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Bis[μ-*N*,*N*-bis(2-hydroxyethyl)dithiocarbamato]-1:2κ^3*S*,*S*′:*S*′;2:1κ^3*S*,*S*′:*S*′-bis{[*N*,*N*-bis(2-hydroxyethyl)dithiocarbamato-κ^2*S*,*S*′]cadmium(**II**)}

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Key indicators

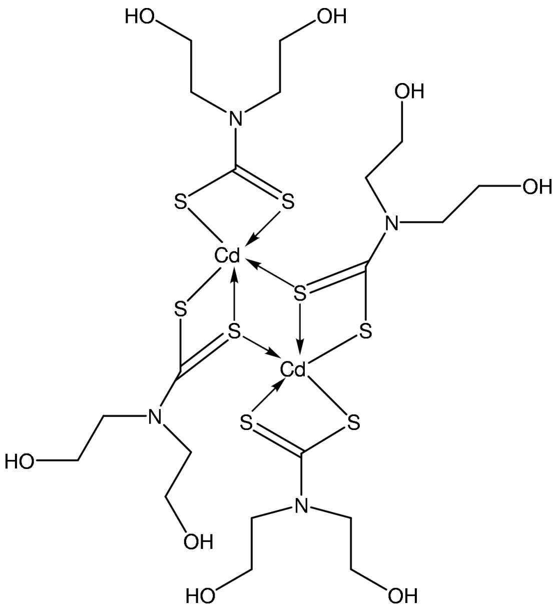
Single-crystal X-ray study
T = 223 K
Mean σ(C–C) = 0.005 Å
R factor = 0.041
wR factor = 0.100
Data-to-parameter ratio = 25.3

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

The dinuclear title compound, $[Cd_2(C_5H_{10}NO_2S_2)_4]$, is disposed about a centre of inversion and features both bidentate bridging and chelating dithiocarbamate ligands. A three-dimensional network structure arises as a result of substantial hydrogen-bonding interactions.

Comment

Monomeric, dimeric, cyclotetrameric, polymeric, two-dimensional and three-dimensional structures are all featured amongst the zinc-triad 1,1-dithiolates (Tiekink, 2002). The challenge is to rationalize the fascinating structural diversity and some progress has been made to achieve that aim (*e.g.* Cox & Tiekink, 1999; Lai *et al.*, 2002; Tiekink, 2003; Lai *et al.*, 2004). The structure of the title compound, (I), a known species (Pages *et al.*, 1985; Marino *et al.*, 1999), has been examined in this context and found to adopt the common structural type found for compounds of the general formula $[Cd(S_2CNR_2)_2]_2$ (Tiekink, 2003). Thus, the centrosymmetric molecule (Fig. 1 and Table 1) features a tridentate dithiocarbamate ligand that chelates one Cd atom and simultaneously bridges to the centrosymmetrically related partner. The two remaining dithiocarbamate ligands are chelating.



(I)

The coordination geometry about the Cd atom is defined by five S atoms, which define an environment intermediate between square pyramidal and trigonal bipyramidal, with a leaning to the former description. This, again, is consistent

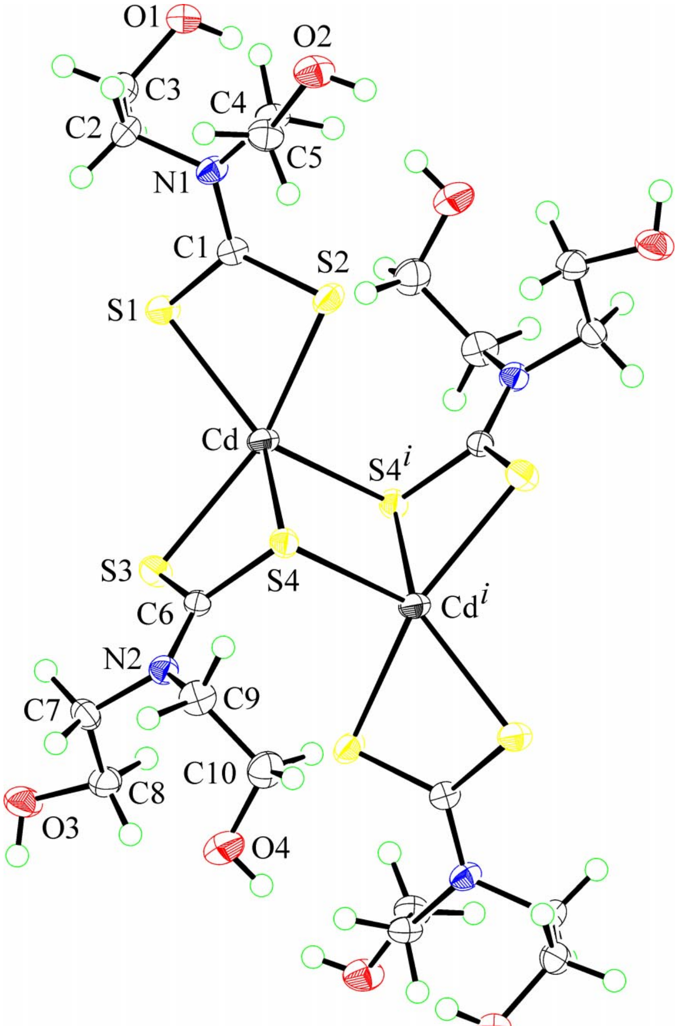


Figure 1
The molecular structure and crystallographic numbering scheme for (I). The molecule is disposed about a centre of inversion [symmetry code: (i) $-x$, $-y$, $-z$]. Displacement ellipsoids are shown at the 50% probability level (Johnson, 1976).

with the literature precedents (Tiekink, 2003). The interesting feature of this structure is the presence of hydrogen bonding between molecules, owing to the presence of hydrogen-bonding functionality in the N-bound residues.

A view of the unit-cell contents is shown in Fig. 2. The structure can be thought of as being comprised of layers held together primarily by O—H···O interactions in the *ab* plane; see Table 2 for geometric parameters describing the hydrogen-bonding interactions. Successive layers stack parallel to the *c* direction, held together by O—H···O interactions.

Experimental

$CdCl_2$ (0.046 g, 0.25 mmol) was added to a solution of $NH(CH_2CH_2OH)_2$ (0.105 g, 1 mmol) and CS_2 (0.091 g, 1.2 mmol) in methanol (15 ml). The mixture was stirred for 2 h at room temperature and the precipitate was filtered off. Colourless crystals were obtained from the slow evaporation of the filtrate [m.p. 428–430 K (decomposition); *cf*. literature 426 K (decomposition) (Marino *et al.*, 1999)].

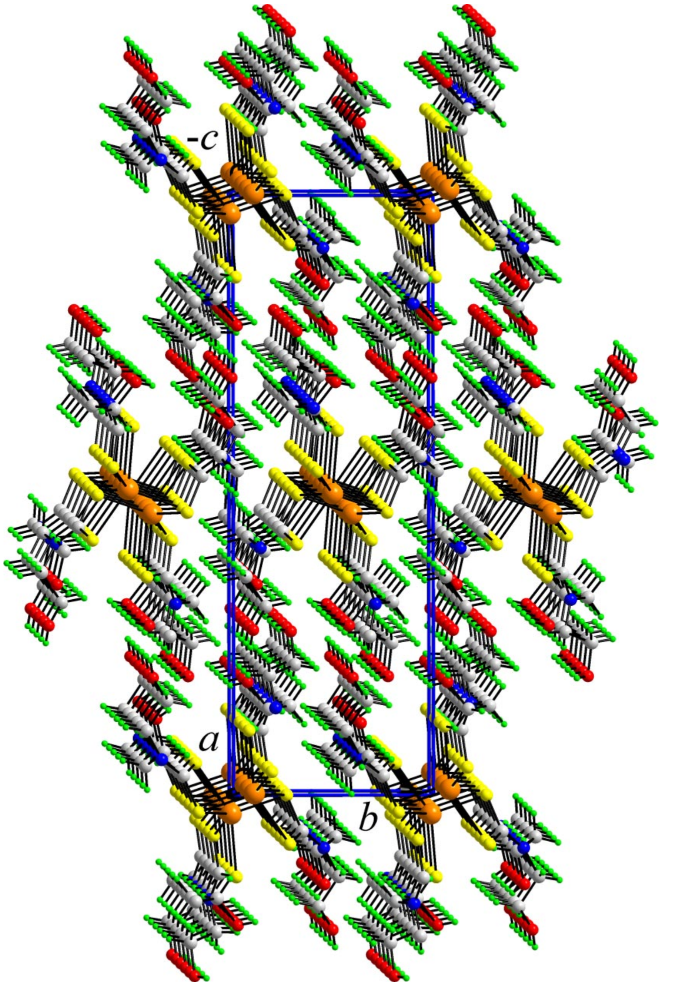


Figure 2
A view of the unit-cell contents (*DIAMOND*; Crystal Impact, 2002). Colour codes: Cd orange, S yellow, O red, N blue, C grey and H green.

Crystal data

$[Cd_2(C_5H_{10}NO_2S_2)_4]$
M_r = 945.84
Monoclinic, $P2_1/c$
a = 8.1588 (10) Å
b = 8.3040 (10) Å
c = 25.008 (3) Å
β = 93.956 (2)°
V = 1690.3 (4) Å^3
Z = 2

D_x = 1.858 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 946 reflections
θ = 2.6–29.9°
μ = 1.80 mm^{-1}
T = 223 (2) K
Plate, colourless
0.34 × 0.23 × 0.07 mm

Data collection

Bruker AXS SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\rm min}$ = 0.630, $T_{\rm max}$ = 0.882
13 581 measured reflections

4909 independent reflections
4665 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.029
$\theta_{\rm max}$ = 30.0°
$h = -11 \rightarrow 10$
$k = -9 \rightarrow 11$
$l = -33 \rightarrow 34$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.100
S = 1.33
4909 reflections
194 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0385P)^2 + 1.1441P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max}$ = 0.52 e Å^{-3}
$\Delta\rho_{\rm min}$ = −1.13 e Å^{-3}

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Table 1
Selected geometric parameters (Å, °).

Cd—S1	2.5673 (8)	S2—C1	1.720 (3)
Cd—S2	2.6389 (9)	S3—C6	1.712 (3)
Cd—S3	2.5915 (8)	S4—C6	1.756 (3)
Cd—S4	2.8021 (9)	N1—C1	1.334 (4)
Cd—S4^{i}	2.5892 (8)	N2—C6	1.330 (4)
S1—C1	1.730 (3)		
S1—Cd—S2	69.73 (2)	Cd—S2—C1	84.15 (10)
S1—Cd—S3	103.44 (3)	Cd—S3—C6	91.01 (10)
S1—Cd—S4	130.58 (3)	Cd—S4—C6	83.40 (10)
S1—Cd—S4^{i}	131.35 (3)	Cd^{i}—S4—C6	100.52 (9)
S2—Cd—S3	149.42 (3)	Cd—S4—Cd^{i}	82.64 (2)
S2—Cd—S4	94.24 (2)	S1—C1—S2	119.25 (16)
S2—Cd—S4^{i}	103.45 (2)	S1—C1—N1	119.9 (2)
S3—Cd—S4	66.99 (2)	S2—C1—N1	120.9 (2)
S3—Cd—S4^{i}	102.79 (3)	S3—C6—S4	118.58 (16)
S4—Cd—S4^{i}	97.36 (2)	S3—C6—N2	121.1 (2)
Cd—S1—C1	86.20 (10)	S4—C6—N2	120.3 (2)

Symmetry code: (i) $-x, -y, -z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{ii}	0.83	1.95	2.732 (4)	158
O2—H2···O3^{iii}	0.83	1.85	2.677 (4)	173
O3—H3···O1^{iv}	0.83	1.86	2.676 (3)	169
O4—H4···O2^{iv}	0.83	2.16	2.964 (4)	162

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

The C- and O-bound H atoms were included in the riding-model approximation, with C—H = 0.98 Å and O—H = 0.84 Å, and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C) and $1.5U_{\rm eq}$(O). The deepest hole in the final difference map was 0.06 Å from the Cd atom.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *PATTY* in *DIRDIF*92 (Beurskens *et al.*, 1992); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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