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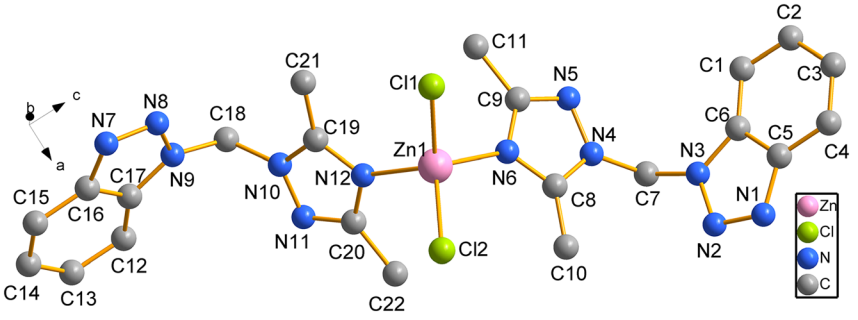
Crystal structure of dichlorido-(1-((3,5-dimethyl-2,3-dihydro-1*H*-1,2,3-triazol-1-yl)methyl)-1*H*-benzo[*d*][1,2,3]triazole-k^1*N*)zinc(II), $C_{22}H_{24}ZnN_{12}Cl_2$



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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, β = 92.102(3)°, 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-1*H*-triazole-1-yl) methyl]-1*H*-benzotriazole (dtmb) was prepared according to the literature method with some modifications.[2] The ligand 1-[(3,5-dimethyl-1*H*-triazole-1-yl)methyl]-1*H*-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.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.28 × 0.21 × 0.19 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	3.52 mm^{-1}
Diffractometer, scan mode:	Xcalibur, ω
θ_{max}, completeness:	67.1°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9,733, 4,634, 0.038
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3,867
$N(param)_{refined}$:	338
Programs:	SHELX[1]

2 Experimental details

H atoms were generated geometrically and introduced 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

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

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

Atom	x	y	z	U_{iso}*/U_{eq}
Zn1	0.45933 (6)	0.20817 (5)	0.25717 (2)	0.03402 (17)
Cl1	0.24722 (15)	0.13393 (12)	0.29365 (5)	0.0541 (3)
Cl2	0.62042 (16)	0.06042 (12)	0.23485 (5)	0.0570 (3)
N1	1.0670 (6)	0.2610 (4)	0.45826 (16)	0.0602 (12)
N2	1.0337 (5)	0.3111 (5)	0.41720 (15)	0.0576 (11)
N3	0.9158 (5)	0.3937 (4)	0.42228 (13)	0.0466 (9)
N4	0.7220 (4)	0.4169 (3)	0.35620 (12)	0.0394 (8)
N5	0.5755 (5)	0.4704 (4)	0.36065 (13)	0.0465 (9)
N6	0.5658 (4)	0.3250 (3)	0.30510 (11)	0.0353 (7)
N7	−0.0565 (6)	0.2636 (4)	0.03692 (17)	0.0600 (12)
N8	−0.0143 (5)	0.3149 (4)	0.07724 (15)	0.0532 (10)
N9	0.1053 (4)	0.3948 (4)	0.06901 (13)	0.0427 (9)
N10	0.2869 (4)	0.4016 (3)	0.13821 (11)	0.0362 (8)
N11	0.4472 (4)	0.4157 (3)	0.13093 (12)	0.0380 (8)
N12	0.4042 (4)	0.3069 (3)	0.19695 (11)	0.0324 (7)
C1	0.7590 (6)	0.4642 (5)	0.49329 (18)	0.0545 (13)
H1	0.6945	0.5214	0.4779	0.065*
C2	0.7511 (8)	0.4405 (6)	0.5415 (2)	0.0659 (16)
H2	0.6775	0.4821	0.5594	0.079*
C3	0.8506 (8)	0.3554 (5)	0.56451 (18)	0.0645 (17)
H3	0.8415	0.3431	0.5973	0.077*
C4	0.9588 (8)	0.2907 (5)	0.54090 (18)	0.0627 (16)
H4	1.0238	0.2344	0.5567	0.075*
C5	0.9693 (6)	0.3119 (4)	0.49128 (16)	0.0485 (11)
C6	0.8703 (6)	0.3968 (4)	0.46910 (15)	0.0438 (11)
C7	0.8627 (6)	0.4652 (5)	0.38219 (16)	0.0521 (12)
H7A	0.9496	0.4724	0.3602	0.063*
H7B	0.8379	0.5450	0.3935	0.063*
C8	0.7170 (5)	0.3315 (4)	0.32265 (13)	0.0350 (9)
C9	0.4861 (6)	0.4122 (4)	0.32903 (15)	0.0406 (10)
C10	0.8530 (5)	0.2577 (5)	0.30884 (17)	0.0499 (12)
H10A	0.9456	0.3076	0.3056	0.075*
H10B	0.8275	0.2190	0.2788	0.075*
H10C	0.8749	0.1983	0.3331	0.075*
C11	0.3119 (6)	0.4407 (5)	0.3213 (2)	0.0593 (14)
H11A	0.2900	0.4592	0.2881	0.089*
H11B	0.2849	0.5083	0.3407	0.089*
H11C	0.2490	0.3728	0.3303	0.089*
C12	0.2473 (7)	0.4608 (5)	−0.00485 (19)	0.0581 (14)
H12	0.3171	0.5169	0.0090	0.070*
C13	0.2428 (9)	0.4347 (6)	−0.0536 (2)	0.076 (2)
H13	0.3137	0.4739	−0.0732	0.092*
C14	0.1354 (10)	0.3515 (7)	−0.0742 (2)	0.082 (2)
H14	0.1357	0.3384	−0.1072	0.098*
C15	0.0322 (9)	0.2903 (5)	−0.0479 (2)	0.0714 (19)
H15	−0.0380	0.2348	−0.0620	0.086*
C16	0.0334 (6)	0.3125 (4)	0.00152 (18)	0.0504 (12)
C17	0.1390 (6)	0.3964 (4)	0.02149 (15)	0.0423 (10)
C18	0.1699 (6)	0.4658 (4)	0.10808 (16)	0.0471 (11)
H18A	0.0828	0.4920	0.1276	0.057*
H18B	0.2201	0.5366	0.0952	0.057*
C19	0.2622 (5)	0.3386 (4)	0.17776 (14)	0.0359 (9)
C20	0.5137 (5)	0.3556 (4)	0.16727 (14)	0.0365 (9)
C21	0.1030 (5)	0.3099 (5)	0.19575 (17)	0.0518 (12)
H21A	0.0539	0.3816	0.2072	0.078*
H21B	0.1143	0.2531	0.2215	0.078*
H21C	0.0370	0.2762	0.1703	0.078*
C22	0.6913 (5)	0.3448 (6)	0.17417 (18)	0.0549 (13)
H22A	0.7259	0.3881	0.2024	0.082*
H22B	0.7422	0.3775	0.1468	0.082*
H22C	0.7199	0.2620	0.1778	0.082*

1-[(benzotriazol-1-yl)methyl]-1*H*-imidazole as ligand.[5] In addition, benzotriazole derivatives exhibit a wide range of biological activities, including antibacterial,[6] antidiabetic[7] and anti-cancer.[8]

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 around Zn1 are of length: Zn1–Cl1: 2.2340(13) Å; Zn1–Cl2: 2.2317(13) Å; Zn1–N6: 2.047(3) 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 benzotriazole ring and the imidazole ring is 58.80(13)°. The distance between the benzotriazole rings of two adjacent molecules is 3.5608 Å and 3.5853 Å, respectively, so it can be inferred that there may be two kinds of π–π 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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