APPLIED ORGANOMETALLIC CHEMISTRY
Appl. Organometal. Chem. 2005; **19**: 173–174
Main Group Metal Compounds
Published online in Wiley InterScience (www.interscience.wiley.com). DOI:10.1002/aoc.699

Crystallographic report

[Bis(3-pyridylacrylato)cadmium(II)]$_n$

Yu-Mei Song, Rui Shi, Xi-Sen Wang, Hong Zhao and Ren-Gen Xiong*

Coordination Chemistry Institute, The State Key Laboratory of Coordination Chemistry Nanjing University, 210093 Nanjing, People's Republic of China

Received 14 April 2004; Revised 5 May 2004; Accepted 6 May 2004

In [bis(3-pyridylacrylato)cadmium(II)]$_n$, the local coordination geometry around the cadmium center is based on an octahedron. The carboxylate acts as a tridentate ligand by bridging two cadmium atoms and binds a third cadmium atom via the pyridyl group with the result that a two-dimensional layered network is formed. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; *in situ* synthesis; deammoniation; cadmium

COMMENT

We have recently combined metal salts with potential 'spacer' organic ligands under hydrothermal conditions to produce a range of new materials.[1] Surprisingly, the reaction of $Cd(ClO_4)_2{\cdot}6H_2O$ with the ligand 3-(3-pyridyl)-3-aminopropionic acid gives the deammoniated product rather than amino-group-remaining product.[2] In the layer structure of [bis(3-pyridylacrylato)cadmium(II)]$_n$, the cadmium atom is located on a centre of inversion and has a distorted octahedral geometry, as shown in Fig. 1. Each carboxylate ligand acts as a bidentate linker to bridge two cadmium centers and the pyridyl group binds to a third cadmium atom, resulting in the formation of two-dimensional layer structure (Fig. 2).

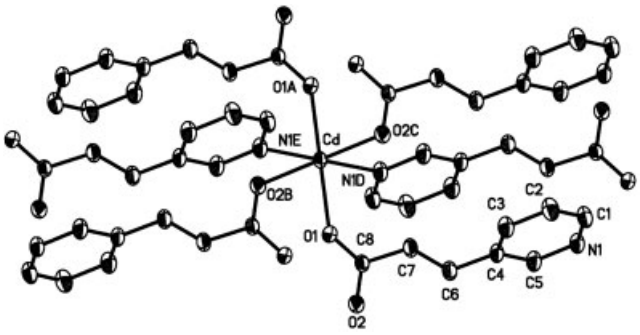

Figure 1. Coordination geometry for [bis(3-pyridylacrylato)cadmium(II)]$_n$; hydrogen atoms are omitted for clarity. Selected geometric parameters: Cd–O1 2.2833(14), Cd–O1A 2.3246(13), Cd–N1D 2.3926(15), C7–C6 1.324(2) Å; O1–Cd–O2B 90.12(5), O1–Cd–N1D 91.66(5), O1A–Cd–N1D 83.41(5)°. Symmetry operations A: $1-x$, $1-y$, $-z$; B: $2-x$, $1-y$, $-z$; C: $x-1$, y, z; D: $1-x$, $1-y$, $1-z$; E: x, y, $z-1$.

EXPERIMENTAL

Hydrothermal treatment of $Cd(ClO_4)_2{\cdot}6H_2O$ (1.0 mmol) and 3-(3-pyridyl)-3-aminopropionic acid (1 mmol) over 1 day at 140 °C gave colorless crystalline needles. The yield was about 35% based 3-(3-pyridyl)-3-aminopropionic acid. Intensity data were collected at 293(2) K on a Bruker AXS Smart CCD for a colorless block $0.1 \times 0.2 \times 0.3$ mm^3. $C_{16}H_{12}CdN_2O_4$, $M = 408.68$, triclinic, $P\bar{1}$, $a = 5.0270(4)$, $b = 8.1075(6)$, $c = 9.5250(7)$ Å, $\alpha = 69.442(1)$, $\beta = 80.550(1)$, $\gamma = 76.004(1)°$, $V = 351.35(5)$ Å^3, $Z = 1$, 2423 unique data ($\theta_{max} = 33.4°$), $R = 0.026$ (2418 [$I \geq 2\sigma(I)$] data), $wR = 0.065$ (all data).

Programs used: SAINT, SADABS, SHELX-97 and ORTEP. CCDC deposition number: 235636.

*Correspondence to: Ren-Gen Xiong, Coordination Chemistry Institute, The State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, People's Republic of China.
E-mail: xiongrg@netra.nju.edu.cn
Contract/grant sponsor: Distinguished Young Scholar Fund; Contract/grant number: 20225103.
Contract/grant sponsor: Specialized Research Fund for the Doctoral Program of Higher Education; Contract/grant number: 20030284001.

Acknowledgements

This work was supported by an award from the Distinguished Young Scholar Fund to R.-G. Xiong (no. 20225103) and by the Specialized Research Fund for the Doctoral Program of Higher Education (no. 20030284001).

REFERENCES

1. Xiong RG, Xue X, Zhao H, You XZ, Abrahams BF, Xue Z. *Angew. Chem. Int. Ed. Engl.* 2002; **41**: 3800.
2. Qu ZR, Zhao H, Wang YP, Wang XS, Ye Q, Li YH, Xiong RG, Abrahams BF, Liu ZG, You XZ. *Chem. Eur. J.* 2004; **10**: 53.

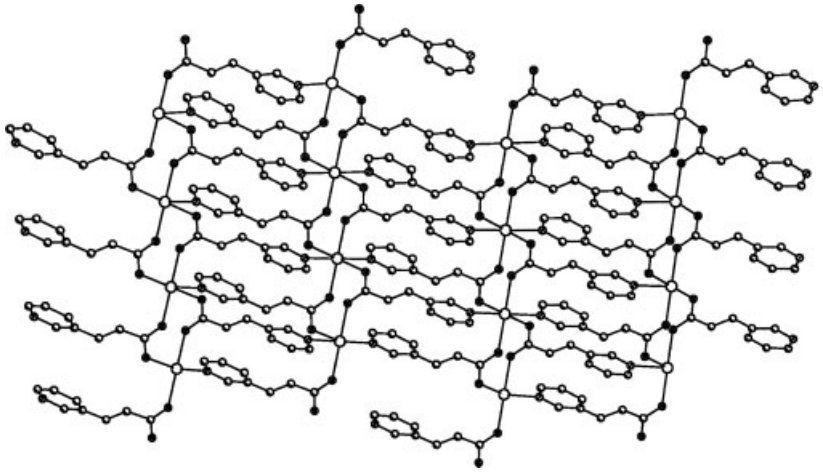

Figure 2. Two-dimensional layer structure of [bis(3-pyridylacrylato)cadmium(II)]$_n$; hydrogen atoms are omitted for clarity.