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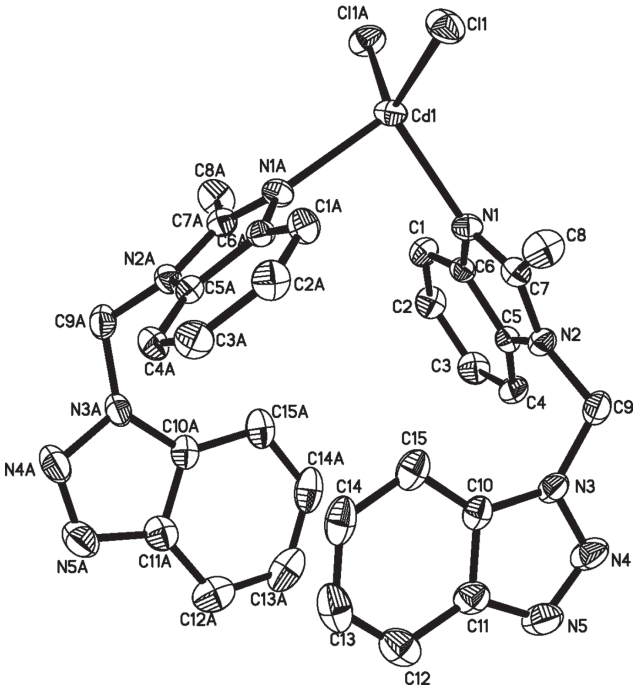
Crystal structure of dichlorido bis[1-[(2-methyl-1*H*-benzoimidazol-1-yl)methyl]-1*H*-benzotriazole-κ^1*N*] cadmium(II), $C_{30}H_{26}CdCl_2N_{10}$



https://doi.org/10.1515/ncrs-2017-0211
Received July 17, 2017; accepted January 15, 2018; available online February 9, 2018

Abstract

$[Cd(C_{15}H_{13}N_5)_2Cl_2]$, monoclinic, *C*2/*c* (no. 15), $a = 15.6291(6)$ Å, $b = 12.8859(4)$ Å, $c = 14.7622(5)$ Å, $\beta = 97.781(3)°$, $V = 2945.65(18)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0381$, $\omega R_{ref}(F^2) = 0.0738$, $T = 293(2)$ K.

CCDC no.: 1816964

The crystal structure is shown in the figure. Hydrogen atoms are omitted for clarity. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	Prism, colorless
Size:	$0.21 \times 0.19 \times 0.17$ mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.96 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
θ_{max}, completeness:	26.4°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6801, 3025, 0.034
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2438
$N(param)_{refined}$:	196
Programs:	CrysAlis^{PRO} [1], SHELX [2]

Source of material

The educt 1-[(2-methyl-1*H*-benzoimidazol-1-yl)methyl]-1*H*-benzotriazole (0.04 mmol, 0.0105 g) in methanol (6 mL) was added dropwise to a methanol solution (6 mL) of $CdCl_2$ (0.04 mmol, 0.0073 g) in methanol. The resulting solution was allowed to stand at room temperature. After 3 weeks colourless crystals were obtained.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Discussion

In the past decades, the design and synthesis of coordination complexes have received rather considerable attention in the field of material chemistry and crystal engineering [3–5]. The incorporation of the biologically active heterocyclic ring moieties such as benzotriazole and benzoimidazole in the molecular structure of this N-donor derivative represents an interesting strategy to design new pharmaceutical candidates [6, 7]. On the other hand, Cd(II)-connected coordination polymers have attracted considerable interest owing to its various coordination modes, and special physical properties [8]. We are engaged in the synthesis of unsymmetrical N-heterocyclic ligands and corresponding complexes [9].

The title compound contains a mononuclear complex. As is shown in the figure, the Cd(II) atom (located at a twofold axis) is four-coordinated by two N atoms from two

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.37392(19)	0.4388(2)	0.56583(18)	0.0425(7)
H1	0.3465	0.4919	0.5935	0.051*
C2	0.3278(2)	0.3729(3)	0.50334(19)	0.0475(8)
H2	0.2684	0.3813	0.4893	0.057*
C3	0.3692(2)	0.2939(3)	0.46099(19)	0.0516(9)
H3	0.3365	0.2512	0.4188	0.062*
C4	0.4566(2)	0.2775(2)	0.47995(17)	0.0443(8)
H4	0.4840	0.2248	0.4518	0.053*
C5	0.50210(18)	0.3440(2)	0.54362(16)	0.0333(6)
C6	0.46220(18)	0.4234(2)	0.58606(16)	0.0317(6)
C7	0.59858(19)	0.4303(2)	0.63924(17)	0.0376(7)
C8	0.6834(2)	0.4612(3)	0.6892(2)	0.0564(9)
H8A	0.6772	0.5250	0.7212	0.085*
H8B	0.7239	0.4708	0.6465	0.085*
H8C	0.7040	0.4080	0.7321	0.085*
C9	0.65733(19)	0.2823(2)	0.55599(18)	0.0453(8)
H9A	0.6592	0.2848	0.4906	0.054*
H9B	0.7125	0.3068	0.5866	0.054*
C10	0.63057(18)	0.1343(3)	0.66508(17)	0.0404(7)
C11	0.6249(2)	0.0290(3)	0.6480(2)	0.0495(8)
C12	0.6102(2)	−0.0408(3)	0.7167(2)	0.0627(10)
H12	0.6057	−0.1118	0.7057	0.075*
C13	0.6029(2)	−0.0001(4)	0.8005(2)	0.0668(11)
H13	0.5929	−0.0445	0.8476	0.080*
C14	0.6097(2)	0.1054(4)	0.8178(2)	0.0630(11)
H14	0.6048	0.1294	0.8763	0.076*
C15	0.6235(2)	0.1765(3)	0.75099(18)	0.0547(9)
H15	0.6278	0.2474	0.7625	0.066*
Cd1	0.5000	0.59851(2)	0.7500	0.03882(12)
Cl1	0.62784(6)	0.69694(7)	0.80860(5)	0.0544(2)
N1	0.52437(15)	0.47625(18)	0.64584(13)	0.0361(6)
N2	0.58901(15)	0.34993(19)	0.57868(13)	0.0358(6)
N3	0.64384(16)	0.1765(2)	0.58312(14)	0.0424(6)
N4	0.6466(2)	0.0997(2)	0.52021(16)	0.0586(8)
N5	0.6350(2)	0.0112(2)	0.55770(18)	0.0643(8)

crystallogaphically dependent 1-[(2-methyl-1*H*-benzoimidazol-1-yl)methyl]-1*H*-benzotriazole ligands and two crystallogaphically dependent chlorido ligands in a distorted tetrahedral coordination environment (with Cd-N bond length of 2.269(2) Å, and a Cd—Cl bond length of 2.4251(8) Å). The bond angles around Cd(II) ion range from 92.07 to 116.93°. In addition, the benzoimidazol rings in adjacent molecules are parallel, with an average interplanar distance of 3.485 Å. Thus π−π interactions are not to be ruled out. Bond lengths and agles are in accord with related structures [10, 11].

Acknowledgements: This work was financially supported by the Foundation for Henan Provincial Institute of Henan University of Chinese Medicine (2014KYYWF-QN11). The authors thank the Professor Hong-Wei Hou and Yu Zhu of Zhengzhou University for their help.

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