Crystal structure of dichlorido-(1-((3,5-dimethyl-2,3-dihydro-1H,1,2,3-triazol-1-yl)methyl)-1H-benzo[d][1,2,3]triazole-k\(^1\)N)zinc(II), C\(_{22}\)H\(_{24}\)ZnN\(_{12}\)Cl\(_2\)

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Abstract

C\(_{22}\)H\(_{24}\)ZnN\(_{12}\)Cl\(_2\), monoclinic, \(P2_1/n\) (no. 14), \(a = 8.3494(3)\) Å, \(b = 11.1678(3)\) Å, \(c = 27.8876(8)\) Å, \(\beta = 92.102(3)^\circ\), \(Z = 4\), \(V = 2598.62(15)\) Å\(^3\), \(R_{gt}(F) = 0.0572\), \(wR_{ref}(F^2) = 0.1535\), \(T = 293(2)\) K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of materials

All starting materials are commercially available without further purification. 1-[(3,5-dimethyl-1H-triazole-1-yl)methyl]-1H-benzotriazole (dtmb) was prepared according to the literature method with some modifications.\(^2\) The ligand 1-[(3,5-dimethyl-1H-triazole-1-yl)methyl]-1H-benzotriazole (0.04 mmol, 0.0091 g) was dissolved in 2 mL of methanol solution and the solution was slowly added to 2 mL of ZnCl\(_2\) (0.04 mmol, 0.0054 g) of methanol solution. The prepared solution was placed at room temperature and colorless crystals were obtained after 2 weeks.

2 Experimental details

H atoms were generated geometrically and introduced as riding atoms with C–H = 0.93 Å and \(U_{eq}(H) = 1.2\) times \(U_{eq}(C)\) for aromatic H atoms, with C–H = 0.97 Å and \(U_{eq}(H) = 1.2\) times \(U_{eq}(C)\) for methylene H atoms, and with C–H = 0.96 Å and \(U_{eq}(H) = 1.5\) times \(U_{eq}(C)\) for methyl H atoms.

3 Comment

As a type of nitrogen heterocyclic compound, benzotriazole derivatives exhibit strong coordination abilities and can effectively interact with transition metals to form a variety of metal complexes. For example, the Fei Wang team successfully synthesized four metal complexes by substituting benzotriazole as a ligand,\(^3\) the Juan Xiao team successfully synthesized three copper metal complexes by benzotriazole-5-carboxylic acid as a ligand,\(^4\) the Chun-Li Liu team successfully synthesized two zinc metal complexes by

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In addition, benzo triazole derivatives exhibit a wide range of biological activities, including antibacterial, antimicrobial and anti-cancer.\(^5\)

X-ray crystallographic analysis shows that the title complex has a mononuclear asymmetric unit structure centered on Zn(II). As shown in the figure the Zn(II) is coordinated with two Cl ions (Cl1, and Cl2) and two N atoms (N6 and N12 from two dtmb ligands, respectively). The Zn–Cl and Zn–N bonds are around Zn1 are of length: Zn1–Cl1: 2.2340(13) Å; Zn1–Cl2: 2.2371(13) Å; Zn1–N6: 2.0473(10) Å; Zn1–N12: 2.048(3) Å. The range of bond angles around the metal center Zn(II) is 105.75(14)°–114.54(10)°. In each dtmb ligand, the angle between the benzo triazole ring and the imidazole ring is 58.8(13)°. The distance between the benzo triazole rings of two adjacent molecules is 3.560 Å and 3.585 Å, respectively, so it can be inferred that there may be two kinds of \(\pi–\pi\) interaction between the two molecules.

**Author contribution:** All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

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### References


