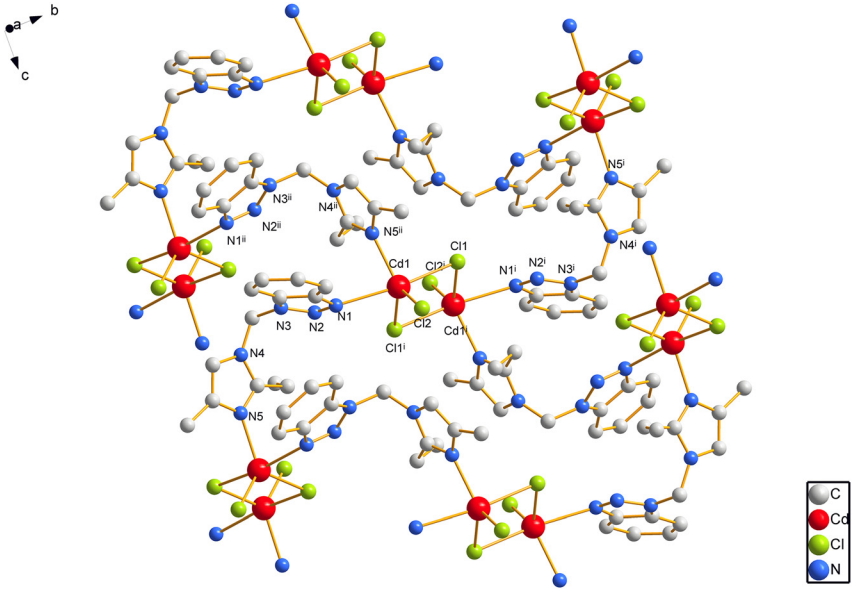
Jun-Ya Du, Tan-peng Zhou, Jing Yang* and Xia Wang

Crystal structure of poly[chlorido-μ_2-chlorido-(μ_2-1-[(2-ethyl-4-methyl-1*H*-imidazol-1-yl)methyl]-1*H*-benzotriazole-κ*N:N*')cadmium(II)], $C_{13}H_{15}CdN_5Cl_2$



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Abstract

$C_{13}H_{15}CdN_5Cl_2$, monoclinic, $P2_1/c$ (no. 14), a = 11.5514(4) Å, b = 16.7843(5) Å, c = 8.9691(3) Å, β = 101.927(3)°, Z = 4, V = 1701.41(10) Å^3, $R_{gt}(F)$ = 0.0379, $wR_{ref}(F^2)$ = 0.1020, 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.

***Corresponding author: Jing Yang**, College of Pharmacy, Henan University of Chinese Medicine, Zhengzhou, 450046, P.R. China, E-mail: candyyjing@163.com. https://orcid.org/0000-0002-4427-2214
Jun-Ya Du, **Tan-peng Zhou and Xia Wang**, College of Pharmacy, Henan University of Chinese Medicine, Zhengzhou, 450046, P.R. China. https://orcid.org/0000-0002-7929-0383 (X. Wang)

Table 1: Data collection and handling.

Crystal:	Prism, colourless
Size:	0.25 × 0.17 × 0.10 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	13.17 mm^{-1}
Diffractometer, scan mode:	Xcalibur, ω-scans
θ_{max}, completeness:	67.1°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6530, 3045, 0.038
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2516
$N(param)_{refined}$:	192
Programs:	CrysAlis^{PRO} [1], SHELX [2]

1 Source of materials

All starting materials are commercially available. The 1-[(2-ethyl-4-methyl-1*H*-imidazol-1-yl)methyl]-1*H*-benzotriazole (emimb) was prepared according to the literature method with some modifications [3]. Emimb (0.02 mmol, 0.0048 g) was dissolved in 2 mL of methanol solution and the solution was slowly add to 2 mL of $CdCl_2$ (0.02 mmol, 0.0037 g) of methanol solution. The prepared solution was placed at room temperature and colorless crystals were obtained after 2 weeks.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.6279 (4)	0.8134 (3)	0.3193 (5)	0.0403 (10)
C2	0.6310 (4)	0.7357 (3)	0.2687 (5)	0.0401 (10)
C3	0.5308 (5)	0.6956 (4)	0.1896 (6)	0.0538 (13)
H3	0.5340	0.6437	0.1544	0.065*
C4	0.4285 (5)	0.7381 (4)	0.1679 (8)	0.0675 (18)
H4	0.3592	0.7146	0.1149	0.081*
C5	0.4234 (5)	0.8163 (4)	0.2226 (7)	0.0649 (16)
H5	0.3506	0.8421	0.2074	0.078*
C6	0.5221 (5)	0.8557 (3)	0.2975 (7)	0.0548 (13)
H6	0.5187	0.9077	0.3319	0.066*
C7	0.8043 (5)	0.6381 (3)	0.3085 (5)	0.0422 (10)
H7A	0.8881	0.6459	0.3126	0.051*
H7B	0.7708	0.6116	0.2133	0.051*
C8	0.6988 (4)	0.5321 (3)	0.4287 (6)	0.0415 (10)
H8	0.6424	0.5181	0.3429	0.050*
C9	0.7086 (5)	0.5027 (3)	0.5691 (6)	0.0426 (10)
C10	0.8497 (4)	0.5910 (3)	0.5825 (5)	0.0369 (9)
C11	0.6381 (5)	0.4398 (4)	0.6247 (7)	0.0632 (16)
H11A	0.5712	0.4264	0.5458	0.095*
H11B	0.6110	0.4589	0.7124	0.095*
H11C	0.6863	0.3933	0.6519	0.095*
C12	0.9571 (4)	0.6403 (3)	0.6353 (6)	0.0482 (12)
H12A	0.9662	0.6502	0.7437	0.058*
H12B	0.9465	0.6914	0.5836	0.058*
C13	1.0696 (6)	0.6016 (6)	0.6064 (12)	0.107 (3)
H13A	1.0662	0.5987	0.4987	0.161*
H13B	1.0767	0.5488	0.6487	0.161*
H13C	1.1369	0.6327	0.6537	0.161*
Cd1	0.84244 (3)	0.96958 (2)	0.41888 (3)	0.03804 (13)
Cl1	0.98139 (10)	1.09584 (7)	0.41601 (14)	0.0486 (3)
Cl2	0.68886 (12)	1.02310 (8)	0.53875 (15)	0.0537 (3)
N1	0.7413 (4)	0.8347 (2)	0.3914 (5)	0.0445 (9)
N2	0.8110 (4)	0.7748 (2)	0.3865 (5)	0.0452 (10)
N3	0.7477 (4)	0.7151 (2)	0.3128 (4)	0.0394 (8)
N4	0.7888 (3)	0.5876 (2)	0.4357 (4)	0.0375 (8)
N5	0.8027 (4)	0.5404 (2)	0.6643 (4)	0.0393 (9)

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.

3 Comment

In recent years, more and more researchers have paid attention to N-heterocyclic complexes [4]. N-heterocyclic compounds. N-heterocyclic imidazoles and benzotriazoles ligands are widely used in complex design and synthesis, since their strong coordination ability and rich functional properties [5–7]. In this study, a Cd(II) complex is synthesized with 1-[(2-ethyl-4-methyl-1H-imidazol-1-yl)methyl]-1*H*-benzotriazole ligand.

X-ray crystallographic analysis shows that the title complex has a two-dimensional network structure containing containing Cd_2Cl_4 units. space group. As shown in the Figure, the central atom Cd(II) is coordinated with three Cl ions (Cl1, Cl1i and Cl2) and two N atoms (N1 and N5ii) from two crystallogaphically dependent emimb ligands, respectively. The Cd–Cl and Cd–N bonds around Cd1 are of length: Cd1–Cl1i: 2.5088(12) Å; Cd1–Cl1: 2.6617(12) Å; Cd1–Cl2: 2.4287(13) Å; Cd1–N1: 2.536(4) Å; Cd1–N5ii: 2.241(4) Å. The range of bond angles around the metal center Cd(II) is 80.84 (14)° –167.52 [8, 9]. In each emimb ligand, the angle between the benzotriazole and the imidazole ring is 80.410 (141)°, and the adjacent two Cd(II) ions are connected by two Cl ions to form a binuclear structure. The dinuclear Cd(II) unit extends infinitely by connecting the (emimb) ligand to form a two-dimensional structure.

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

References

1. Agilent Technologies. *CrysAlis$_{PRO}$ Software System, Version 171.37.35*; Agilent Technologies UK Ltd: Oxford, UK, 2014.
2. Sheldrick G. M. A short history of *SHELX*. *Acta Crystallogr.* 2008, *A64*, 112–122.
3. Katritzky A. R., Drewniak-Deyrup M., Lan X. F., Brunner F. Chemistry of benzotriazole. Preparation, lithiation and transformation of *N*-(benzotriazol-1-ylmethyl) heterocycles. *J. Heterocycl. Chem.* 1989, *26*, 829–836.
4. Panzner M. J., Hindi K. M., Wright B. D., Taylor J. B., Han D. S., Youngs W. J., Cannon C. L. A theobromine derived silver N-heterocyclic carbene: synthesis, characterization, and antimicrobial efficacy studies on cystic fibrosis relevant pathogens. *Dalton Trans.* 2009, *35*, 7308–7313.
5. Wang Y. Z., Zhang J., Yang H. X., Meng X. R. A new Ag complex based on 1-[(1*H*-benzimidazol-1-yl)meth-yl]-1*H*-1,2,4-triazole. *Acta Crystallogr., Sect. E: Struct. Rep. Online* 2011, *E67*, m1788.
6. Asmaa E. N., Abdelnaser A. E., Hassan M. E. Z., Tran D. X., Tran D. K., Mohamed G., Nadia E. W., Yusif E. S., Yasser N. Benzimidazole derivatives suppress fusarium wilt disease *via* interaction with ERG6 of fusarium equiseti and activation of the antioxidant defense system of pepper plants. *J. Fungi.* 2023, *9*, 244.

7. Smirnova K. S., Lider E. V., Kozlova S. G., Sukhikh T. S., Kuratieva N. V., Pozdniakov I. P., Potapov A. S. Zinc complexes with 1-(1*H*-benzimidazol-1-ylmethyl)-1*H*-benzotriazole: the structure, quantum chemical calculations, and luminescence properties. *Russ. Chem. Bull. Int. Ed.* 2020, *10*, 1873–1883.
8. Wang X., Shi X. J., Yang H. X., Hu F., Pan L. *catena*–Poly [chloridocadmium(II)]bis-{μ-1-[(2-ethyl-1*H*-imidazole-1-yl)meth-yl]-1*H*-benzotriazole}[chloridocadmium(II)]di-μ-chlorido]. *Acta Crystallogr. Sec. E.* 2011, *67*, m846.
9. Liang G., Liu Y., Zhang X., Yi Z. Anion-dependent assemblies of a ser=s of Cd(II) coordination complexes based on an asymmetric multi-dentate ligand and inorganic SBUs: syntheses, crystal structures, and fluorescent properties. *CrystEngComm* 2014, *42*, 9896.