APPLIED ORGANOMETALLIC CHEMISTRY
Appl. Organometal. Chem. 2003; **17**: 249–250
Published online in Wiley InterScience (www.interscience.wiley.com). DOI:10.1002/aoc.419

Crystallographic report

Polymeric [bis(*N*,*N*-diethyldithiocarbamato)(*trans*-1,2-bis(4-pyridyl)ethylene)cadmium(II)]

Jishan Chai, Chian Sing Lai, Jiayi Yan and Edward R. T. Tiekink*

Department of Chemistry, National University of Singapore, Singapore 117543, Singapore

Received 19 December 2002; Revised 6 January 2003; Accepted 7 January 2003

The linear polymeric structure of $[Cd(S_2CNEt_2)_2(trans\text{-}NC_5H_4C(H)=C(H)C_5H_4N)]_\infty$ shows bidentate coordination by the dithiocarbamate ligands and a distorted octahedral geometry for cadmium, defined by a trans-N_2S_4 donor set. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; cadmium; dithiocarbamate; diimine adduct; polymer

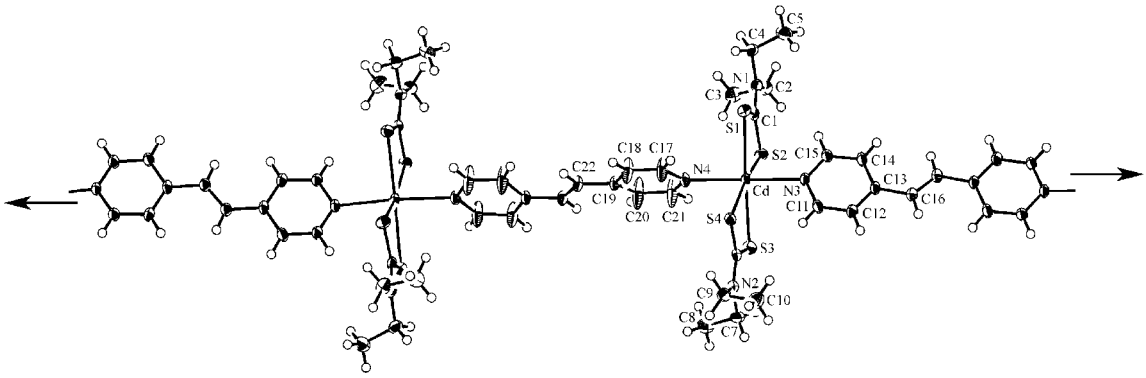

Figure 1. Polymeric structure of $[Cd(S_2CNEt_2)_2(trans\text{-}NC_5H_4C(H)=C(H)C_5H_4N)]_\infty$. Key geometric parameters: Cd–S(1) 2.6475(9), Cd–S(2) 2.6685(9), Cd–S(3) 2.6641(10), Cd–S(4) 2.6711(9), Cd–N(3) 2.420(3), Cd–N(4) 2.420(3), S(1)–C(1) 1.727(3), S(2)–C(1) 1.724(4), S(3)–C(6) 1.720(4), S(4)–C(6) 1.728(4), C(1)–N(1) 1.326(4), C(6)–N(2) 1.331(4) Å; S(1)–Cd–S(2) 68.05(3), S(1)–Cd–S(3) 166.83(3), S(1)–Cd–S(4) 125.37(3), S(1)–Cd–N(3) 91.07(7), S(1)–Cd–N(4) 88.91(7), S(2)–Cd–S(3) 98.83(3), S(2)–Cd–S(4) 166.46(3), S(2)–Cd–N(3) 91.63(7), S(2)–Cd–N(4) 92.76(7), S(3)–Cd–S(4) 67.71(3), S(3)–Cd–N(3) 90.47(7), S(3)–Cd–N(4) 90.63(7), S(4)–Cd–N(3) 89.96(7), S(4)–C–dN(4) 86.19(7), N(3)–Cd–N(4) 175.26(10)°.

COMMENT

Thus far, most diimine adducts of cadmium 1,1-dithiolates are mononuclear (e.g. see Ref. 1) with the exception being for the polymeric structure of $[Cd(S_2CO^iPr)_2(4,4'\text{-bipy})]_\infty$.[2] The structure of the title compound, $[Cd(S_2CNEt_2)_2(trans\text{-}NC_5H_4C(H)=C(H)C_5H_4N)]_\infty$ (Fig. 1), also forms a linear polymeric structure, propagated along the crystallographic *a*-axis, in which each diimine molecule is disposed about a crystallographic centre of inversion. The cadmium atom exists in an octahedral environment defined by a *trans*-N_2S_4 donor set.

EXPERIMENTAL

Yellow crystals were isolated from a 2/1 chloroform/toluene solution containing equimolar amounts of $Cd(S_2CNEt_2)_2$[3] and *trans*-$NC_5H_4C(H)=C(H)C_5H_4N$ (Aldrich); m.p. 198–200 °C. IR (KBr): ν(C–S) 987 and ν(C–N) 1422 and 1490 cm^{-1}. Intensity data were

*Correspondence to: Edward R. T. Tiekink, Department of Chemistry, National University of Singapore, Singapore 117543, Singapore.
E-mail: chmtert@nus.edu.sg
Contract/grant sponsor: National University of Singapore; Contract/grant number: R-143-000-151-112.

collected at 223 K on a Bruker AXS SMART CCD diffractometer for a yellow plate $0.03 \times 0.26 \times 0.34\ mm^3$. $C_{22}H_{30}CdN_4S_4$, $M = 591.14$, monoclinic, $C2/c$, $a = 21.0620(17)$, $b = 19.2248(17)$, $c = 15.1653(13)$ Å, $\beta = 122.439(2)^\circ$, $V = 5182.5(8)$ Å^3, $Z = 8$, 7585 unique data ($\theta_{max}30.1^\circ$), $R = 0.084$ (all data), $wR = 0.127$ (all data), $\rho_{max} = 1.38\ e^-$ Å^{-3} (near cadmium). Programs used: teXsan, DIRDIF, SHELXL, and ORTEP. CCDC deposition number: 200066.

Acknowledgements

The National University of Singapore is thanked for support (R-143-000-151-112).

REFERENCES

1. Guo T, Lai CS, Tan XJ, Teo CS, Tiekink ERT. *Acta Crystallogr. Sect. E* 2002; **58**: m439.
2. Abrahams BF, Hoskins BF, Winter G. *Aust. J. Chem.* 1990; **43**: 1759.
3. Dee CM, Tiekink ERT. *Z. Kristallogr.* 2002; **217**: 85.