# Crystal structure of 4-[(2-phenylbenzimidazole)-methyl]benzoic acid cadmium(II), $C_{42}H_{30}CdN_4O_4$

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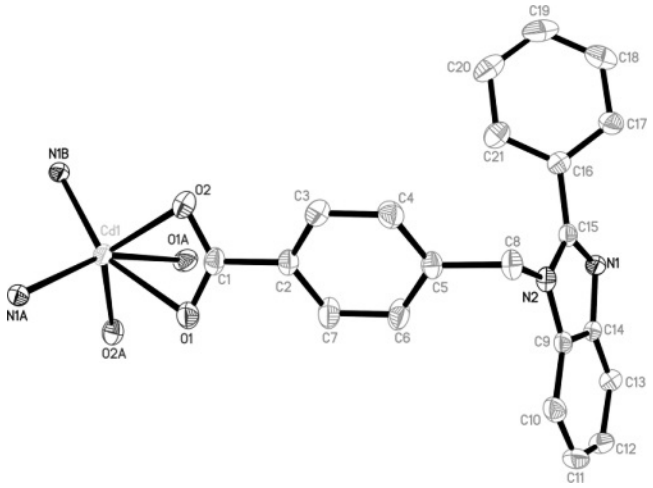
Received February 19, 2012, accepted June 12, 2012, available online October 19, 2012, CCDC no. 905693




**Abstract**

$C_{42}H_{30}CdN_4O_4$, monoclinic, *C*2/*c* (no. 15), $a$ = 9.6025(3) Å, $b$ = 21.6248(5) Å, $c$ = 16.4162(5) Å, $\beta$ = 96.440(3)°, $V$ = 3387.4 Å$^3$, $Z$ = 4, $R_{gt}(F)$ = 0.0340, $wR_{ref}(F^2)$ = 0.0880, $T$ = 293 K.

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

| | |
|---|---|
| Crystal: | colourless blocks, size 0.17×0.18×0.2 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 6.96 cm$^{-1}$ |
| Diffractometer, scan mode: | Oxford Diffraction Gemini R Ultra, $\omega$ |
| $2\theta_{max}$: | 58.52° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 11416, 4015 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 3239 |
| $N(param)_{refined}$: | 231 |
| Programs: | SHELX [3] |

**Source of material**

A mixture of 2-phenylbenzimidazole (1.98 g, 10mmol) and NaOH (0.44 g, 11mmol) in DMSO (10 mL) was stirred at 70 °C for 2 h, and then methyl-4-(bromomethyl)benzoate (3.5 g, 10mmol) was added [1]. The mixture was cooled to room temperature after stirring at 70 °C for 2 h and then poured into 200 mL of water, and the white solid formed immediately. Then the isolated products were heated and refluxed at 90 °C in ethanol (100 ml) and sodium hydroxide aqueous solution. After ethanol was removed by evaporation, the pH value was adjusted to 2-3 via diluted hydrochloric acid solution as soon as the reaction was completed. Meanwhile, a large quantity of white powder was deposited. After the sample was filtrated, washed by water and dried, the target HL ligand was obtained with a yield of 73%. A mixture containing $Cd(OAc)_2$ (27.0 mg, 0.1mmol), HL (131.2 mg, 0.2mmol), NaOH (8 mg, 0.2mmol), and water (10 mL) was sealed in a Teflon reactor (15 mL), which was heated at 150 °C for 3 days and then it was cooled to room temperature at 10 °C/h. Colourless block crystals were collected in a 42% yield.

**Experimental details**

All H atoms bound to carbon were refined using a riding model with $d$(C–H) = 0.93 Å, $U_{iso}$ = 1.2 $U_{eq}$(C) for aromatic and 0.97 Å, $U_{iso}$ =1.5 $U_{eq}$(C) for $CH_2$ atoms.

**Discussion**

Benzimidazole ligand as a typical rigid ligand is an excellent candidate for the construction of extended architectures [2]. The structure of the title compound contains one $Cd^{2+}$ ion and two L anions. In this compound, Cd1 is in an octahedral coordination sphere, which is defined by four oxygen atoms (Co1–O1 = 2.389, Co1–O2 = 2.396, Co1–O1A = 2.389 and Co1–O2A = 2.396 Å) and two nitrogen atoms (Co1–N1A = 2.262 and Co1–N1B = 2.262 Å). The C–O and C–N bond lengths are in the range of 1.2 to 1.3 Å and 1.3 Å to 1.5 Å, respectively. The bond distances and bond angles are all in a normal range.

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

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(10) | 8*f* | 0.4845 | 0.1809 | 0.5102 | 0.054 |
| H(11) | 8*f* | 0.6238 | 0.2606 | 0.4724 | 0.064 |
| H(12) | 8*f* | 0.5497 | 0.3272 | 0.3689 | 0.061 |
| H(8A) | 8*f* | 0.1187 | 0.1018 | 0.5014 | 0.048 |
| H(8B) | 8*f* | 0.2701 | 0.1208 | 0.5384 | 0.048 |
| H(6) | 8*f* | 0.4322 | 0.0874 | 0.4041 | 0.062 |
| H(7) | 8*f* | 0.5159 | –0.0034 | 0.3554 | 0.061 |
| H(4) | 8*f* | 0.1355 | –0.0067 | 0.5015 | 0.056 |
| H(3) | 8*f* | 0.2146 | –0.0975 | 0.4489 | 0.06 |
| H(13) | 8*f* | 0.3231 | 0.3223 | 0.3023 | 0.049 |
| H(21) | 8*f* | 0.0387 | 0.0625 | 0.3505 | 0.059 |
| H(20) | 8*f* | –0.1754 | 0.0171 | 0.309 | 0.076 |
| H(19) | 8*f* | –0.3751 | 0.0756 | 0.289 | 0.081 |
| H(18) | 8*f* | –0.3675 | 0.1792 | 0.319 | 0.072 |
| H(17) | 8*f* | –0.1562 | 0.2263 | 0.3623 | 0.052 |

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

| Atom | Site | *x* | *y* | *z* | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Cd(1) | 4*e* | ½ | –0.20428(1) | ¼ | 0.0367(2) | 0.0268(1) | 0.0378(2) | 0 | –0.0004(1) | 0 |
| O(1) | 8*f* | 0.5484(2) | –0.11851(8) | 0.3405(1) | 0.047(1) | 0.0399(9) | 0.055(1) | 0.0079(8) | –0.0012(9) | –0.0102(8) |
| O(2) | 8*f* | 0.3371(2) | –0.15962(8) | 0.3335(1) | 0.054(1) | 0.0346(9) | 0.060(1) | –0.0026(8) | 0.0044(9) | –0.0109(8) |
| N(1) | 8*f* | 0.1313(2) | 0.23248(8) | 0.3374(1) | 0.030(1) | 0.0312(9) | 0.035(1) | 0.0009(8) | 0.0000(8) | –0.0012(8) |
| N(2) | 8*f* | 0.2093(2) | 0.16218(8) | 0.4310(1) | 0.040(1) | 0.0294(9) | 0.031(1) | 0.0060(8) | 0.0029(8) | –0.0021(7) |
| C(14) | 8*f* | 0.2685(2) | 0.24712(9) | 0.3668(1) | 0.031(1) | 0.030(1) | 0.035(1) | 0.0018(9) | 0.003(1) | –0.0096(9) |
| C(10) | 8*f* | 0.4523(3) | 0.2085(1) | 0.4688(2) | 0.040(1) | 0.051(2) | 0.041(1) | 0.012(1) | –0.006(1) | –0.010(1) |
| C(11) | 8*f* | 0.5340(3) | 0.2559(1) | 0.4455(2) | 0.031(1) | 0.066(2) | 0.060(2) | 0.001(1) | –0.009(1) | –0.020(2) |
| C(12) | 8*f* | 0.4885(3) | 0.2969(1) | 0.3837(2) | 0.038(2) | 0.052(2) | 0.062(2) | –0.010(1) | 0.006(1) | –0.014(1) |
| C(9) | 8*f* | 0.3174(2) | 0.20405(9) | 0.4265(1) | 0.034(1) | 0.033(1) | 0.034(1) | 0.0050(9) | 0.003(1) | –0.0096(9) |
| C(8) | 8*f* | 0.2130(3) | 0.1096(1) | 0.4880(1) | 0.051(2) | 0.037(1) | 0.032(1) | 0.011(1) | 0.006(1) | –0.000(1) |
| C(5) | 8*f* | 0.2705(3) | 0.0506(1) | 0.4551(1) | 0.044(1) | 0.032(1) | 0.033(1) | 0.008(1) | 0.004(1) | 0.0026(9) |
| C(6) | 8*f* | 0.3867(3) | 0.0504(1) | 0.4127(2) | 0.066(2) | 0.028(1) | 0.066(2) | –0.001(1) | 0.029(2) | –0.000(1) |
| C(7) | 8*f* | 0.4363(3) | –0.0041(1) | 0.3829(2) | 0.062(2) | 0.034(1) | 0.062(2) | 0.004(1) | 0.029(1) | 0.000(1) |
| C(2) | 8*f* | 0.3697(3) | –0.0596(1) | 0.3932(1) | 0.042(1) | 0.031(1) | 0.034(1) | 0.006(1) | 0.000(1) | –0.0013(9) |
| C(4) | 8*f* | 0.2101(3) | –0.0055(1) | 0.4699(2) | 0.044(2) | 0.043(1) | 0.057(2) | 0.001(1) | 0.018(1) | 0.003(1) |
| C(1) | 8*f* | 0.4229(3) | –0.1167(1) | 0.3537(2) | 0.052(2) | 0.029(1) | 0.038(1) | 0.006(1) | –0.004(1) | 0.001(1) |
| C(3) | 8*f* | 0.2581(3) | –0.0602(1) | 0.4389(2) | 0.049(2) | 0.032(1) | 0.068(2) | –0.003(1) | 0.006(1) | 0.000(1) |
| C(13) | 8*f* | 0.3543(3) | 0.2942(1) | 0.3431(2) | 0.039(1) | 0.038(1) | 0.044(1) | –0.003(1) | 0.002(1) | –0.004(1) |
| C(15) | 8*f* | 0.0999(2) | 0.1815(1) | 0.3765(1) | 0.035(1) | 0.030(1) | 0.033(1) | 0.0047(9) | 0.004(1) | –0.0053(9) |
| C(16) | 8*f* | –0.0358(3) | 0.1495(1) | 0.3594(1) | 0.040(1) | 0.037(1) | 0.029(1) | –0.005(1) | 0.006(1) | 0.0004(9) |
| C(21) | 8*f* | –0.0423(3) | 0.0864(1) | 0.3440(2) | 0.057(2) | 0.040(1) | 0.049(2) | –0.006(1) | 0.004(1) | 0.003(1) |
| C(20) | 8*f* | –0.1705(4) | 0.0595(1) | 0.3187(2) | 0.076(2) | 0.047(2) | 0.067(2) | –0.025(2) | 0.007(2) | –0.004(1) |
| C(19) | 8*f* | –0.2902(4) | 0.0942(2) | 0.3079(2) | 0.054(2) | 0.082(2) | 0.066(2) | –0.033(2) | 0.009(2) | –0.001(2) |
| C(18) | 8*f* | –0.2855(3) | 0.1560(2) | 0.3248(2) | 0.039(2) | 0.084(2) | 0.058(2) | –0.004(1) | 0.012(1) | 0.004(2) |
| C(17) | 8*f* | –0.1591(3) | 0.1842(1) | 0.3507(2) | 0.039(2) | 0.048(1) | 0.045(1) | –0.004(1) | 0.010(1) | –0.001(1) |

*Acknowledgments.* We thank the Science Foundation for Young Teachers of Northeast Normal University (no.20060304) and the Analysis and Testing Foundation of Northeast Normal University for support.

## References

1. Yue, S. M.; Su, Z. M.; Ma, J. F.; Liao, Y.; Kan,Y. H.; Zhang ,H. J.: Crystal Structure and Electronic Structure of a Luminescent Compound 2-(2-pyridyl) benzimidazole. Chinese J. Struct. Chem. **22** (2003) 174.
2. Ma, J. F.; Liu, J. F.; Xing ,Y.; Jia, H. Q.; Lin,Y. H.: Networks with hexagonal circuits in coordination polymers of metal ions (ZnII, CdII) with 1,1'-(1,4-butanediyl)*bis*(imidazole). J.Chem. Soc., Dalton Trans. (2000) 2403.
3. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112-122.