

catena-Poly[[aqua(1*H*-imidazole- κ *N*)cadmium(II)]- μ -thiodiacetato- κ^4 O,*S*,O':O'']

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Key indicators

Single-crystal X-ray study
 T = 295 K
 Mean σ (C–C) = 0.004 Å
 R factor = 0.019
 wR factor = 0.046
 Data-to-parameter ratio = 16.5

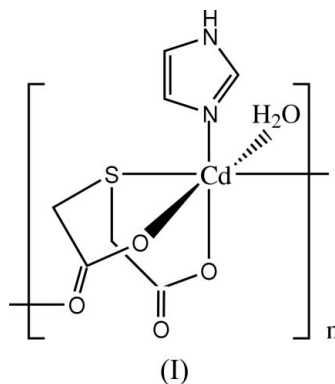
For details of how these key indicators were
 automatically derived from the article, see
<http://journals.iucr.org/e>.

In the title complex, $[\text{Cd}(\text{C}_4\text{H}_4\text{O}_4\text{S})(\text{C}_3\text{H}_4\text{N}_2)(\text{H}_2\text{O})]_n$, the Cd^{II} atom is surrounded by one imidazole ligand, one water molecule and two thiodiacetate dianions in a distorted octahedral CdNO_4S coordination. Each thiodiacetate dianion coordinates to two independent Cd atoms, one as a tridentate chelate, the other in a monodentate fashion through a carboxylate O atom. The thiodiacetate dianions bridge neighbouring Cd^{II} atoms, forming zigzag polymeric chains.

Received 11 November 2005
 Accepted 15 November 2005
 Online 23 November 2005

Comment

Non-covalent interactions are fundamental to interpreting and predicting relationships between chemical structure and function. As part of our ongoing investigations into such interactions in metal complexes, the title Cd^{II} compound incorporating an imidazole ligand, (I), has been prepared and its X-ray crystal structure is presented here.



The Cd^{II} atom is coordinated by one imidazole ligand, one water molecule, and two thiodiacetate dianions (TDA) related by a twofold screw axis (Fig. 1). Each TDA coordinates to two independent Cd atoms, one in a tridentate chelating mode through the thioether donor atom and the O atoms of two terminal carboxylate groups, the other in a monodentate fashion, through a terminal carboxylate O atom. The chelating TDA displays a facial configuration, a feature commonly found in metal-TDA complexes (Baggio *et al.*, 1999; Pan *et al.*, 2005); the two five-membered rings are nearly perpendicular to each other, the dihedral angle being $87.65(6)^\circ$. The TDA dianions also act as bridging ligands in (I). Neighbouring Cd^{II} atoms, related by a twofold axis, are bridged by TDA, forming zigzag polymeric chains along the *c* axis (Fig. 2). Both coordinated and uncoordinated O atoms of the same carboxylate groups are hydrogen-bonded to the imidazole ligands of neighbouring polymeric chains (Fig. 2). The crystal structure is also stabilized by hydrogen bonding-interactions between

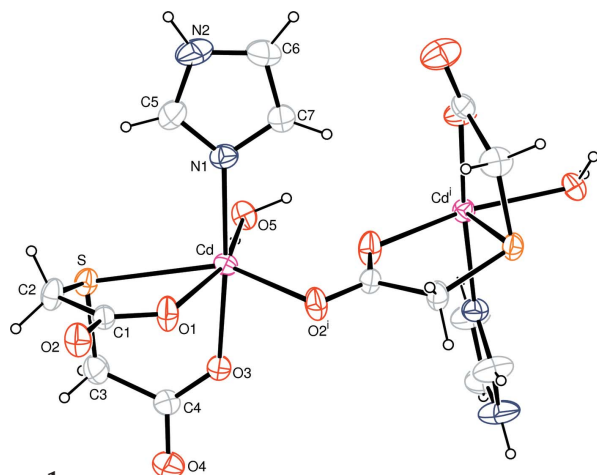


Figure 1
The molecular structure of (I), with 40% probability displacement ellipsoids [symmetry code: (i) $1 - x, 1 - y, z - \frac{1}{2}$].

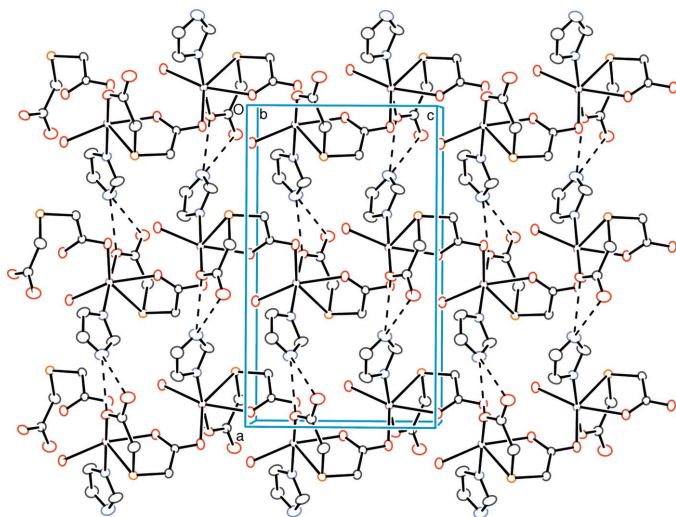


Figure 2
The packing of (I), viewed along the crystallographic *b* axis, showing the N—H...O hydrogen bonds (dashed lines) between neighbouring zigzag polymeric chains.

water molecules and the carboxylate O atoms of TDA dianions (Table 2).

Experimental

$\text{Cd}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ (0.62 g, 2 mmol), Na_2CO_3 (0.21 g, 2 mmol) and H_2TDA (0.30 g, 2 mmol) were dissolved in a water/ethanol solution (20 ml, 1:3) and imidazole (0.13 g, 2 mmol) added. The mixture was refluxed for 4 h, and filtered after cooling to room temperature. Colorless single crystals of (I) were obtained after 2 weeks.

Crystal data

$[\text{Cd}(\text{C}_4\text{H}_4\text{O}_4\text{S})(\text{C}_3\text{H}_4\text{N}_2)(\text{H}_2\text{O})]$
 $M_r = 346.63$
 Orthorhombic, $Pca2_1$
 $a = 14.928$ (5) Å
 $b = 8.326$ (3) Å
 $c = 8.830$ (3) Å
 $V = 1097.5$ (7) Å³
 $Z = 4$
 $D_x = 2.098$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 10095 reflections
 $\theta = 3.4$ – 27.5°
 $\mu = 2.19$ mm⁻¹
 $T = 295$ (3) K
 Needle, colorless
 $0.26 \times 0.11 \times 0.08$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.554$, $T_{\max} = 0.821$
 10262 measured reflections

2388 independent reflections
 2329 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$
 $\theta_{\max} = 27.5^\circ$
 $h = -19 \rightarrow 19$
 $k = -10 \rightarrow 10$
 $l = -10 \rightarrow 11$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.019$
 $wR(F^2) = 0.046$
 $S = 1.06$
 2388 reflections
 145 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2 + 0.1379P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.38$ e Å⁻³
 $\Delta\rho_{\min} = -0.71$ e Å⁻³
 Absolute structure: Flack (1983), 1050 Friedel Pairs
 Flack parameter: -0.02 (2)

Table 1

Selected geometric parameters (Å, °).

| | | | |
|------------------------|-------------|-----------------------|-------------|
| Cd—O1 | 2.354 (2) | Cd—O5 | 2.3161 (18) |
| Cd—O2 ⁱ | 2.2950 (17) | Cd—N1 | 2.251 (2) |
| Cd—O3 | 2.2433 (19) | Cd—S | 2.8258 (8) |
| O1—Cd—O3 | 87.20 (9) | O5—Cd—N1 | 87.21 (10) |
| O1—Cd—O5 | 160.85 (7) | O1—Cd—S | 71.63 (5) |
| O2 ⁱ —Cd—O1 | 77.52 (15) | O2 ⁱ —Cd—S | 145.57 (12) |
| O2 ⁱ —Cd—O5 | 121.42 (15) | O3—Cd—S | 74.41 (5) |
| O3—Cd—O2 ⁱ | 89.39 (7) | O5—Cd—S | 89.37 (5) |
| O3—Cd—O5 | 90.02 (8) | N1—Cd—O2 ⁱ | 96.02 (8) |
| O1—Cd—N1 | 93.89 (11) | S—Cd—N1 | 100.89 (7) |
| O3—Cd—N1 | 174.58 (7) | | |

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

Table 2

Hydrogen-bond geometry (Å, °).

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|----------------------------|-------------|---------------|-----------------------|-------------------------|
| N2—H2...O3 ⁱⁱ | 0.86 | 2.02 | 2.856 (3) | 165 |
| N2—H2...O4 ⁱⁱⁱ | 0.86 | 2.58 | 3.276 (4) | 138 |
| O5—H5A...O4 ⁱⁱⁱ | 0.83 | 1.91 | 2.695 (3) | 157 |
| O5—H5B...O2 ^{iv} | 0.93 | 1.85 | 2.776 (5) | 174 |

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

H atoms of water molecules were located in a difference Fourier map and refined as riding in their as-found relative positions, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$. Other H atoms were placed in calculated positions, with C—H = 0.97 (methylene) or 0.93 Å (aromatic) and N—H = 0.86 Å, and were included in the final cycles of refinement in riding mode with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$ of the carrier atoms.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The project was supported by the National Natural Science Foundation of China (grant No. 20443003).

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