Rabia Usman, Arshad Khan*, Amjad Khan, Moamen S. Refat, Amani M. R. Alsaedi and Faiz-Ur Rahman*

Dichlorido-{2,6-bis(4,5-dihydro-1H-pyrazol-3-yl)pyridine- κ^3N,N',N'' }zinc(II), $C_{11}H_9C_{12}N_5Zn$

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.16 × 0.16 × 0.10 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	2.20 mm ⁻¹
Diffractometer, scan mode:	D8-Apex2 φ and ω
$\theta_{\max}$, completeness:	26.0°, 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	3010, 1330, 0.024
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1092
$N(\text{param})_{\text{refined}}$:	92
Programs:	Bruker [1], SHELX [2], Diamond [3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	1.0000	0.12355 (2)	0.2500	0.04054 (14)
Cl1	1.17845 (6)	0.05810 (3)	0.19852 (8)	0.05287 (19)
N1	1.0000	0.24736 (15)	0.2500	0.0371 (6)
N2	0.91056 (18)	0.15877 (11)	-0.0174 (2)	0.0411 (4)
N3	0.8629 (2)	0.12516 (11)	-0.1714 (2)	0.0457 (5)
H3	0.8592	0.0755	-0.1884	0.055*
C1	0.8218 (2)	0.17826 (16)	-0.2958 (3)	0.0489 (6)
H1	0.7854	0.1679	-0.4127	0.054 (7)*
C2	0.8424 (2)	0.25001 (15)	-0.2219 (3)	0.0458 (6)
H2	0.8230	0.2983	-0.2758	0.051 (7)*
C3	0.8995 (2)	0.23518 (13)	-0.0462 (3)	0.0378 (5)
C4	0.9490 (2)	0.28656 (13)	0.1021 (3)	0.0377 (5)
C5	0.9469 (2)	0.36674 (14)	0.0980 (3)	0.0504 (6)
H5	0.9106	0.3933	-0.0048	0.049 (7)*
C6	1.0000	0.4073 (2)	0.2500	0.0572 (10)
H6	1.0000	0.4616	0.2500	0.088 (14)*

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Abstract

$C_{11}H_9C_{12}N_5Zn$, monoclinic, $C2/c$ (no. 15), $a = 10.256(3)$ Å, $b = 17.110(5)$ Å, $c = 7.967(3)$ Å, $\beta = 104.361(4)^\circ$, $V = 1354.36$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0270$, $wR_{\text{ref}}(F^2) = 0.0659$, $T = 293$ K.

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*Corresponding authors: Arshad Khan, School of Chemistry and Environmental Engineering, Sichuan University of Science & Engineering, Zigong 643000, Sichuan, P. R. China, E-mail: arshadkhan@suse.edu.cn. <https://orcid.org/0000-0001-8716-4312> (A. Khan); and Faiz-Ur Rahman, Inner Mongolia University Research Center for Glycochemistry of Characteristic Medicinal Resources, School of Chemistry and Chemical Engineering, Inner Mongolia University, Hohhot 010021, P. R. China, E-mail: faiz@imu.edu.cn

Rabia Usman, School of Chemistry and Environmental Engineering, Sichuan University of Science & Engineering, Zigong 643000, Sichuan, P. R. China. <https://orcid.org/0000-0002-1387-3519>

Amjad Khan, Department of Chemistry, Oxford University, 12 Mansfield Road, Oxford, Oxfordshire OX1 3TA, UK

Moamen S. Refat and Amani M. R. Alsaedi, Department of Chemistry, College of Science, Taif University, P. O. Box 11099, Taif 21944, Saudi Arabia

The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The ligand 2,6-bis(1-(pyridin-2-yl)pyrazol-3-yl)pyridine (L1) was dissolved in dichloromethane (DCM) and a

methanolic solution of ZnCl₂ was layered over it gently to allow slow diffusion, resulting in colorless block crystals of the mononuclear title complex after a week.

Experimental details

The hydrogen atoms were placed in calculated positions and refined as riding mode, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Comment

Zinc is one of the most precious transition metals and the second most abundant in the human body. In recent years zinc complexes attracted lots of interest with applications in sensor technology [4], batteries [5], and cell imaging [6, 7], etc. Our previous work on the structural characterization of the different classes of compounds [8–12] that may be used as ligands provides motivation to explore the zinc complex with L1 in the current study. Earlier studies reported the iron and cobalt complexes with L1 [13, 14].

Structural analysis revealed that zinc is coordinated by three nitrogen atoms to form a pentacoordinate structure with one half of the complex to form the asymmetric unit (see the figure). The zinc and two chlorido ligands exhibits a bipyramidal geometry in the crystal structure. The ligand L1 exhibits a planar geometry to minimize the nitrogen lone pair interactions thus promoting the $\pi \cdots \pi$ interactions between the neighbouring rings. In the crystal the neighboring complex molecules are associated with each other by classical hydrogen bonds: N3–H3 $\cdots$ Cl1 (2.36 Å). Additionally, $\pi \cdots \pi$ (3.74 Å) interactions also play a crucial role in establishing the crystal structure.

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