Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[bis(μ-1-methyl-1,2,3,4-tetrazol-5-yl-thiolato)cadmium(II)]

Xiu-Ling Zhang,[a] Yue Qiu[a] and Seik Weng Ng[b]*

[a]Department of Chemistry, Dezhou University, Dezhou 253011, People's Republic of China, and [b]Department of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(N–C) = 0.005 Å
R factor = 0.029
wR factor = 0.078
Data-to-parameter ratio = 15.2

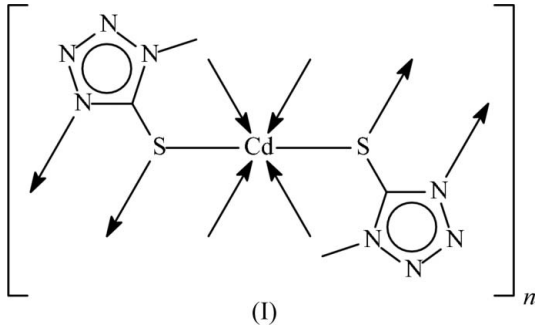
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 6 November 2006
Accepted 7 November 2006

The crystal structure of the title compound, $[Cd(C_2H_3N_4S)_2]_n$, consists of octahedrally coordinated Cd atoms that are linked by the anionic ligands into a layer structure. The Cd atom lies on a special position of site symmetry $\overline{1}$.

Comment

The crystal structures of only a few metal complexes of 1-substituted 1,2,3,4-tetrazol-5-thioles have been reported; the metals comprise gold (Ortner & Abram, 1999), palladium (Kim *et al.*, 2003, 2004, 2005) and platinum (Kim *et al.*, 2003) only. The title compound, (I), adopts a layer structure in which the monoanion binds covalently through the S atom, and datively through the N atom at the 4-position; the S atom also interacts with an adjacent formula unit to generate an octahedral environment about the metal atom, which lies on an inversion centre.



(I)

The synthesis of the compound was reported a long time ago (Agarwala *et al.*, 1967); the present study complements the ^{13}C NMR assignment reported earlier (Kahn & O'Brien, 1991).

Experimental

Cadmium dichloride (18 mg, 0.1 mmol), 5-mercapto-1-methyltetrazole (23 mg, 0.2 mmol) and water (12 m) were placed in a Teflon-lined stainless steel Parr bomb. The bomb was heated at 413 K for 48 h. The bomb was then cooled to room temperature over 36 h. Colourless crystals of (I)) were isolated in about 30% yield.

Crystal data

$[Cd(C_2H_3N_4S)_2]$
M_r = 342.69
Monoclinic, $P2_1/c$
a = 11.431 (2) Å
b = 5.395 (1) Å
c = 7.771 (2) Å
β = 92.00 (3)°
V = 478.95 (17) Å^3
Z = 2
D_x = 2.376 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.69 mm^{-1}
T = 295 (2) K
Block, colourless
0.16 × 0.14 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.353, T_{max} = 0.738
4300 measured reflections
1082 independent reflections
991 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.078
S = 1.09
1082 reflections
71 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0399P)^2 + 0.0392P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.92 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—N1^{i}	2.441 (2)	Cd1—S1^{iii}	2.6685 (8)
Cd1—N1^{ii}	2.441 (2)	Cd1—S1^{iv}	2.6612 (9)
Cd1—S1	2.6612 (9)	Cd1—S1^{v}	2.6685 (8)

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+1, -y+1, -z+1$; (v) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

H atoms were positioned geometrically, with C—H = 0.96 Å, and were included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.5U_{eq}(C). The methyl group was rotated to fit the electron density.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2006).

The authors thank Dezhou University and the University of Malaya for supporting this study.

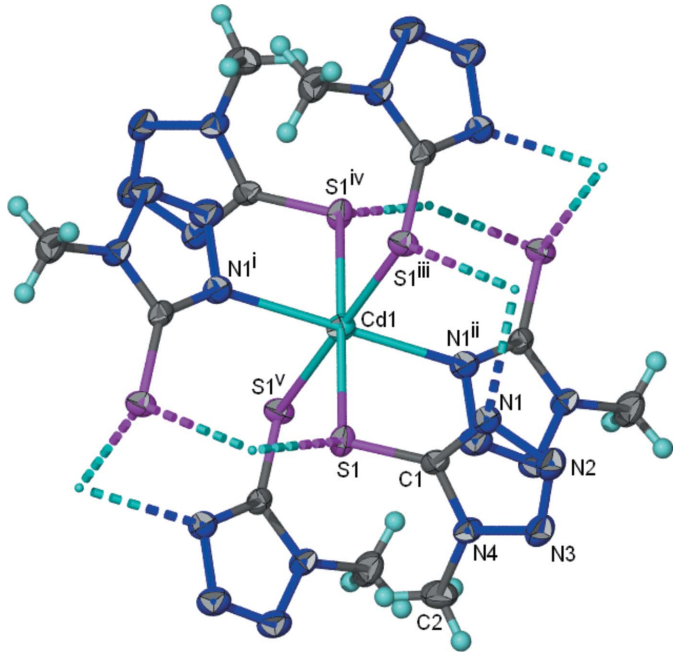


Figure 1
Displacement ellipsoid plot (70% probability) of a fragment of the layer structure of (I). H atoms are drawn as spheres of arbitrary radii. Symmetry codes are as given in Table 1. Dashed lines indicate the bridging Cd—N and Cd—S bonds.

References

Agarwala, U., Narayan, V. A. & Dikshit, S. K. (1967). *Can. J. Chem.* **45**, 1057–1062.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Kahn, O. F. Z. & O'Brien, P. (1991). *Polyhedron*, **10**, 325–332.
Kim, Y.-J., Chang, X.-H., Han, J.-T., Lim, M. S. & Lee, S. W. (2004). *Dalton Trans.* pp. 3699–3708.
Kim, Y.-J., Han, J.-T., Kang, S., Han, W. S. & Lee, S. W. (2003). *Dalton Trans.* pp. 3357–3364.
Kim, Y.-J., Lee, S.-H., Lee, S.-H., Jeon, S.-I., Lim, M. S. & Lee, S. W. (2005). *Inorg. Chim. Acta*, **35**, 650–658.
Ortner, K. & Abram, U. (1999). *Polyhedron*, **18**, 749–754.
Rigaku (2004). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2004). *CrystalStructure*. Rigaku/MSC Inc. The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Westrip, S. P. (2006). *publCIF*. In preparation.