The crystal structure of dichlorido-bis(1-butyl-1H-imidazole-κN)zinc(II), C_{14}H_{24}Cl_{2}ZnN_{4}

Abstract

C_{14}H_{24}Cl_{2}ZnN_{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.

Source of material

In a typical experiment, \( N \)-butyl imidazole (0.744 g; 6 mmol), and zinc chloride (0.136 g; 1 mmol), vanadiumoxo 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_{2}ZnN_{4}: C 43.72, H 6.29, N 14.57; found: C 43.63,

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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(t-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(2)°), 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′-imidazoyl)-2-thiapropene-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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References


