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Crystal structure of poly[μ_2-dichlorido-(μ_2-1-[(2,4-dimethyl-1*H*-triazole-1-yl)methyl]-1*H*-benzotriazole-κ^2N:N′)cadmium(II)], $C_{11}H_{12}CdN_6Cl_2$

https://doi.org/10.1515/ncrs-2024-0082
Received February 22, 2024; accepted April 27, 2024;
published online May 24, 2024

Abstract

$C_{11}H_{12}CdN_6Cl_2$, triclinic, $P\bar{1}$ (no. 2), a = 6.8644(8) Å, b = 10.4577(8) Å, c = 10.6304(12) Å, α = 112.218(9)°, β = 94.638(9)°, γ = 93.289(8)°, Z = 2, V = 700.93(13) Å^3, $R_{gt}(F)$ = 0.0427, $wR_{ref}(F^2)$ = 0.1137, T = 293(2) K.

CCDC no.: 2351582

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

1 Source of materials

1-[(2,4-Dimethyl-1H-triazole-1-yl)methyl]-1H-benzotriazole (dtmb) was prepared according to the literature method with some modifications.[3] The ligand 1-[(2,4-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 $CdCl_2$ (0.04 mmol, 0.0074 g) of methanol solution. The prepared solution was placed at room temperature and colorless crystals were obtained after ten days.

2 Experimental details

H atoms were generated geometrically and refined as riding atoms with C–H = 0.93 Å and the 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.

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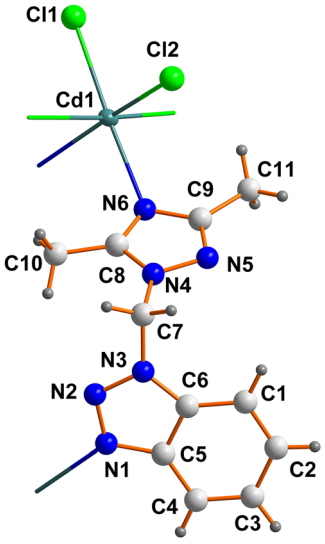
Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.21 × 0.16 × 0.12 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	16.0 mm^{-1}
Diffractometer, scan mode:	Xcalibur, ω
θ_{max}, completeness:	67.1°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4999, 2496, 0.046
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2180
$N(param)_{refined}$:	184
Programs:	CrysAlis^{PRO},[1] SHELX[2]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cd1	1.24229 (6)	0.41604 (4)	0.00383 (4)	0.02454 (19)
Cl1	1.4141 (2)	0.55211 (15)	−0.13167 (15)	0.0306 (3)
Cl2	1.0845 (2)	0.62841 (14)	0.16241 (15)	0.0305 (3)
N1	0.6855 (8)	−0.1936 (5)	0.1586 (5)	0.0280 (11)
N2	0.6556 (7)	−0.0944 (5)	0.1169 (5)	0.0277 (11)
N3	0.6622 (7)	0.0250 (5)	0.2277 (5)	0.0257 (11)
N4	0.8379 (7)	0.2190 (5)	0.2039 (5)	0.0246 (10)
N5	0.9418 (8)	0.3111 (5)	0.3228 (5)	0.0299 (12)
N6	1.0931 (8)	0.2961 (5)	0.1382 (5)	0.0265 (11)
C1	0.7292 (10)	0.0908 (7)	0.4843 (6)	0.0347 (15)
H1	0.7244	0.1863	0.5140	0.042*
C2	0.7634 (10)	0.0264 (7)	0.5729 (6)	0.0365 (15)
H2	0.7822	0.0802	0.6662	0.044*
C3	0.7714 (11)	−0.1182 (8)	0.5292 (7)	0.0382 (16)
H3	0.7925	−0.1569	0.5943	0.046*
C4	0.7489 (10)	−0.2030 (7)	0.3936 (7)	0.0339 (15)
H4	0.7568	−0.2981	0.3648	0.041*
C5	0.7135 (9)	−0.1399 (6)	0.3002 (6)	0.0262 (13)
C6	0.7016 (8)	0.0029 (6)	0.3448 (6)	0.0245 (12)
C7	0.6488 (9)	0.1542 (6)	0.2090 (7)	0.0310 (14)
H7A	0.5663	0.1368	0.1247	0.037*
H7B	0.5865	0.2175	0.2837	0.037*
C8	0.9287 (9)	0.2115 (6)	0.0962 (6)	0.0252 (13)
C9	1.0921 (10)	0.3547 (6)	0.2782 (6)	0.0287 (13)
C10	0.8543 (10)	0.1183 (7)	−0.0458 (6)	0.0333 (14)
H10A	0.7559	0.1611	−0.0814	0.050*
H10B	0.7981	0.0319	−0.0464	0.050*
H10C	0.9607	0.1016	−0.1015	0.050*
C11	1.2531 (11)	0.4570 (8)	0.3748 (6)	0.0405 (17)
H11A	1.3661	0.4094	0.3827	0.061*
H11B	1.2082	0.5001	0.4630	0.061*
H11C	1.2876	0.5267	0.3400	0.061*



3 Comment

Recently, nitrogen heterocyclic compounds have attracted a lot of attention in the field of metal coordination polymers due to their flexible coordination patterns and rich functional properties.[4–6] Among them, triazole and benzotriazole compounds are rich in biological activities such as antibacterial, anti-inflammatory, anti-cancer and anti-diabetes. Metallic polymers synthesized with them as ligands have also been found to have beneficial effects in antibacterial, antioxidant, anti-cancer, hypoglycemic, etc.[7–10] Previously, our group also successfully synthesized complexes with nitrogen heterocycles as ligands, among which complexes were investigated to have better antidiabetic activity.[11]

X-ray crystallographic analysis shows that the title polymer has a two-dimensional network structure centered on a binuclear Cd(II). As shown in the Figure, the central atom Cd(II) is coordinated with four Cl ions (Cl1, Cl1i, Cl2 and Cl2ii) and two N atoms (N1iii and N6) from two dtmb ligands, respectively. The Cd–Cl and Cd–N bonds around Cd1 are of length: Cd1–Cl1: 2.6689(16) Å; Cd1–Cl1i: 2.5630(15) Å; Cd1–Cl2: 2.5861(14) Å; Cd1–Cl2i: 2.6436(16) Å; Cd1–N1iii: 2.423(5) Å; Cd1–N6: 2.471(5) Å. The range of bond angles around the Cd is 84.16(12)°–177.51(12)°.[12] The smallest bond angle is N6–Cd1–Cl2, the largest is N6–Cd1–Cl1, in each dtmb ligand, the angle between the benzotriazole and the triazole ring is 67.0°, and two adjacent cadmium ions are connected by two dtmb ligands in a bidentate bridging coordination mode to form a binuclear structure. The dinuclear Cd(II) asymmetric unit extends indefinitely by connecting two Cl ions to form a two-dimensional structure. In addition, the distance between the benzotriazole rings of two neighboring binuclear units is 3.716 Å, which may have intermolecular p-p interactions, and the two-dimensional mesh structure is expanded into three-dimensional, making the structure more stable.

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.
Research funding: This work was financially supported by the Key Scientific and Research Projects of the Education Department of Henan Province (No. 21A430024).
Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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