# Crystal structure of catena[dichlorido-1,4-bis(2-methylbenzimidazol-1-ylmethyl)benzene-cadmium(II)]–*N,N*-dimethylformamide–water (2:2:1), $[CdCl_2(C_{24}H_{22}N_4)]\cdot C_3N_2O_2H_7\cdot 0.5H_2O$, $C_{54}H_{60}Cd_2Cl_4N_{10}O_3$

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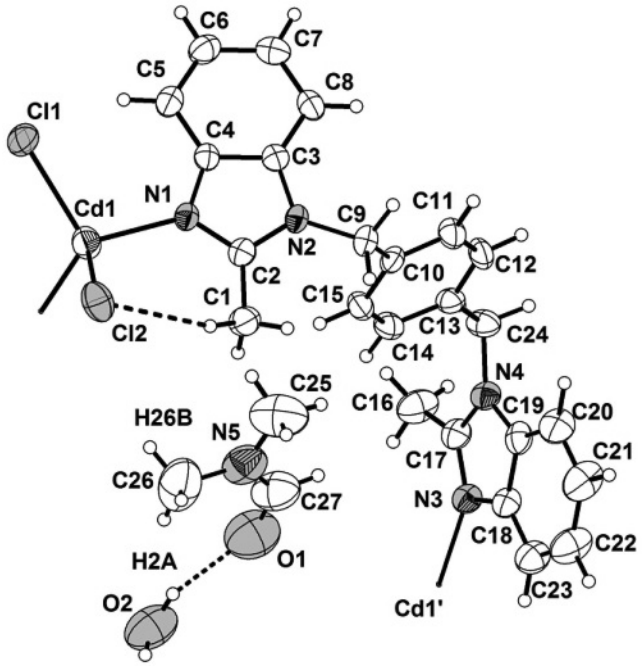


**Abstract**

$C_{54}H_{60}Cd_2Cl_4N_{10}O_3$, monoclinic, $P2_1/c$ (no. 14), $a$ = 9.552(2) Å, $b$ = 26.647(5) Å, $c$ = 11.094(2) Å, $\beta$ = 98.23(3)°, $V$ = 2794.7 Å$^3$, $Z$ = 2, $R_{gt}(F)$ = 0.0485, $wR_{ref}(F^2)$ = 0.0968, $T$ = 293 K.

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | colourless blocks, size 0.18×0.23×0.26 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 10.04 cm$^{-1}$ |
| Diffractometer, scan mode: | Rigaku Saturn, $\omega$ |
| $2\theta_{max}$: | 49.98° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 27495, 4814 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 4316 |
| $N(param)_{refined}$: | 341 |
| Programs: | SHELX [12] |

**Source of material**

A mixture of 1,4-bis(2-methylbenzimidazol-1-ylmethyl) benzene (*bmb*, 73.2 mg, 0.2 mmol), $CdCl_2\cdot H_2O$ (53.2 mg, 0.2 mmol), *N,N*-Dimethylformamide solution (1 mL) and $H_2O$ (9 mL) were placed in a Teflon-lined stainless steel vessel, heated to 130 °C for 4 days, and then cooled to room temperature for 24 h. Colourless block-shaped crystals of the title complex were obtained.

**Experimental details**

Absorption corrections were applied by using multi-scan program. The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

**Discussion**

In recent years, the construction of metal-organic frameworks (MOFs) has received remarkable attention due to their potentially applications in the areas of magnetism, molecular separation, catalysis, luminescence, sorption, and so on [1-4]. In order to build novel molecular architectures, the geometries of organic ligands have a great effect on the structural frameworks of coordination polymers; thus, much effort has been devoted to designing and modifying the organic ligands to control the products [5-8]. According to our recent research [9-11], we anticipate that the semi-rigid *N*-donor ligand 1,4-bis(2-methylbenzimidazol-1-ylmethyl)benzene (*bmb*) would be a powerful precursor for the construction of fascinating structures: (1) the 2-position substituent methyl effectively enhances the donated electrons ability of benzimidazole ring; (2) the flexible –$CH_2$- makes the two methylbenzimidazol groups significantly deviates from coplanarity with a potential tendency to generate various *cis*- and *trans*-conformations when *bmb* coordinates with metal centers. The asymmetric unit of the title structure consists of one *bmb*, two chlorido ligands, one Cd(II) ion, one *N,N*-dimethylformamide molecule and one half water molecule. As shown in the figure, the center Cd(II) ion is four-coordinated in a distorted tetrahedral geometry, ligated by two chlorido ligands and two nitrogen atoms (N1, N4) from *bmb* ligands. The bond lengths are Cd1–Cl1 = 2.4355(6) Å, Cd1–Cl2 = 2.4345(7) Å, Cd1–N1 = 2.2480(14) Å and Cd1–N3 = 2.2405(14) Å, respectively. *bmb* adopts asymmetric *trans*-conformation with the $N_{donor}\cdots N{-}C_{sp3}\cdots C$ torsion angles of 108.4° and 115.4°, respectively. The two methylbenzimidazol arms of *bmb* are bend in opposite directions to bridge two adjacent $Cd^{2+}$ ions to form a zigzag chain. In addition, there exist two kinds of hydrogen bond with C–H···Cl (3.680 Å and 3.728 Å) between the chloride ion and the adjacent C–H group, and O–H···O (2.775 Å) hydrogen bonds between free water molecule and the ketonic oxygen of *N,N*-dimethylformamide molecule.

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**Table 2.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | Occ. | *x* | *y* | *z* | $U_{iso}$ |
|---|---|---|---|---|---|---|
| H(26A) | 4*e* | | 0.6387 | 0.6796 | 0.4188 | 0.187 |
| H(26B) | 4*e* | | 0.5461 | 0.6330 | 0.4425 | 0.187 |
| H(26C) | 4*e* | | 0.6518 | 0.6296 | 0.3470 | 0.187 |
| H(2A) | 4*e* | 0.5 | 0.7232 | 0.7390 | 0.4203 | 0.175 |
| H(2B) | 4*e* | 0.5 | 0.7230 | 0.7688 | 0.3176 | 0.175 |
| H(27) | 4*e* | | 0.8986 | 0.6443 | 0.6438 | 0.121 |
| H(24A) | 4*e* | | 0.1700 | 0.8236 | 0.9519 | 0.061 |
| H(24B) | 4*e* | | 0.0373 | 0.7893 | 0.9548 | 0.061 |
| H(9A) | 4*e* | | 0.8276 | 0.5653 | 0.9732 | 0.049 |
| H(9B) | 4*e* | | 0.8081 | 0.5267 | 1.0759 | 0.049 |
| H(8) | 4*e* | | 0.6537 | 0.5219 | 1.2525 | 0.053 |
| H(1A) | 4*e* | | 0.5592 | 0.6041 | 0.7427 | 0.080 |
| H(1B) | 4*e* | | 0.7105 | 0.5921 | 0.8117 | 0.080 |
| H(1C) | 4*e* | | 0.6394 | 0.6440 | 0.8306 | 0.080 |
| H(6) | 4*e* | | 0.2325 | 0.5276 | 1.2511 | 0.063 |
| H(12) | 4*e* | | 1.0893 | 0.5975 | 1.3881 | 0.059 |

**Table 2.** continued.

| Atom | Site | Occ. | *x* | *y* | *z* | $U_{iso}$ |
|---|---|---|---|---|---|---|
| H(20) | 4*e* | | 0.3031 | 0.8462 | 0.7474 | 0.076 |
| H(11) | 4*e* | | 0.9633 | 0.5439 | 1.2483 | 0.057 |
| H(14) | 4*e* | | 0.8996 | 0.7147 | 1.2089 | 0.056 |
| H(5) | 4*e* | | 0.1971 | 0.5632 | 1.0583 | 0.055 |
| H(15) | 4*e* | | 0.7760 | 0.6614 | 1.0698 | 0.053 |
| H(23) | 4*e* | | 0.4216 | 0.6856 | 0.6196 | 0.072 |
| H(21) | 4*e* | | 0.4684 | 0.8353 | 0.6168 | 0.093 |
| H(7) | 4*e* | | 0.4532 | 0.5060 | 1.3446 | 0.066 |
| H(16A) | 4*e* | | 0.0354 | 0.6564 | 0.9076 | 0.105 |
| H(16B) | 4*e* | | –0.0394 | 0.7084 | 0.9161 | 0.105 |
| H(16C) | 4*e* | | 0.0910 | 0.6940 | 1.0123 | 0.105 |
| H(22) | 4*e* | | 0.5247 | 0.7572 | 0.5517 | 0.090 |
| H(25A) | 4*e* | | 0.7947 | 0.5596 | 0.4542 | 0.191 |
| H(25B) | 4*e* | | 0.6790 | 0.5567 | 0.5410 | 0.191 |
| H(25C) | 4*e* | | 0.8379 | 0.5655 | 0.5952 | 0.191 |

**Table 3.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | Occ. | *x* | *y* | *z* | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C(26) | 4*e* | | 0.6366(3) | 0.6436(1) | 0.4237(2) | 0.095(2) | 0.178(3) | 0.100(2) | 0.007(2) | 0.010(2) | –0.007(2) |
| O(2) | 4*e* | 0.5 | 0.7110(4) | 0.7686(1) | 0.3921(4) | 0.114(2) | 0.096(2) | 0.149(3) | –0.026(2) | 0.048(2) | –0.034(2) |
| C(27) | 4*e* | | 0.8302(3) | 0.6580(1) | 0.5848(2) | 0.112(2) | 0.096(2) | 0.093(2) | –0.037(1) | 0.010(2) | –0.009(2) |
| O(1) | 4*e* | | 0.8245(2) | 0.70322(8) | 0.5751(2) | 0.146(2) | 0.109(2) | 0.157(2) | –0.025(1) | 0.034(1) | –0.024(1) |
| C(24) | 4*e* | | 0.0984(2) | 0.80403(6) | 0.9017(2) | 0.061(1) | 0.0432(9) | 0.0463(9) | 0.0142(8) | 0.0035(8) | –0.0006(8) |
| Cd(1) | 4*e* | | 0.24798(1) | 0.604395(4) | 0.77288(1) | 0.03932(6) | 0.03745(6) | 0.05196(7) | 0.00153(5) | –0.00216(6) | 0.00406(6) |
| Cl(1) | 4*e* | | 0.03406(5) | 0.56157(2) | 0.81274(5) | 0.0452(2) | 0.0532(3) | 0.0909(3) | –0.0101(2) | 0.0016(2) | 0.0062(3) |
| Cl(2) | 4*e* | | 0.31717(5) | 0.58113(2) | 0.57755(4) | 0.0753(3) | 0.0723(3) | 0.0459(2) | 0.0167(3) | –0.0040(2) | –0.0032(2) |
| N(2) | 4*e* | | 0.6343(1) | 0.56712(5) | 1.0220(1) | 0.0279(6) | 0.0388(7) | 0.0382(7) | –0.0009(5) | –0.0006(6) | –0.0040(6) |
| C(10) | 4*e* | | 0.8586(2) | 0.59686(6) | 1.1430(1) | 0.0265(7) | 0.0394(8) | 0.0450(9) | –0.0040(6) | 0.0032(7) | –0.0021(7) |
| C(9) | 4*e* | | 0.7876(2) | 0.56076(6) | 1.0480(1) | 0.0309(7) | 0.0458(9) | 0.0451(9) | 0.0019(7) | 0.0011(7) | –0.0058(8) |
| N(1) | 4*e* | | 0.4198(1) | 0.58655(5) | 0.9274(1) | 0.0311(6) | 0.0393(7) | 0.0397(7) | –0.0001(6) | 0.0009(6) | –0.0015(6) |
| C(3) | 4*e* | | 0.5404(2) | 0.55233(5) | 1.0992(1) | 0.0399(8) | 0.0287(7) | 0.0375(8) | –0.0020(7) | 0.0030(7) | –0.0056(6) |
| C(8) | 4*e* | | 0.5635(2) | 0.53010(6) | 1.2143(1) | 0.0477(9) | 0.0397(9) | 0.0432(9) | 0.0032(8) | –0.0040(8) | 0.0027(7) |
| C(1) | 4*e* | | 0.6225(2) | 0.60881(7) | 0.8172(2) | 0.0496(9) | 0.061(1) | 0.048(1) | –0.0087(9) | 0.0055(8) | 0.0037(9) |
| N(3) | 4*e* | | 0.2240(1) | 0.68790(5) | 0.7819(1) | 0.0443(7) | 0.0348(7) | 0.0514(8) | 0.0038(6) | 0.0080(6) | 0.0071(6) |
| C(19) | 4*e* | | 0.2666(2) | 0.77131(6) | 0.7638(2) | 0.0393(8) | 0.0418(9) | 0.055(1) | 0.0013(7) | –0.0037(8) | 0.0085(8) |
| N(4) | 4*e* | | 0.1671(1) | 0.76397(5) | 0.8418(1) | 0.0438(7) | 0.0359(7) | 0.0524(8) | 0.0087(6) | 0.0042(7) | 0.0050(6) |
| C(6) | 4*e* | | 0.3100(2) | 0.53371(7) | 1.2111(2) | 0.0465(9) | 0.055(1) | 0.059(1) | –0.0022(8) | 0.0187(8) | –0.0004(9) |
| C(4) | 4*e* | | 0.4072(2) | 0.56476(6) | 1.0397(1) | 0.0343(7) | 0.0316(8) | 0.0395(8) | 0.0009(6) | 0.0022(7) | –0.0029(7) |
| C(12) | 4*e* | | 1.0275(2) | 0.61069(6) | 1.3235(2) | 0.0430(9) | 0.0446(9) | 0.054(1) | –0.0003(8) | –0.0143(8) | 0.0098(8) |
| C(13) | 4*e* | | 1.0119(2) | 0.66163(6) | 1.3115(1) | 0.0421(8) | 0.0385(8) | 0.0427(9) | –0.0093(7) | 0.0038(7) | 0.0024(7) |
| C(20) | 4*e* | | 0.3272(2) | 0.81432(7) | 0.7229(2) | 0.064(1) | 0.0330(9) | 0.093(1) | 0.0075(9) | 0.011(1) | 0.0136(9) |
| C(18) | 4*e* | | 0.3012(2) | 0.72340(6) | 0.7256(2) | 0.0405(8) | 0.0344(8) | 0.054(1) | 0.0034(7) | 0.0054(8) | 0.0097(7) |
| C(11) | 4*e* | | 0.9513(2) | 0.57841(6) | 1.2393(2) | 0.0453(9) | 0.0324(8) | 0.062(1) | –0.0014(7) | –0.0054(8) | 0.0009(8) |
| C(14) | 4*e* | | 0.9144(2) | 0.68026(6) | 1.2163(2) | 0.0511(9) | 0.0325(8) | 0.054(1) | –0.0029(7) | 0.0041(8) | 0.0044(8) |
| C(2) | 4*e* | | 0.5578(2) | 0.58733(6) | 0.9209(1) | 0.0386(8) | 0.0378(8) | 0.0386(8) | –0.0033(7) | 0.0028(7) | –0.0060(7) |
| C(5) | 4*e* | | 0.2876(2) | 0.55531(6) | 1.0963(2) | 0.0369(8) | 0.047(1) | 0.054(1) | 0.0000(7) | 0.0063(8) | –0.0039(8) |
| C(17) | 4*e* | | 0.1464(2) | 0.71403(6) | 0.8500(2) | 0.0443(9) | 0.0446(9) | 0.0479(9) | 0.0075(8) | 0.0012(8) | 0.0079(8) |
| C(15) | 4*e* | | 0.8398(2) | 0.64827(6) | 1.1332(2) | 0.0437(8) | 0.0372(9) | 0.0483(9) | 0.0011(7) | –0.0033(8) | 0.0063(8) |
| C(23) | 4*e* | | 0.3982(2) | 0.71733(7) | 0.6456(2) | 0.059(1) | 0.052(1) | 0.072(1) | 0.0037(9) | 0.016(1) | 0.006(1) |
| C(21) | 4*e* | | 0.4243(2) | 0.80735(7) | 0.6447(2) | 0.071(1) | 0.049(1) | 0.120(2) | –0.002(1) | 0.038(1) | 0.027(1) |
| C(7) | 4*e* | | 0.4435(2) | 0.52099(7) | 1.2682(2) | 0.065(1) | 0.052(1) | 0.049(1) | –0.0048(9) | 0.0120(9) | 0.0089(8) |
| C(16) | 4*e* | | 0.0498(2) | 0.69120(8) | 0.9284(2) | 0.077(1) | 0.059(1) | 0.081(1) | 0.005(1) | 0.039(1) | 0.013(1) |
| C(22) | 4*e* | | 0.4592(2) | 0.76014(8) | 0.6057(2) | 0.075(1) | 0.063(1) | 0.096(1) | 0.005(1) | 0.043(1) | 0.020(1) |
| N(5) | 4*e* | | 0.7446(2) | 0.62697(9) | 0.5164(2) | 0.092(1) | 0.123(2) | 0.064(1) | –0.015(1) | 0.025(1) | –0.003(1) |
| C(25) | 4*e* | | 0.7659(3) | 0.5725(1) | 0.5277(3) | 0.173(3) | 0.115(2) | 0.094(2) | –0.044(2) | 0.020(2) | –0.009(2) |

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