catena-Poly[[bis(*μ*-3-dimethylamino-*N*-salicylidenepropylamine)isothiocyanato-dicadmium(II)]-*μ*-isothiocyanato]

Wen-Xuan Cai, Qi-Wei Zhang, Hong Su and Yun-Long Feng*

Zhejiang Key Laboratory for Reactive Chemistry on Solid Surfaces, Institute of Physical Chemistry, Zhejiang Normal University, Jinhua, Zhejiang 321004, People's Republic of China

Correspondence e-mail: sky37@zjun.cn

The deprotonated 3-dimethylamino-*N*-salicylidenepropylamine Schiff base chelates to a Cd atom in the polymeric title compound with a dinuclear building block, $[Cd_2(NCS)_2(C_{12}H_{17}N_2O)_2]_n$. The O atom of the Schiff base also engages in bridging. The bridging NCS group links adjacent dinuclear entities into a helical chain that runs along the *b* axis of the monoclinic unit cell.

Comment

The deprotonated *N*-(salicylidene)-3-dimethylaminopropylamine Schiff base chelates to copper in the isothiocyanate complex, which exists as a centrosymmetric dinuclear compound having Cu in a square-pyramidal geometry (Lin & Feng, 2005). We present here the crystal structure of the analogous polymeric title compound with a dinuclear building block, (I), with Cd as the metal atom.

(I)
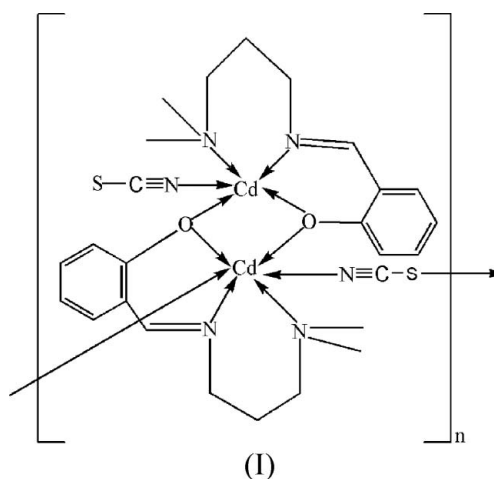
In compound (I), the deprotonated *N*-(salicylidene)-3-(dimethylamino)propylamine Schiff bases are each *O,N,N'*-chelated to a Cd atom (Fig. 1). The O atoms of the Schiff bases also engage in bridging. The set of two O and two N atoms comprises an approximate square around the Cd atom, above which lies the NCS group. For one Cd site, the geometry isoctahedral, as the NCS group behaves as a bridge [Cd—N = 2.310 (3) and Cd—S = 2.8165 (8) Å], the bridging linking adjacent dinuclear entities into a helical chain that runs along the *b* axis of the monoclinic unit cell (Fig. 2). For the other Cd site, the geometry is square pyramidal, with the N atom of the NCS group at the apical site. However, the geometry is distorted towards octahedral, owing to the proximity of the S atom that is involved in bridging [Cd—N = 2.219 (3) and Cd···S = 3.2814 (10) Å].
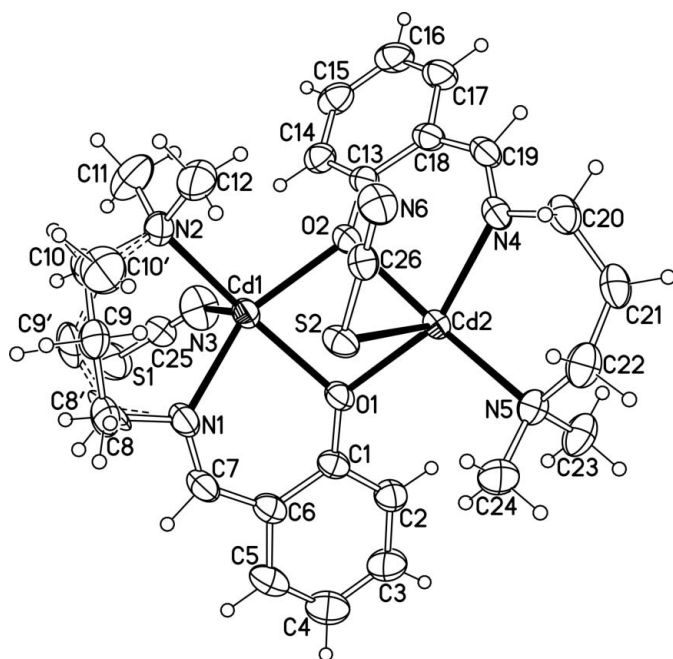
Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. The minor component of the disordered trimethylene linkage is shown with dashed bonds. [Symmetry code (i): $\frac{3}{2} - x, y - \frac{1}{2}, \frac{3}{2} - z$.]
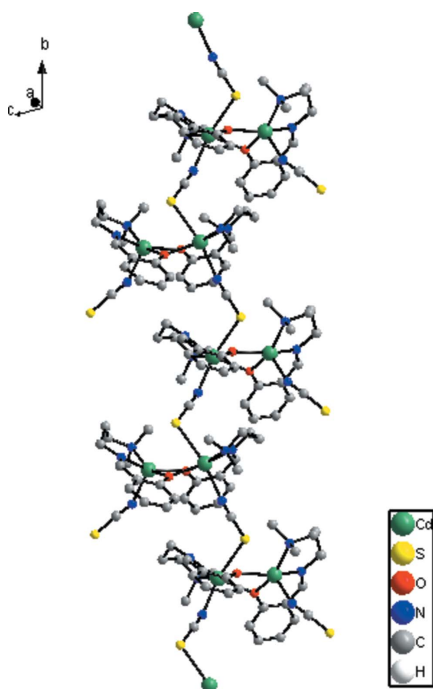

Figure 2
The helical chain structure of (I). H atoms have been omitted

Experimental

The Schiff base ligand N-(salicylidene)-3-dimethylaminopropylamine was prepared by refluxing 3-dimethylamino-1-propylamine (0.125 ml, 1.0 mmol) and salicyladehyde (0.105 ml, 1.0 mmol) in ethanol (10 ml)

for 30 min. $Cd(CH_3COO)_2 \cdot 2H_2O$ (0.267 g, 1.0 mmol) was then added dropwise. A yellow mixture was obtained by refluxing for about an hour, and this was cooled to room temperature and filtered. Yellow crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of the yellow filtrate in air (yield 47%).

Crystal data

$[Cd_2(NCS)_2(C_{12}H_{17}N_2O)_2]$	$Z = 4$
$M_r = 751.55$	$D_x = 1.624$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 14.9782$ (15) Å	$\mu = 1.55$ mm^{-1}
$b = 12.7398$ (13) Å	$T = 273$ (2) K
$c = 21.7317$ (15) Å	Prism, yellow
$\beta = 132.148$ (4)°	$0.40 \times 0.38 \times 0.20$ mm
$V = 3074.5$ (5) Å^3	

Data collection

Bruker APEX-II area-detector diffractometer	20224 measured reflections
φ and ω scans	7274 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	5081 reflections with $I > 2\sigma(I)$
$T_{min} = 0.543$, $T_{max} = 0.733$	$R_{int} = 0.021$
	$\theta_{max} = 27.9°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 0.5071P]$
$R[F^2 > 2\sigma(F^2)] = 0.028$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.075$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.06$	$\Delta\rho_{max} = 0.95$ e Å^{-3}
7274 reflections	$\Delta\rho_{min} = -0.78$ e Å^{-3}
374 parameters	
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

Cd1—N3	2.219 (3)	Cd2—O1	2.2586 (17)
Cd1—O2	2.2420 (18)	Cd2—O2	2.2759 (19)
Cd1—O1	2.2446 (19)	Cd2—N4	2.287 (2)
Cd1—N1	2.286 (2)	Cd2—N6^i	2.310 (3)
Cd1—N2	2.344 (2)	Cd2—N5	2.352 (2)
Cd1···Cd2	3.4302 (4)	Cd2—S2	2.8165 (8)

Symmetry code: (i) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$.

H atoms were positioned geometrically (C—H = 0.93–0.97 Å), and were included in the refinement in the riding-model approximation, with U_{iso}(H) restrained to 1.2–1.5 times U_{eq}(C). The methyl groups were rotated to fit the electron density. One of the trimethylene linkages is disordered over two positions and the site occupancy factors refined to 0.61 (1):0.39 (1). The pairs of bond distances (N1–C8/N1–C8′, C8–C9/C8′–C9′, C9–C10/C9′–C10′ and C10–N2/C10′–N2) were restrained to within 0.01 Å of each other.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

metal-organic papers

References

Bruker (2004). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.

Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Lin, H. & Feng, Y.-L. (2005). *Chin. J. Struct. Chem.* **24**, 346–348.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.