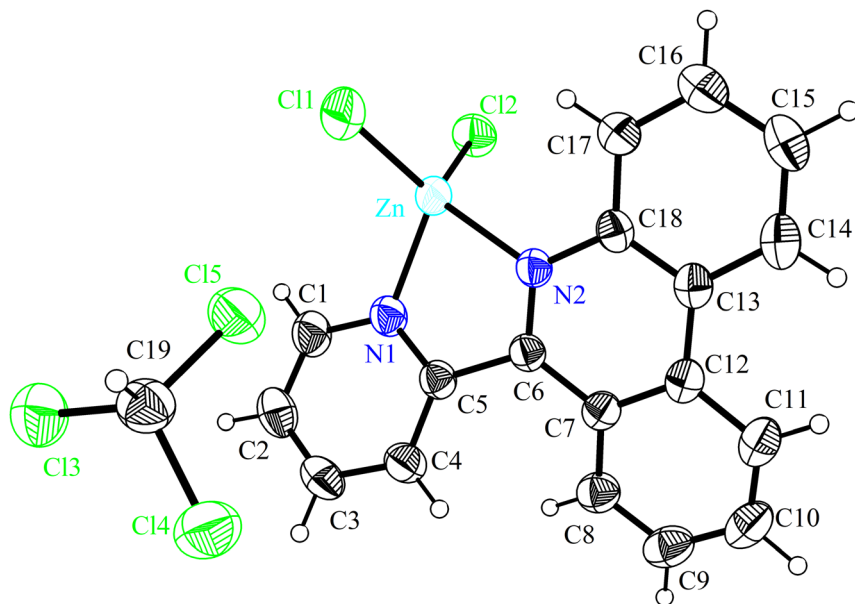


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# The crystal structure of dichlorido-[6-(pyridin-2-yl)phenanthridine- $\kappa^2N, N'$ ]zinc(II)-chloroform (1/1), $C_{19}H_{13}N_2ZnCl_5$



<https://doi.org/10.1515/ncrs-2025-0118>

Received March 6, 2025; accepted April 2, 2025;

published online April 23, 2025

## Abstract

$C_{19}H_{13}N_2ZnCl_5$ , monoclinic,  $I2/a$ ,  $a = 15.2859(2)$  Å,  $b = 14.7894(1)$  Å,  $c = 18.0569(2)$  Å,  $\beta = 97.311(1)^\circ$ ,  $V = 4048.92(8)$  Å<sup>3</sup>,  $Z = 8$ ,  $R_g(F) = 0.0260$ ,  $wR_{ref}(F^2) = 0.0722$ ,  $T = 296$  K.

CCDC no.: 2417280

The molecular structure is shown in the figure. Table 1 contains crystallographic data.

Table 1 contains the crystallographic data. The list of the atoms including atomic coordinates and displacement parameters can be found in the cif- file attached to this article.

**Table 1:** Data collection and handling.

|                                                       |                                                            |
|-------------------------------------------------------|------------------------------------------------------------|
| Crystal:                                              | Clear yellowish colourless block                           |
| Size:                                                 | 0.15 × 0.15 × 0.14 mm                                      |
| Wavelength:                                           | Cu Kα radiation (1.54184 Å)                                |
| $\mu$ :                                               | 7.82 mm <sup>-1</sup>                                      |
| Diffractometer, scan mode:                            | Rigaku Synergy, $\omega$ scans                             |
| $\theta_{max}$ , completeness:                        | 77.6°, 100 %                                               |
| $N(hkl)_{measured}$ , $N(hkl)_{unique}$ , $R_{int}$ : | 25,997, 4,217, 0.035                                       |
| Criterion for $I_{obs}$ , $N(hkl)_{gt}$ :             | $I_{obs} > 2 \sigma(I_{obs})$ , 3,828                      |
| $N(param)_{refined}$ :                                | 245                                                        |
| Programs:                                             | Rigaku, <sup>1</sup> SHELX, <sup>2</sup> Olex <sup>3</sup> |

## 1 Source of materials

All chemicals were purchased from commercial sources and used as received without further purification. 6-(Pyridin-2-yl)phenanthridine was prepared as reported.<sup>4,5</sup> A solution of 6-(pyridin-2-yl)phenanthridine (0.01 mmol) in chloroform (4 mL) was added to a stirred solution of  $ZnCl_2$  (0.01 mmol) in acetonitrile (2 mL) at room temperature for 2 h. After filtration, slow diffusion of diethyl ether into the filtrate over 72 h afforded block yellow crystals.

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## 2 Experimental details

The structure solution followed standard methods; the SHELXL<sup>2</sup> refinement package were employed to refine the crystal structure. The Olex2<sup>3</sup> was used to visualize the crystal structure. All hydrogen atoms were placed in idealized positions. Their  $U_{iso}$  values were set to  $1.2U_{eq}$  of the parent atoms.

## 3 Comment

Symmetric chelating ligands such as 2,2'-bipyridine and phenanthroline play important roles in the fields of coordination chemistry, supramolecular chemistry, catalytic chemistry, and optoelectronic materials.<sup>6,7</sup> Asymmetric chelating ligands with flexible and versatile structures can provide richer electronic and spatial effects and shows potential application value in the field of functional complexes.<sup>8,9</sup> The unsymmetric chelating ligand composed of phenanthrene ring and pyridine ring coordinated with Zn(II) to form the planar structure and the rigid structures of the complex can reduce the non-radiative transition process, thereby improving the luminescence efficiency of the Zn(II) complex.<sup>10</sup>

Each Zn(II) shows a tetrahedral coordination geometry and is ligated by one N atom from one pyridine, one N atom from phenanthridine moiety,<sup>11</sup> and two chlorido ligands (see the Figure). In addition, there is a free chloroform molecule present in the crystal structure. For  $C_{19}H_{13}N_2ZnCl_5$ , The Zn–Cl bond lengths range are 2.1970(5)–2.2182(6) Å, while the Zn–N bond lengths are 2.0500(15)–2.0673(13) Å. The Cl–Zn–Cl, and N–Zn–N angles are 116.82(2) and 80.07(6)°, respectively, while those for N–Zn–Cl are 111.10(5)–115.96(5)°. The C–N–Zn angles range from 113.20(11) to 125.51(13)°. It should be noted that the above bond lengths and angles are consistent with the reported Zn-based complexes.<sup>12</sup>

**Acknowledgments:** We gratefully acknowledge support by the NSFC of China (21703291), the NSF of Guangdong Province (2017A030310258), the Education Department of Guangdong Province (2022ZDJS027) and Jiangmen Municipal Science and Technology Bureau (Jiangke 2020-135, Jiangke 2021-76).

**Conflict of interest:** The authors declare no conflicts of interest regarding this article.

**Research funding:** NSFC of China (21703291), the NSF of Guangdong Province (2017A030310258), the Education Department of Guangdong Province (2022ZDJS027) and Jiangmen Municipal Science and Technology Bureau (Jiangke 2020-135, Jiangke 2021-76).

**Author contribution:** All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

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