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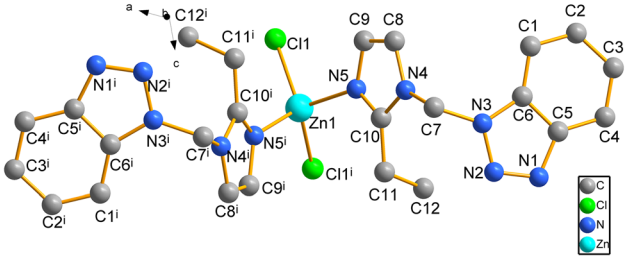
Crystal structure of dichlorido-1-[(2-ethylimidazole-1-yl)methyl]-1*H*–benzotriazole κ^1*N* zinc(II), $C_{24}H_{26}ZnN_{10}Cl_2$



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Abstract

$C_{24}H_{26}ZnN_{10}Cl_2$, monoclinic, *C*2/*c* (no. 15), *a* = 29.9014(12) Å, *b* = 7.0183(2) Å, *c* = 13.6656(5) Å, *β* = 115.518(5)°, *Z* = 4, *V* = 2588,06(19) Å^3, $R_{gt}(F)$ = 0.0439, $wR_{ref}(F^2)$ = 0.1315, T = 293(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.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.12 × 0.10 × 0.09 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	3.51 mm^{-1}
Diffractometer, scan mode:	Xcalibur, *ω*
θ_{max}, completeness:	67.1°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4,747, 2,321, 0.037
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1,987
$N(param)_{refined}$:	170
Programs:	SHELX[1]

1 Source of materials

All starting materials are commercially available. The 1-[(2-ethylimidazole-1-yl)methyl]-1H–benzotriazole (eimb) was prepared according to the literature method with some modifications.[2] The ligand 1-[(2-ethylimidazole-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 two weeks.

2 Experimental details

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

3 Comment

Due to their flexible coordination patterns, some nitrogen-containing heterocyclic compounds are unique in the field of coordination chemistry and are widely used in the design and synthesis of multifunctional complexes.[3–5] Among them, benzotriazole compounds have good binding system and strong electron transfer ability, and the N atom on the triazole ring contains lone pair electrons, and it is easy to form strong coordination bonds. Imidazole and triazole have similar strong coordination ability.[6–8]

X-ray crystal analysis shows that the title complex is a mononuclear complex with zinc as the central atom. As shown in Figure 1, the central atom Zn(II) (located at a twofold axis) is connected to two Cl ions (Cl1 and Cl1i) and

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.27157 (12)	−0.0072 (4)	−0.0309 (3)	0.0359 (7)
H1	0.2921	−0.0102	−0.0662	0.043*
C2	0.22236 (13)	0.0312 (5)	−0.0843 (3)	0.0449 (8)
H2	0.2088	0.0531	−0.1586	0.054*
C3	0.19100 (14)	0.0390 (5)	−0.0315 (3)	0.0516 (9)
H3	0.1575	0.0656	−0.0716	0.062*
C4	0.20896 (15)	0.0083 (5)	0.0777 (4)	0.0520 (10)
H4	0.1885	0.0154	0.1130	0.062*
C5	0.25958 (13)	−0.0345 (5)	0.1344 (3)	0.0407 (8)
C6	0.28941 (11)	−0.0419 (4)	0.0798 (2)	0.0309 (6)
C7	0.38177 (11)	−0.1156 (5)	0.1518 (3)	0.0400 (7)
H7A	0.3766	−0.2002	0.0918	0.048*
H7B	0.4053	−0.1761	0.2178	0.048*
C8	0.40365 (11)	0.1197 (5)	0.0405 (2)	0.0366 (7)
H8	0.3892	0.0573	−0.0260	0.044*
C9	0.42970 (10)	0.2834 (5)	0.0623 (2)	0.0347 (7)
H9	0.4366	0.3539	0.0128	0.042*
C10	0.42846 (9)	0.1935 (4)	0.2141 (2)	0.0284 (6)
C11	0.43463 (11)	0.1885 (5)	0.3279 (2)	0.0349 (7)
H11A	0.4673	0.2361	0.3755	0.042*
H11B	0.4325	0.0575	0.3482	0.042*
C12	0.39540 (13)	0.3078 (5)	0.3438 (3)	0.0469 (8)
H12A	0.3631	0.2578	0.2992	0.070*
H12B	0.3974	0.4375	0.3237	0.070*
H12C	0.4012	0.3028	0.4186	0.070*
Cl1	0.50742 (3)	0.69785 (12)	0.12254 (6)	0.0503 (3)
N1	0.28803 (13)	−0.0792 (5)	0.2419 (2)	0.0558 (8)
N2	0.33286 (11)	−0.1114 (5)	0.2556 (2)	0.0506 (8)
N3	0.33539 (9)	−0.0894 (4)	0.15874 (19)	0.0362 (6)
N4	0.40263 (9)	0.0626 (4)	0.13652 (19)	0.0316 (6)
N5	0.44464 (8)	0.3300 (4)	0.17030 (19)	0.0307 (5)
Zn1	0.5000	0.52085 (7)	0.2500	0.0298 (2)

two N atoms (N5 and N5i, each from two eimb ligands). The Zn–Cl and Zn–N bonds around Zn1 are of length: Zn1–Cl1: 2.2270(8) Å; Zn1–Cl1i: 2.2270(8) Å; Zn1–N5: 2.041(2) Å; Zn1–N5i: 2.041(2) Å. The range of bond angles around Zn1 is 97.99(14)°–116.88(7)°. The smallest bond angle is N5–Zn1–N5i, the largest is N5i–Zn1–Cl1 and N5–Zn1–Cl1i. The dihedral angle of the benzotriazole and imidazole rings in each ligand is 70.0°. The central atom zinc (II) ion forms a mononuclear structure with the two ligands in a monodentate coordination. In addition, the distance between the adjacent benzotriazole rings is 3.672 and 3.649 Å, indicating that there may be intermolecular π-π interactions between the adjacent zinc units.[9,10]

Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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