Poly[[dichloridozinc(II)]- μ -1,4-bis(pyridin-2-ylmethoxy)benzene- κ^2 N:N']**

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Comment

The metal-organic frameworks are determined by many factors, in which the organic ligands as building blocks and the kinds of metal ions are most important. Many pyridyl-containing ligands with strong coordination ability and functional characteristics have been studied over the recent years (Wang *et al.*, 2007). The flexible bipyridyl ligands could react with transitional metals to construct the helical-like structures. Recently, as a continuation of previous works (Liu *et al.*, 2010*a*, *b*), we report the crystal structure of the title compound here.

In the title compound, $[(ZnCl_2)(C_{18}H_{16}N_2O_2)]_n$, each Zn^{II} atom is four-coordinated by two Cl atoms and two N atoms from different 1,4-bis(pyridin-2-ylmethoxy)benzene ligands to form a distorted tetrahedral geometry configuration. The Zn-Cl bond lengths are 2.228 (1) and 2.253 (1) Å, and Zn-N bond lengths are 2.090 (2) and 2.080 (2) Å. The Cl(1)-Zn-Cl(2) bond angle (110.45 °) and the N(1)-Zn-N(2) bond angle (111.03 °) are nearly equal to 120 ° in order to minimize the steric hindrance (Fig. 1, Table 1).

The ligand is oriented in a divergent fashion, in which the dihedral angles between two terminal pyridine rings with the linking benzene ring are 7.86 (12) and 70.74 (11)°. In the crystal packing, the flexible ligands link the Zn^{II} atoms to generate an infinite chain running along [001].

Experimental

The 1,4-bis(pyridin-2-ylmethoxy)benzene ligand was synthesized as the reference method (Liu *et al.*, 2010*a*,*b*). The title compound was produced by reaction of $ZnCl_2$ (0.50 mmol, 0.068 g) in water (5 mL) and 1,4-bis(pyridin-2-ylmethoxy)benzene (0.5 mmol, 0.146 g) in 5 mL methanol under constant stirring, and filtered after stirring for about one hour. The filtrate was maintained for about one week under the room temperature to give colorless block-like crystals suitable for X-ray analysis.

Refinement

The anomalous reflection data (4 -5 6), (-3 2 0) and (2 -3 1) have been omitted during the refinement. H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic); C—H = 0.97 Å (methylene), and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

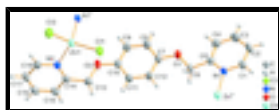


Fig. 1. The molecular structure of the title compound, showing displacement ellipsoids at the 50% probability level for non-H atoms [Symmetry code I = x, y, z-1; II = x, y, z+1].

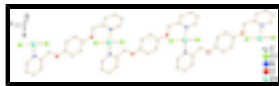


Fig. 2. A partial packing view, showing the chain structure along *b* axis.

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Crystal data

| | |
|---|---|
| $[\text{ZnCl}_2(\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_2)]$ | $Z = 2$ |
| $M_r = 428.62$ | $F(000) = 436$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.591 \text{ Mg m}^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| $a = 8.8797 (18) \text{ \AA}$ | Cell parameters from 6941 reflections |
| $b = 10.458 (2) \text{ \AA}$ | $\theta = 3.6\text{--}27.5^\circ$ |
| $c = 10.561 (2) \text{ \AA}$ | $\mu = 1.69 \text{ mm}^{-1}$ |
| $\alpha = 87.55 (3)^\circ$ | $T = 293 \text{ K}$ |
| $\beta = 73.50 (3)^\circ$ | Block, colorless |
| $\gamma = 72.31 (3)^\circ$ | $0.21 \times 0.19 \times 0.17 \text{ mm}$ |
| $V = 894.9 (3) \text{ \AA}^3$ | |

Data collection

| | |
|---|--|
| Rigaku R-Axis RAPID diffractometer | 4028 independent reflections |
| Radiation source: fine-focus sealed tube graphite | 3222 reflections with $I > 2\sigma(I)$ |
| ω scan | $R_{\text{int}} = 0.028$ |
| Absorption correction: multi-scan (ABSCOR; Higashi, 1995) | $\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.6^\circ$ |
| $T_{\text{min}} = 0.719$, $T_{\text{max}} = 0.760$ | $h = -10 \rightarrow 11$ |
| 8755 measured reflections | $k = -13 \rightarrow 13$ |
| | $l = -13 \rightarrow 13$ |

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.032$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.073$ | H-atom parameters constrained |
| $S = 1.05$ | $w = 1/[\sigma^2(F_o^2) + (0.0311P)^2 + 0.1894P]$ |
| 4028 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 226 parameters | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| 0 restraints | $\Delta\rho_{\text{max}} = 0.32 \text{ e \AA}^{-3}$ |
| | $\Delta\rho_{\text{min}} = -0.29 \text{ e \AA}^{-3}$ |

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|------------|------------|------------|----------------------------------|
| C1 | 0.8929 (3) | 0.5157 (2) | 1.3377 (2) | 0.0426 (5) |
| H1 | 0.8933 | 0.5634 | 1.4099 | 0.051* |
| C2 | 0.9801 (3) | 0.3817 (2) | 1.3198 (3) | 0.0503 (6) |
| H2 | 1.0380 | 0.3394 | 1.3786 | 0.060* |
| C3 | 0.9800 (3) | 0.3111 (2) | 1.2128 (3) | 0.0508 (6) |
| H3 | 1.0393 | 0.2203 | 1.1976 | 0.061* |
| C4 | 0.8915 (3) | 0.3759 (2) | 1.1287 (2) | 0.0438 (6) |
| H4 | 0.8894 | 0.3293 | 1.0565 | 0.053* |
| C5 | 0.8052 (3) | 0.5115 (2) | 1.1526 (2) | 0.0331 (5) |
| C6 | 0.7058 (3) | 0.5875 (2) | 1.0652 (2) | 0.0369 (5) |
| H6A | 0.5895 | 0.6153 | 1.1133 | 0.044* |
| H6B | 0.7376 | 0.6674 | 1.0367 | 0.044* |
| C7 | 0.6566 (3) | 0.5573 (2) | 0.8599 (2) | 0.0377 (5) |
| C8 | 0.6904 (3) | 0.4718 (2) | 0.7515 (2) | 0.0415 (5) |
| H8 | 0.7590 | 0.3840 | 0.7478 | 0.050* |
| C9 | 0.6227 (3) | 0.5165 (2) | 0.6498 (2) | 0.0401 (5) |
| H9 | 0.6442 | 0.4583 | 0.5782 | 0.048* |
| C10 | 0.5228 (3) | 0.6472 (2) | 0.6532 (2) | 0.0353 (5) |
| C11 | 0.4855 (3) | 0.7321 (2) | 0.7619 (2) | 0.0438 (6) |
| H11 | 0.4157 | 0.8194 | 0.7658 | 0.053* |
| C12 | 0.5525 (3) | 0.6863 (2) | 0.8651 (2) | 0.0448 (6) |
| H12 | 0.5270 | 0.7432 | 0.9386 | 0.054* |
| C13 | 0.3676 (3) | 0.8196 (2) | 0.5444 (2) | 0.0373 (5) |
| H13A | 0.4243 | 0.8803 | 0.5609 | 0.045* |
| H13B | 0.2650 | 0.8351 | 0.6145 | 0.045* |
| C14 | 0.3322 (3) | 0.8458 (2) | 0.4139 (2) | 0.0325 (5) |
| C15 | 0.1734 (3) | 0.8713 (2) | 0.4044 (2) | 0.0396 (5) |
| H15 | 0.0900 | 0.8629 | 0.4778 | 0.047* |
| C16 | 0.1382 (3) | 0.9091 (2) | 0.2865 (3) | 0.0450 (6) |
| H16 | 0.0322 | 0.9250 | 0.2792 | 0.054* |
| C17 | 0.2624 (3) | 0.9227 (2) | 0.1811 (3) | 0.0460 (6) |
| H17 | 0.2419 | 0.9512 | 0.1013 | 0.055* |
| C18 | 0.4196 (3) | 0.8933 (2) | 0.1949 (2) | 0.0407 (5) |

supplementary materials

| | | | | |
|-----|-------------|--------------|--------------|--------------|
| H18 | 0.5040 | 0.9021 | 0.1225 | 0.049* |
| C11 | 0.76914 (7) | 0.83611 (6) | 0.47450 (6) | 0.04153 (14) |
| C12 | 0.81884 (8) | 0.89409 (6) | 0.12085 (6) | 0.04904 (16) |
| N1 | 0.8066 (2) | 0.58173 (17) | 1.25574 (17) | 0.0322 (4) |
| N2 | 0.4562 (2) | 0.85272 (17) | 0.30782 (18) | 0.0329 (4) |
| O1 | 0.7344 (2) | 0.50350 (16) | 0.95442 (16) | 0.0488 (4) |
| O2 | 0.4678 (2) | 0.68394 (15) | 0.54293 (15) | 0.0416 (4) |
| Zn1 | 0.70586 (3) | 0.78909 (2) | 0.29601 (3) | 0.03361 (9) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|---------------|---------------|--------------|
| C1 | 0.0489 (14) | 0.0418 (12) | 0.0389 (13) | -0.0072 (11) | -0.0224 (11) | 0.0025 (10) |
| C2 | 0.0581 (16) | 0.0458 (14) | 0.0492 (16) | -0.0070 (12) | -0.0297 (13) | 0.0140 (12) |
| C3 | 0.0563 (16) | 0.0348 (12) | 0.0540 (17) | -0.0014 (12) | -0.0184 (13) | 0.0058 (11) |
| C4 | 0.0527 (14) | 0.0372 (12) | 0.0387 (14) | -0.0083 (11) | -0.0142 (11) | -0.0014 (10) |
| C5 | 0.0334 (11) | 0.0354 (11) | 0.0295 (11) | -0.0095 (9) | -0.0089 (9) | 0.0034 (9) |
| C6 | 0.0449 (13) | 0.0384 (11) | 0.0287 (12) | -0.0084 (10) | -0.0169 (10) | -0.0003 (9) |
| C7 | 0.0503 (13) | 0.0351 (11) | 0.0323 (12) | -0.0120 (11) | -0.0201 (11) | 0.0018 (9) |
| C8 | 0.0590 (15) | 0.0292 (11) | 0.0384 (13) | -0.0087 (11) | -0.0219 (12) | 0.0011 (9) |
| C9 | 0.0594 (15) | 0.0318 (11) | 0.0343 (13) | -0.0152 (11) | -0.0192 (11) | -0.0026 (9) |
| C10 | 0.0442 (13) | 0.0363 (11) | 0.0307 (12) | -0.0130 (10) | -0.0181 (10) | 0.0022 (9) |
| C11 | 0.0543 (15) | 0.0378 (12) | 0.0378 (13) | -0.0029 (11) | -0.0218 (12) | -0.0034 (10) |
| C12 | 0.0567 (15) | 0.0397 (12) | 0.0347 (13) | 0.0002 (11) | -0.0226 (12) | -0.0082 (10) |
| C13 | 0.0384 (12) | 0.0391 (11) | 0.0310 (12) | -0.0038 (10) | -0.0127 (10) | -0.0028 (9) |
| C14 | 0.0351 (11) | 0.0269 (10) | 0.0356 (12) | -0.0034 (9) | -0.0161 (10) | -0.0033 (8) |
| C15 | 0.0367 (12) | 0.0382 (12) | 0.0448 (14) | -0.0080 (10) | -0.0164 (10) | -0.0017 (10) |
| C16 | 0.0382 (13) | 0.0423 (13) | 0.0575 (16) | -0.0031 (11) | -0.0271 (12) | -0.0031 (11) |
| C17 | 0.0532 (15) | 0.0444 (13) | 0.0433 (14) | -0.0020 (12) | -0.0321 (13) | 0.0031 (11) |
| C18 | 0.0440 (13) | 0.0407 (12) | 0.0342 (13) | -0.0026 (11) | -0.0175 (11) | 0.0029 (10) |
| C11 | 0.0482 (3) | 0.0434 (3) | 0.0426 (3) | -0.0150 (3) | -0.0264 (3) | 0.0013 (2) |
| C12 | 0.0539 (4) | 0.0542 (3) | 0.0416 (3) | -0.0198 (3) | -0.0154 (3) | 0.0129 (3) |
| N1 | 0.0331 (9) | 0.0344 (9) | 0.0291 (9) | -0.0069 (8) | -0.0127 (8) | 0.0033 (7) |
| N2 | 0.0343 (9) | 0.0324 (9) | 0.0307 (10) | -0.0022 (8) | -0.0155 (8) | -0.0011 (7) |
| O1 | 0.0704 (12) | 0.0377 (8) | 0.0383 (10) | -0.0005 (8) | -0.0320 (9) | -0.0043 (7) |
| O2 | 0.0607 (10) | 0.0338 (8) | 0.0359 (9) | -0.0084 (8) | -0.0287 (8) | -0.0001 (6) |
| Zn1 | 0.03523 (15) | 0.03499 (14) | 0.03301 (15) | -0.00713 (11) | -0.01731 (11) | 0.00198 (10) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|-------|-----------|----------|-----------|
| C1—N1 | 1.348 (3) | C11—C12 | 1.387 (3) |
| C1—C2 | 1.371 (3) | C11—H11 | 0.9300 |
| C1—H1 | 0.9300 | C12—H12 | 0.9300 |
| C2—C3 | 1.376 (4) | C13—O2 | 1.426 (3) |
| C2—H2 | 0.9300 | C13—C14 | 1.495 (3) |
| C3—C4 | 1.374 (3) | C13—H13A | 0.9700 |
| C3—H3 | 0.9300 | C13—H13B | 0.9700 |
| C4—C5 | 1.387 (3) | C14—N2 | 1.346 (3) |
| C4—H4 | 0.9300 | C14—C15 | 1.385 (3) |

| | | | |
|------------|-------------|-------------------------|-------------|
| C5—N1 | 1.344 (3) | C15—C16 | 1.381 (3) |
| C5—C6 | 1.496 (3) | C15—H15 | 0.9300 |
| C6—O1 | 1.410 (3) | C16—C17 | 1.364 (4) |
| C6—H6A | 0.9700 | C16—H16 | 0.9300 |
| C6—H6B | 0.9700 | C17—C18 | 1.384 (3) |
| C7—C12 | 1.377 (3) | C17—H17 | 0.9300 |
| C7—O1 | 1.378 (3) | C18—N2 | 1.341 (3) |
| C7—C8 | 1.390 (3) | C18—H18 | 0.9300 |
| C8—C9 | 1.373 (3) | C11—Zn1 | 2.2271 (7) |
| C8—H8 | 0.9300 | C12—Zn1 | 2.2530 (10) |
| C9—C10 | 1.380 (3) | N1—Zn1 ⁱ | 2.0898 (18) |
| C9—H9 | 0.9300 | N2—Zn1 | 2.0803 (18) |
| C10—C11 | 1.381 (3) | Zn1—N1 ⁱⁱ | 2.0898 (18) |
| C10—O2 | 1.383 (3) | | |
| N1—C1—C2 | 123.2 (2) | C7—C12—H12 | 119.7 |
| N1—C1—H1 | 118.4 | C11—C12—H12 | 119.7 |
| C2—C1—H1 | 118.4 | O2—C13—C14 | 109.20 (17) |
| C1—C2—C3 | 118.5 (2) | O2—C13—H13A | 109.8 |
| C1—C2—H2 | 120.8 | C14—C13—H13A | 109.8 |
| C3—C2—H2 | 120.8 | O2—C13—H13B | 109.8 |
| C4—C3—C2 | 119.4 (2) | C14—C13—H13B | 109.8 |
| C4—C3—H3 | 120.3 | H13A—C13—H13B | 108.3 |
| C2—C3—H3 | 120.3 | N2—C14—C15 | 120.9 (2) |
| C3—C4—C5 | 119.4 (2) | N2—C14—C13 | 118.31 (19) |
| C3—C4—H4 | 120.3 | C15—C14—C13 | 120.6 (2) |
| C5—C4—H4 | 120.3 | C16—C15—C14 | 120.4 (2) |
| N1—C5—C4 | 121.7 (2) | C16—C15—H15 | 119.8 |
| N1—C5—C6 | 116.45 (18) | C14—C15—H15 | 119.8 |
| C4—C5—C6 | 121.9 (2) | C17—C16—C15 | 118.5 (2) |
| O1—C6—C5 | 108.69 (18) | C17—C16—H16 | 120.8 |
| O1—C6—H6A | 110.0 | C15—C16—H16 | 120.8 |
| C5—C6—H6A | 110.0 | C16—C17—C18 | 118.8 (2) |
| O1—C6—H6B | 110.0 | C16—C17—H17 | 120.6 |
| C5—C6—H6B | 110.0 | C18—C17—H17 | 120.6 |
| H6A—C6—H6B | 108.3 | N2—C18—C17 | 123.1 (2) |
| C12—C7—O1 | 125.3 (2) | N2—C18—H18 | 118.4 |
| C12—C7—C8 | 119.3 (2) | C17—C18—H18 | 118.4 |
| O1—C7—C8 | 115.4 (2) | C5—N1—C1 | 117.94 (18) |
| C9—C8—C7 | 120.1 (2) | C5—N1—Zn1 ⁱ | 127.03 (14) |
| C9—C8—H8 | 119.9 | C1—N1—Zn1 ⁱ | 114.79 (14) |
| C7—C8—H8 | 119.9 | C18—N2—C14 | 118.08 (19) |
| C8—C9—C10 | 120.5 (2) | C18—N2—Zn1 | 115.68 (15) |
| C8—C9—H9 | 119.8 | C14—N2—Zn1 | 125.98 (14) |
| C10—C9—H9 | 119.8 | C7—O1—C6 | 117.33 (17) |
| C9—C10—C11 | 119.8 (2) | C10—O2—C13 | 116.16 (17) |
| C9—C10—O2 | 115.81 (19) | N2—Zn1—N1 ⁱⁱ | 111.05 (7) |
| C11—C10—O2 | 124.4 (2) | N2—Zn1—C11 | 115.74 (6) |

supplementary materials

| | | | |
|-------------|-----------|---------------------------|------------|
| C10—C11—C12 | 119.6 (2) | N1 ⁱⁱ —Zn1—C11 | 107.18 (6) |
| C10—C11—H11 | 120.2 | N2—Zn1—C12 | 103.67 (6) |
| C12—C11—H11 | 120.2 | N1 ⁱⁱ —Zn1—C12 | 108.57 (6) |
| C7—C12—C11 | 120.6 (2) | C11—Zn1—C12 | 110.47 (3) |

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

Fig. 1

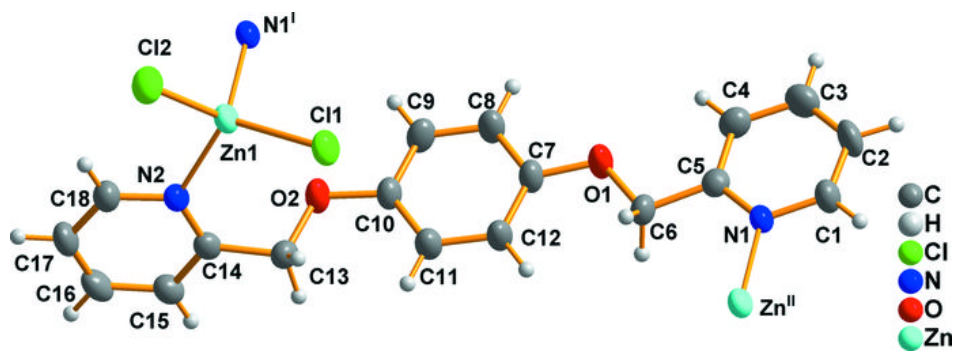


Fig. 2

