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Crystal structure of dichloride-bis(1-propylimidazole- κ^1N)zinc(II), $C_{12}H_{20}Cl_2N_4Zn$

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Abstract

$C_{12}H_{20}Cl_2N_4Zn$, monoclinic, $P2_1/n$ (no. 14), $a = 9.9915(9)$ Å, $b = 13.0923(12)$ Å, $c = 13.1894(13)$ Å, $\beta = 98.794(2)^\circ$, $V = 1705.0(3)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0453$, $wR_{ref}(F^2) = 0.1248$, $T = 298(2)$ K.

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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

A solution of vanadiumoxy acetylacetonate (0.5 mmol) in H_2O (10 mL) was successively added 1-propylimidazole (6 mmol) and zinc chloride (0.5 mmol), and then maintained for 4 h at 60 °C with consistent stirring, and then filtered hot. The filtrate was left to slowly evaporate at room

Table 1: Data collection and handling.

Crystal:	White block
Size:	0.26 × 0.24 × 0.21 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.75 mm ^{−1}
Diffraction, scan mode:	φ and ω
θ_{max} , completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	8268, 2985, 0.046
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1973
$N(param)_{refined}$:	174
Programs:	Bruker [1], SHELX [2]

temperature for 3 days, and then the precipitated orange green rod crystals of the title compound were filtered off. Yield: 35.2%. Anal. Calcd. for $C_{12}H_{20}Cl_2N_4Zn$: C, 40.42; H, 5.65; N, 15.71; found: C, 40.59; H, 5.63; N, 15.67.

Experimental details

All hydrogen atomic positions were taken from a difference Fourier map. Hydrogen atoms were assigned with common isotropic displacement factors $U_{iso}(H) = 1.2$ times $U_{eq}(C, \text{imidazole ring and methylene carbon})$ and $U_{iso}(H) = 1.5$ times $U_{eq}(C, \text{methyl carbon})$. All the H atoms were refined as riding on their parent atom.

Comment

In the present scenario, zinc complexes have attracted interest owing to their bio-compatibility, low cost, varying coordination numbers and geometries, thermodynamic stability and catalytic properties [3, 4]. Up to date,

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lots of outstanding work about organic–inorganic hybrid zinc complexes have been presented, especially in the field of metal-organic frameworks [5–7]. Additionally, imidazole derivatives as a class of versatile ligands can be used not only as solvent, but also as ligands and organic base in the preparation of organic–inorganic hybrid materials, including some polyoxometalates [8–10].

The molecular structure of the title zinc complex is shown in the figure. Single crystal X-ray diffraction analysis demonstrates that the asymmetric unit of the title structure contains one zinc(II) cation, two 1-propylimidazole ligands

and two chlorido ligands. The bond distances of Zn–N are 1.995(4) to 2.015(4) Å, bond lengths of Zn–Cl are 2.2390(13) and 2.2456(13) Å, respectively, which are similar with those of the reported dichloro-bis(1-octadecylimidazole)zinc compound [11]. In the title complex, the bond angles of N(3)–Zn(1)–N(1), N(1)–Zn(1)–Cl(2), N(3)–Zn(1)–Cl(2), N(3)–Zn(1)–Cl(1), Cl(2)–Zn(1)–Cl(1) and N(1)–Zn(1)–Cl(1) are 111.69(16)°, 106.83(11)°, 107.67(12)°, 106.33(12)°, 116.83(5)° and 107.47(12)°, respectively, which suggests a distorted tetrahedral geometry. Additionally, there are intermolecular weak C–H···Cl hydrogen-bonding interactions between adjacent complex molecules.

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

Atom	X	Y	Z	U _{iso} */U _{eq}
Zn1	1.03894 (5)	0.77306 (4)	0.45279 (4)	0.0469 (2)
N1	0.9173 (4)	0.7500 (3)	0.5592 (3)	0.0519 (10)
N2	0.8331 (4)	0.6768 (4)	0.6849 (3)	0.0610 (11)
N3	0.9372 (4)	0.8306 (3)	0.3234 (3)	0.0520 (10)
N4	0.8253 (4)	0.9382 (3)	0.2150 (3)	0.0624 (11)
Cl1	1.11689 (13)	0.61988 (9)	0.41220 (9)	0.0603 (4)
Cl2	1.19362 (14)	0.88879 (10)	0.51772 (10)	0.0667 (4)
C1	0.9075 (5)	0.6651 (4)	0.6103 (4)	0.0576 (13)
H1	0.947834	0.603798	0.595958	0.069*
C2	0.8444 (6)	0.8196 (4)	0.6033 (4)	0.0713 (15)
H2	0.831500	0.887295	0.582735	0.086*
C3	0.7929 (6)	0.7756 (5)	0.6818 (5)	0.0783 (17)
H3	0.740312	0.807061	0.725105	0.094*
C4	0.8024 (6)	0.5989 (5)	0.7587 (5)	0.0833 (18)
H4A	0.749356	0.630487	0.805942	0.100*
H4B	0.746949	0.546195	0.721550	0.100*
C5	0.9238 (9)	0.5497 (6)	0.8194 (5)	0.113 (3)
H5A	0.892115	0.502770	0.867505	0.136*
H5B	0.967772	0.509108	0.772566	0.136*
C6	1.0226 (9)	0.6130 (6)	0.8751 (7)	0.136 (3)
H6A	1.065441	0.653127	0.828262	0.204*
H6B	1.089219	0.571617	0.916245	0.204*
H6C	0.980435	0.657502	0.918710	0.204*
C7	0.8884 (5)	0.9235 (4)	0.3097 (4)	0.0621 (14)
H7	0.897184	0.973325	0.360600	0.075*
C8	0.9015 (6)	0.7828 (4)	0.2290 (4)	0.0648 (14)
H8	0.921617	0.715726	0.213854	0.078*
C9	0.8335 (6)	0.8494 (4)	0.1638 (4)	0.0730 (16)
H9	0.798240	0.836998	0.095544	0.088*
C10	0.7603 (7)	1.0330 (5)	0.1736 (6)	0.096 (2)
H10A	0.693603	1.015798	0.114661	0.115*
H10B	0.711949	1.062172	0.225136	0.115*
C11	0.8440 (9)	1.1059 (8)	0.1446 (10)	0.181 (5)
H11A	0.785477	1.152842	0.101589	0.217*
H11B	0.878038	1.143253	0.206749	0.217*
C12	0.9591 (12)	1.0904 (7)	0.0932 (8)	0.184 (5)
H12A	1.025693	1.050246	0.135883	0.277*
H12B	0.997435	1.155350	0.079743	0.277*
H12C	0.931148	1.055318	0.029579	0.277*

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