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Bis(tetraethylammonium) bis(2-thioxo-1,3-dithiole-4,5-dithiolato)cadmium(II)

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Key indicators

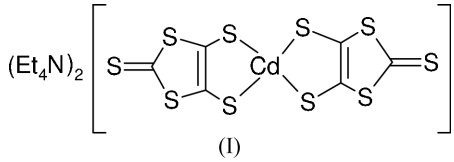
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.038
wR factor = 0.095
Data-to-parameter ratio = 19.0

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

The title complex, $(C_8H_{20}N)_2[Cd(C_3S_5)_2]$, has the Cd atom in a distorted tetrahedral geometry, due to the relatively small bite angles, 88.61 (4)–88.78 (4)°, of the 2-thioxo-1,3-dithiole-4,5-dithiolate ligands.

Comment

Many 4,5-dimercapto-1,3-dithiol-2-thione (H_2dmit) derivatives have been extensively studied as heterocyclic compounds, coordination compounds, precursors of tetrathiafulvalene derivatives and organic conductors. We are interested in the third-order non-linear optical properties of $dmit^{2-}$ coordination complexes and report here the structure of the new complex $(Et_4N)_2[Cd(dmit)_2]$, (I).



(I)

In (I), there are two sets of $[Cd(dmit)_2]^{2-}$ anions, approximately orthogonal to one another and running along diagonals of the *ab* plane, with the cations occupying the voids created by this packing arrangement. The structure of the $[Cd(dmit)_2]^{2-}$ anion is the same as reported in $(Bu_4N)_2[Cd(dmit)_2]$ (Zhai *et al.*, 1999), the cadmium ion being coordinated by four S atoms with a distorted tetrahedral configuration.

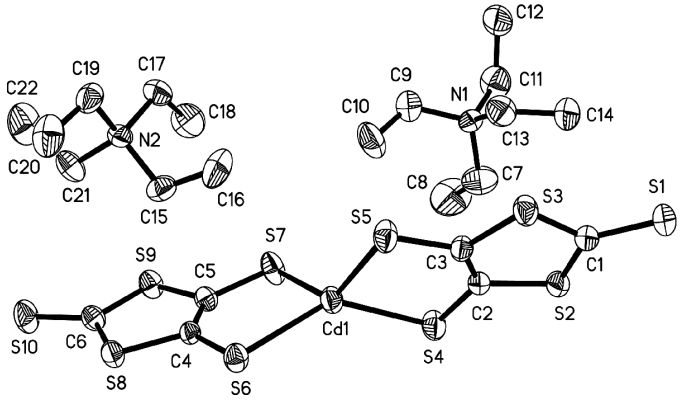


Figure 1
The components of the title complex salts, showing the atom-labelling scheme and ellipsoids plotted at the 30% probability level.

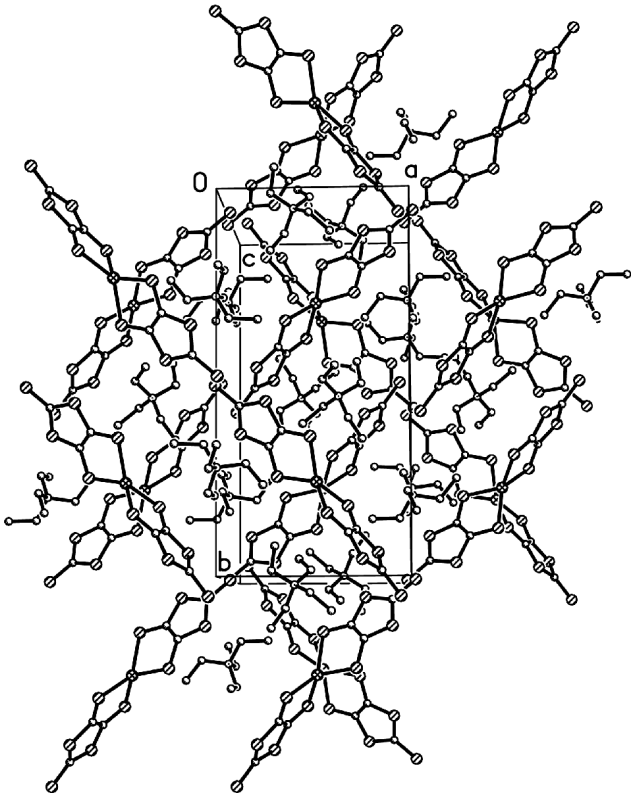


Figure 2
The unit cell of the title compound viewed along the *c* axis.

Experimental

Compound (I) was synthesized according to the procedure of Steimeck & Kirmse (1979) and recrystallized from acetone to give block-shaped single crystals.

Crystal data

$(C_8H_{20}N)[Cd(C_3S_5)_2]$
M_r = 765.56
Monoclinic, $P2_1/c$
a = 9.9739 (14) Å
b = 20.116 (2) Å
c = 17.033 (4) Å
β = 90.860 (16)°
V = 3417 (1) Å^3
Z = 4
D_x = 1.488 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 35 reflections
θ = 5.3–12.5°
μ = 1.27 mm^{-1}
T = 293 (2) K
Block, dark red
0.42 × 0.40 × 0.38 mm

Data collection

Bruker *P*4 diffractometer
ω scans
Absorption correction: multi-scan (*XSCANS*; Bruker, 1996)
T_{min} = 0.573, T_{max} = 0.620
7577 measured reflections
6020 independent reflections
4621 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 25.0°
$h = -11 \rightarrow 1$
$k = -23 \rightarrow 1$
$l = -20 \rightarrow 20$
3 standard reflections
every 97 reflections
intensity decay: 0.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.095
S = 1.02
6017 reflections
317 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0398P)^2 + 3.2613P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.83 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0063 (3)

Table 1
Selected geometric parameters (Å, °).

C1—S1	1.649 (4)	C4—S8	1.753 (4)
C1—S3	1.711 (4)	C5—S7	1.737 (4)
C1—S2	1.718 (4)	C5—S9	1.743 (4)
C2—C3	1.349 (5)	C6—S10	1.658 (4)
C2—S4	1.736 (4)	C6—S9	1.708 (4)
C2—S2	1.753 (4)	C6—S8	1.715 (4)
C3—S5	1.737 (4)	S4—Cd1	2.5293 (12)
C3—S3	1.750 (4)	S5—Cd1	2.5189 (12)
C4—C5	1.356 (5)	S6—Cd1	2.5330 (11)
C4—S6	1.739 (4)	S7—Cd1	2.5162 (13)
S1—C1—S3	123.9 (3)	S10—C6—S8	124.5 (3)
S1—C1—S2	124.6 (3)	S9—C6—S8	112.2 (2)
S3—C1—S2	111.5 (2)	C1—S2—C2	99.07 (19)
C3—C2—S4	128.5 (3)	C1—S3—C3	99.28 (19)
C3—C2—S2	115.0 (3)	C2—S4—Cd1	96.70 (13)
S4—C2—S2	116.5 (2)	C3—S5—Cd1	96.57 (13)
C2—C3—S5	129.4 (3)	C4—S6—Cd1	96.74 (13)
C2—C3—S3	115.1 (3)	C5—S7—Cd1	97.19 (14)
S5—C3—S3	115.5 (2)	C6—S8—C4	98.68 (19)
C5—C4—S6	128.6 (3)	C6—S9—C5	98.9 (2)
C5—C4—S8	114.8 (3)	S7—Cd1—S5	131.48 (5)
S6—C4—S8	116.6 (2)	S7—Cd1—S4	105.67 (4)
C4—C5—S7	128.7 (3)	S5—Cd1—S4	88.78 (4)
C4—C5—S9	115.5 (3)	S7—Cd1—S6	88.61 (4)
S7—C5—S9	115.8 (2)	S5—Cd1—S6	111.09 (4)
S10—C6—S9	123.4 (3)	S4—Cd1—S6	138.13 (4)
S4—C2—C3—S5	0.4 (6)	C4—C5—S7—Cd1	−2.4 (4)
S2—C2—C3—S5	−178.5 (2)	S9—C5—S7—Cd1	175.18 (19)
S4—C2—C3—S3	177.6 (2)	S10—C6—S8—C4	−176.6 (3)
S2—C2—C3—S3	−1.3 (4)	S9—C6—S8—C4	1.7 (3)
S6—C4—C5—S7	−0.8 (6)	C5—C4—S8—C6	−0.6 (3)
S8—C4—C5—S7	176.9 (2)	S6—C4—S8—C6	177.3 (2)
S6—C4—C5—S9	−178.4 (2)	S10—C6—S9—C5	176.3 (3)
S8—C4—C5—S9	−0.7 (4)	S8—C6—S9—C5	−2.0 (3)
S1—C1—S2—C2	178.7 (3)	C4—C5—S9—C6	1.7 (3)
S3—C1—S2—C2	−1.7 (3)	S7—C5—S9—C6	−176.2 (2)
C3—C2—S2—C1	1.9 (4)	C5—S7—Cd1—S5	−114.31 (14)
S4—C2—S2—C1	−177.1 (2)	C5—S7—Cd1—S4	143.07 (14)
S1—C1—S3—C3	−179.3 (3)	C5—S7—Cd1—S6	3.00 (14)
S2—C1—S3—C3	1.2 (3)	C3—S5—Cd1—S7	−107.34 (14)
C2—C3—S3—C1	0.1 (4)	C3—S5—Cd1—S4	2.64 (14)
S5—C3—S3—C1	177.7 (2)	C3—S5—Cd1—S6	144.83 (14)
C3—C2—S4—Cd1	2.1 (4)	C2—S4—Cd1—S7	130.47 (14)
S2—C2—S4—Cd1	−179.0 (2)	C2—S4—Cd1—S5	−2.54 (14)
C2—C3—S5—Cd1	−2.6 (4)	C2—S4—Cd1—S6	−123.56 (14)
S3—C3—S5—Cd1	−179.8 (2)	C4—S6—Cd1—S7	−3.24 (13)
C5—C4—S6—Cd1	3.3 (4)	C4—S6—Cd1—S5	131.25 (13)
S8—C4—S6—Cd1	−174.26 (18)	C4—S6—Cd1—S4	−115.43 (13)

H atoms were geometrically positioned (C—H = 0.96–0.97Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$. Three reflections were omitted from the final refinement.

Data collection: *XSCANS* (Bruker, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXTL* (Bruker, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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