Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(*N*-methylpyridinium) bis(2-thioxo-1,3-dithione-4,5-dithiolato)cadmate(II)

Yan-Ling Wang,[a]* Yong-Jin Wang,[b] Rui-He Wang,[a] Jun Yao[a] and Xiu-Tai Zhao[a]

[a]School of Petroleum Engineering, China University of Petroleum (East China), Dongying 257061, People's Republic of China, and [b]R&D Department, Qilu Antibiotics Pharmaceutical Co. Ltd, Jinan 250105, People's Republic of China

Correspondence e-mail: wangyl@hdpu.edu.cn

Received 11 December 2006
Accepted 19 December 2006

Key indicators

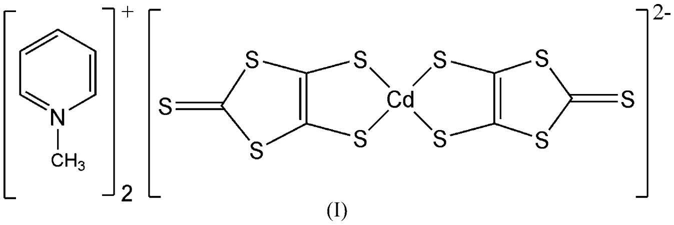
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.035
wR factor = 0.088
Data-to-parameter ratio = 21.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title complex, $(C_6H_8N)_2[Cd(C_3S_5)_2]$, the Cd^{II} ion is coordinated by four dmit (2-thioxo-1,3-dithione-4,5-dithiolate) S atoms in a distorted tetrahedral geometry. The *N*-methylpyridinium cations link with the Cd^{II} complex anion *via* weak C—H···S hydrogen bonding.

Comment

Metal complexes with 2-thioxo-1,3-dithio-4,5-dithiolate (dmit) have attracted much attention because of promising conductivity and optical properties (Steimeck & Kirmse, 1979; Li *et al.*, 1996; Xia *et al.*, 1997; Dai *et al.*, 2000; Sun *et al.*, 2001). Of these complexes, $[Cd(dmit)_2]^{2-}$ salts have been reported as promising organic optical materials (Zhai *et al.*, 1999). As part of an investigation on organometallic materials, the crystal structure of the title compound, (I), is presented here.



(I)

The asymmetric unit of (I) is shown in Fig. 1. The structure of the $[Cd(dmit)_2]^{2-}$ anion in (I) is similar to those reported previously for $[Cd(dmit)_2]^{2-}$ and $[Zn(dmit)_2]^{2-}$ (Wang *et al.*, 1985; Chohan *et al.*, 1997; Zhai *et al.*, 1999; Harrison *et al.*, 2000; Comerlato *et al.*, 2002; Wang *et al.*, 2005). The Cd^{II} ion is coordinated by four S atoms in a distorted tetrahedral geometry. The S—Cd—S bond angles, ranging from 90.19 (3) to 116.79 (3)°, are far from the typical tetrahedral angle. The two planar dmit ligands form a dihedral angle of 87.94 (4)°.

Weak C—H···S hydrogen bonding is observed between the Cd^{II} complex anion and *N*-methylpyridinium cations (Table 1).

Experimental

Compound (I) was prepared according to the literature procedure (Steimeck & Kirmse, 1979). Single crystals of (I) were obtained by evaporation of an acetone solution of (I) at room temperature.

Crystal data

$(C_6H_8N)_2[Cd(C_3S_5)_2]$
$M_r = 693.33$
Monoclinic, $P2_1/c$
$a = 14.4624$ (12) Å
$b = 13.5970$ (11) Å
$c = 14.1880$ (11) Å
$\beta = 109.369$ (1)°
$V = 2632.1$ (4) Å^3
$Z = 4$
$D_x = 1.750$ Mg m^{-3}
Mo *Kα* radiation
$\mu = 1.64$ mm^{-1}
$T = 293$ (2) K
Plate, purple–red
0.24 × 0.23 × 0.05 mm

doi:10.1107/S1600536806055346

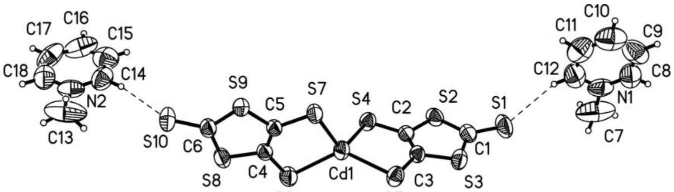


Figure 1
The molecular structure of (I) with 50% probability displacement ellipsoids (arbitrary spheres for H atoms). Dashed lines indicate the weak C—H···S hydrogen bonding.

Data collection

Bruker APEX2 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
$T_{\min} = 0.694$, $T_{\max} = 0.917$
13401 measured reflections
6032 independent reflections
4441 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.088$
$S = 1.01$
6032 reflections
282 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 1.0462P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.53$ e Å^{-3}
$\Delta\rho_{\min} = -0.40$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···S1	0.93	2.84	3.737 (6)	161
C14—H14···S10	0.93	2.74	3.650 (5)	167

Methyl H atoms were placed in calculated positions with C—H = 0.96 Å and torsion angles were refined to fit the electron density; $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C). Other H atoms were placed in calculated positions with C—H = 0.93 Å and refined in riding mode with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This work was sponsored by the Scientific Research Foundation for PhD, China University of Petroleum (East China).

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.

Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2005). *APEX2*. Version 2.0-2. Bruker AXS Inc., Madison, Wisconsin, USA.

Chohan, Z. H., Howie, R. A., Wardell, J. L., Wilkens, R. & Doidge-Harrison, S. M. S. V. (1997). *Polyhedron*, **16**, 2689–2696.

Comerlato, N. M., Harrison, W. T. A., Howie, R. A., Low, J. N., Silvino, A. C., Wardell, J. L. & Wardell, S. M. S. V. (2002). *Acta Cryst.* C**58**, m105–m108.

Dai, J., Bian, G. Q., Wang, X., Xu, Q. F., Zhou, M. Y., Munakata, M., Maekawa, M., Tong, M. H., Sun, Z. R. & Zeng, H. P. (2000). *J. Am. Chem. Soc.* **122**, 11007–11008.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Harrison, W. T. A., Howie, R. A., Wardell, J. L., Wardell, S. M. S. V., Comerlato, N. M., Costa, L. A. S., Silvino, A. C., de Oliveira, A. I. & Silva, R. M. (2000). *Polyhedron*, **19**, 821–827.

Li, H., Huang, C. H., Xu, J., Li, T., Zhao, X. & Xia, X. (1996). *J. Chem. Soc. Faraday Trans.* **92**, 2585–2592.

Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

Steimeck, G. & Kirmse, R. (1979). *Phosphorus Sulfur*, **7**, 49–55.

Sun, Z. R., Tong, M. H., Zeng, H. P., Ding, L. G., Wang, Z. G., Xu, Z. Z., Dai, J. & Bian, G. Q. (2001). *Chem. Phys. Lett.* **342**, 323–327.

Wang, H. H., Zhu, D. B., Zhu, N. J. & Fu, H. (1985). *Acta Phys. Chim. Sin.* **1**, 378–383.

Wang, Y.-L., Yu, W.-T., Xu, D., Wang, X.-Q., Guo, W.-F. & Zhang, G.-H. (2005). *Acta Cryst.* E**61**, m2408–m2410.

Xia, W. S., Huang, C. H. & Zhou, D. J. (1997). *Langmuir*, **13**, 80–84.

Zhai, J., Huang, C. H., Wei, T. X., Gan, L. B. & Cao, H. (1999). *Polyhedron*, **18**, 1513–1518.