Zongmu Li*

The crystal structure of dichlorido-bis(1-butyl-1*H*-imidazole- κN)zinc(II), $C_{14}H_{24}Cl_2ZnN_4$

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Abstract

$C_{14}H_{24}Cl_2ZnN_4$, orthorhombic, *Pbca* (no. 61), $a = 13.3238(11)$ Å, $b = 15.9366(13)$ Å, $c = 18.0943(16)$ Å, $V = 3842.1(6)$ Å³, $Z = 8$, $R_{gt}(F) = 0.0393$, $wR_{ref}(F^2) = 0.1053$, $T = 298(2)$ K.

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Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

In a typical experiment, *N*-butyl imidazole (0.744 g; 6 mmol), and zinc chloride (0.136 g; 1 mmol), vanadiumoxy acetylacetonate (0.132 g; 0.5 mmol) and 5 mL water were added successively in a 25 mL round-bottom flask. The mixture was heated to 60 °C for 60 min, resulting in a blue-turquoise coloured solution. The resulting mixture was filtrated and the filtrate stood by slow evaporation for five days. Crystals of the title complex were obtained.

Yield: 74% (base on Zn element), and elemental analysis: calc. for $C_{14}H_{24}Cl_2ZnN_4$: C 43.72, H 6.29, N 14.57; found: C 43.63,

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.21 × 0.20 × 0.18 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	1.56 mm ⁻¹
Diffractometer, scan mode:	Bruker SMART, φ and ω -scans
θ_{max} , completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	17488, 3387, 0.059
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 2163
$N(param)_{refined}$:	193
Programs:	Bruker programs [1], SHELX [2]

H 6.38, N 14.73. The elemental analyses were performed with PERKIN ELMER MODEL 2400 SERIES II.

Experimental details

Hydrogen atoms were geometrically assigned with common isotropic displacement factors $U_{iso}(H) = 1.5$ times U_{eq} (C, methyl) and $U_{iso}(H) = 1.2$ times U_{eq} (C, methyne and imidazole ring).

Comment

Organic inorganic zinc compounds have attracted much interest due to their diverse applications, such as in the field of electrocatalysis [3], chemical gas sensors [4], energy storage [5] and catalytic properties [6, 7]. A variety of organic inorganic hybrids containing zinc complexes have been demonstrated [8, 9]. In addition imidazole derivatives can be used as solvent and ligands [10–12]. However, to the best of our

*Corresponding author: Zongmu Li, Department of Chemical Engineering, Zibo Vocational Institute, Zibo 255314, China, e-mail: lizmzb@163.com

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

Atom	x	y	z	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Zn1	0.27259(3)	0.01046(3)	0.54028(2)	0.04888(18)
Cl1	0.12184(8)	0.00207(7)	0.59470(7)	0.0712(3)
Cl2	0.39173(8)	−0.07427(7)	0.58430(6)	0.0694(3)
N1	0.3192(2)	0.13022(19)	0.54875(17)	0.0528(8)
N2	0.4098(3)	0.2424(2)	0.5307(2)	0.0672(10)
N3	0.2525(2)	−0.00860(19)	0.43056(18)	0.0509(8)
N4	0.1766(3)	−0.0171(2)	0.32355(17)	0.0599(9)
C1	0.4012(3)	0.1601(3)	0.5192(2)	0.0618(11)
H1	0.447705	0.127911	0.493442	0.074*
C2	0.2720(3)	0.1975(3)	0.5803(2)	0.0657(12)
H2	0.210971	0.195981	0.605144	0.079*
C3	0.3284(4)	0.2663(3)	0.5695(3)	0.0736(14)
H3	0.314003	0.320299	0.585685	0.088*
C4	0.4937(4)	0.2950(3)	0.5055(3)	0.0982(19)
H4A	0.467129	0.347662	0.487012	0.118*
H4B	0.527288	0.267020	0.464858	0.118*
C5	0.5684(4)	0.3131(3)	0.5645(3)	0.0772(14)
H5A	0.618203	0.351553	0.544920	0.093*
H5B	0.534487	0.341231	0.604919	0.093*
C6	0.6205(4)	0.2383(3)	0.5939(4)	0.0990(18)
H6A	0.649307	0.206765	0.553243	0.119*
H6B	0.572228	0.202425	0.618657	0.119*
C7	0.7022(5)	0.2614(5)	0.6473(5)	0.168(4)
H7A	0.752512	0.293663	0.622120	0.252*
H7B	0.731881	0.211270	0.666948	0.252*
H7C	0.674330	0.294035	0.686865	0.252*
C8	0.1661(3)	−0.0149(2)	0.3967(2)	0.0512(10)
H8	0.104569	−0.017579	0.420893	0.061*
C9	0.3228(4)	−0.0060(3)	0.3765(3)	0.0675(12)
H9	0.391622	−0.001345	0.384100	0.081*
C10	0.2779(4)	−0.0112(3)	0.3105(3)	0.0734(13)
H10	0.309270	−0.010906	0.264545	0.088*
C11	0.0964(4)	−0.0262(3)	0.2685(2)	0.0813(15)
H11A	0.110616	0.009783	0.226562	0.098*
H11B	0.033257	−0.008150	0.289981	0.098*
C12	0.0863(4)	−0.1158(4)	0.2422(3)	0.0943(17)
H12A	0.042092	−0.116885	0.199557	0.113*
H12B	0.151619	−0.135624	0.226238	0.113*
C13	0.0462(4)	−0.1748(4)	0.2992(3)	0.1025(18)
H13A	−0.020701	−0.156635	0.313032	0.123*
H13B	0.088154	−0.171095	0.342891	0.123*
C14	0.0410(6)	−0.2657(4)	0.2754(4)	0.151(3)
H14A	−0.009331	−0.271921	0.237793	0.227*
H14B	0.024026	−0.300088	0.317087	0.227*
H14C	0.104952	−0.282686	0.256092	0.227*

knowledge, imidazole-zinc complexes of organic-inorganic hybrids are rare. This contribution is part of our continuing interest in synthesis, characterization and understanding of imidazole complexes.

The molecular structure of title complex is shown in the figure. The asymmetric unit of the title structure contains two 1-butylimidazole ligands, one zinc cation and two chlorine anions. The Zn center adopts a tetrahedral

geometry. The bond distances of Zn-N are 2.013(3) Å and 2.026(3) Å, which are longer than those reported for dichloro-bis(1,2-dimethylimidazole)zinc [Zn-N, 2.006(3) Å, 2.008(3) Å] and equivalent to those reported for dichloro-bis(1-octadecylimidazole)zinc [13, 14]. The bond angles around the zinc(II) ion are N(1)–Zn(1)–N(3) (104.92(13)°), N(1)–Zn(1)–Cl(2) (109.11(10)°), N(3)–Zn(1)–Cl(2) (110.68(10)°), N(1)–Zn(1)–Cl(1) (107.43(10)°), N(3)–Zn(1)–Cl(1) (107.63(10)°), Cl(2)–Zn(1)–Cl(1) (116.41(5)°), which are similar with those of dichloro-(1,3-bis(5'-methyl-4'-imidazolyl)-2-thiapropane-*N,N'*)-zinc complex [15]. In one of the two 1-butylimidazole ligands, the butyl chain plane (C5/C6/C7) is tilted by 70.55(2)° from the imidazole ring plane (C1/N1/C2/N2/C3), and in the other ligand, the dihedral angle of the alkyl chain (C11/C12/C13) and the imidazole ring plane (C8/N3/C9/N4/C10) is 74.43(2)°.

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