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Crystallographic report

Bis{4-[*N*,*N*-bis(2-cyanoethyl)amino]pyridine} dichlorozinc(II)

Jun Ni, Wei Xu, Zheng Xue, Yi-Zhi Li, Hui-Lan Chen and Zhi-Lin Wang*

Coordination Chemistry Institute, State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, People's Republic of China

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In $(C_{11}H_{12}N_4)_2ZnCl_2$, the zinc(II) center is coordinated by the pyridine nitrogen atoms of two 4-[*N*,*N*-bis(2-cyanoethyl)amino]pyridine ligands and two chlorine atoms in a tetrahedral geometry.

KEYWORDS: 4-[*N*,*N*-bis(2-cyanoethyl)amino]pyridine; crystal structure; hydrogen bonds; zinc(II)

COMMENT

The 4-[*N*,*N*-bis(2-cyanoethyl)amino]pyridine molecule comprises a pyridine ring 'head' and two cyanoethyl group 'tails', and as such can be used to form different hydrogen bonding patterns leading to distinct packing structures.[1–3] Here, we report a new mononuclear zinc complex, $(C_{11}H_{12}N_4)_2ZnCl_2$, as shown in Fig. 1. The zinc(II) atom is tetrahedrally coordinated by two pyridine nitrogen atoms and two chlorine atoms with the range of tetrahedral angles being 107.08(6) to 117.40(3)°. The crystal structure is stabilized by a complex network of CN···H interactions.

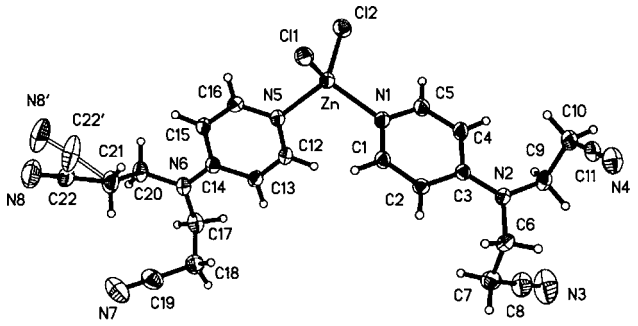

Figure 1. Molecule structure of $(C_{11}H_{12}N_4)_2ZnCl_2$, with displacement ellipsoids drawn at the 30% probability level. Selected bond distances (Å) and angles (°): Zn–Cl1 2.2411(8), Zn–Cl2 2.2429(8), Zn–N1 2.010(2), Zn–N5 2.033(2), Cl1–Zn–Cl2 117.40(3), Cl1–Zn–N1 108.50(7), Cl1–Zn–N5 107.24(7), Cl2–Zn–N1 108.17(6), Cl2–Zn–N5 107.08(6), N1–Zn–N5 108.12(9).

EXPERIMENTAL

A mixture of 4-[*N*,*N*-bis(2-cyanoethyl)amino]pyridine (400 mg, 2 mmol) and $ZnCl_2$ (136 mg, 1 mmol) was dissolved in methanol (25 ml). The reaction mixture was refluxed for 3 h and then filtered, yielding a white product. Yield: 456 mg (85%). Analysis. Found: C, 49.18; H, 4.47; N, 20.92. Calc.: C, 49.23; H, 4.51; N, 20.88%. The resultant colorless filtrate was left to stand at room temperature. Well-defined block-shaped colorless single crystals of the title compound were obtained within 1 week by slow evaporation of the above filtrate. Intensity data for $(C_{11}H_{12}N_4)_2ZnCl_2$ were collected at 293 K on a Bruker Smart Apex CCD diffractometer for a colorless crystal with dimensions of $0.10 \times 0.15 \times 0.20$ mm^3. $C_{22}H_{24}Cl_2N_8Zn$, $M = 536.76$, triclinic, $P\bar{1}$, $a = 9.447(1)$, $b = 10.699(1)$, $c = 12.231(1)$ Å, $\alpha = 94.79(1)$, $\beta = 90.10(1)$, $\gamma = 96.77(1)°$, $V = 1223.2(2)$ Å^3, $Z = 2$, 4244 unique data (θ_{max} 25.0°), 3434 data with $I \geq 2\sigma(I)$, $R = 0.038$ (obs. data), and $wR = 0.093$ (all data). Programs used: SMART, SAINT, and SHELXTL. CCDC deposition number: 230571. The C22 and N8 atoms in one ligand are distorted and were refined over two sites with site occupancies, from refinement, equal to 0.567(16) and 0.433(16) respectively.

*Correspondence to: Zhi-Lin Wang, Coordination Chemistry Institute, State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, People's Republic of China.
E-mail: wangzl@nju.edu.cn
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