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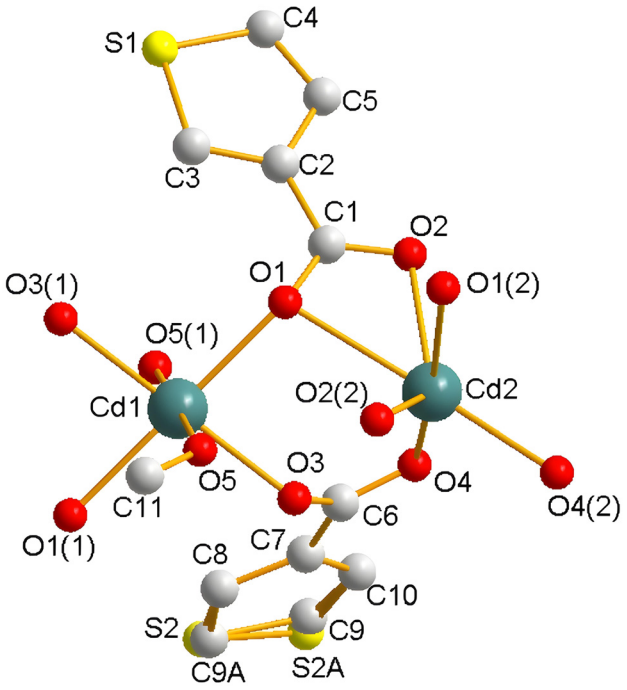
Crystal structure of poly(3-thiophenecarboxylato-$\kappa^3O,O':O'$)-(methanol-κO)cadmium(II), $C_{11}H_{10}O_5S_2Cd$



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Abstract

$C_{11}H_{10}O_5S_2Cd$, monoclinic, $C2/c$ (no. 15), a = 18.303(5) Å, b = 10.806(3) Å, c = 13.859(4) Å, β = 95.074(4)°, V = 2730.4(14) Å^3, Z = 8, $R_{gt}(F)$ = 0.0186, w$R_{ref}(F^2)$ = 0.0488, T = 273.15 K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	White block
Size:	0.25 × 0.20 × 0.20 mm
Wavelength:	MoKα radiation (0.71073 Å)
μ:	1.92 mm^{-1}
Diffractometer, scan mode:	φ and ω
θ_{max}, completeness:	26.3°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8700, 2782, 0.017
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2585
$N(param)_{refined}$:	194
Programs:	Bruker,[1] Olex2[2]

1 Source of materials

3-Thiophenecarboxylic acid (4.0 mmol) was dissolved in 15 mL of anhydrous methanol. $Cd(CH_3COO)_2{\cdot}2H_2O$ (2.0 mmol) dissolved in 15 mL of anhydrous methanol was added dropwise to the above 3-thiophenecarboxylic acid solution and stirred for 5 h at 50 °C, cooled and filtered. The filtrate was left for slow evaporation at room temperature. The white block crystals were formed 15 days later. Yield: 32.17 %. Anal. Calcd. for $(C_{11}H_{10}O_5S_2Cd)_n$: C, 33.13; H, 2.53; S, 16.08; found: C, 33.15; H, 2.50; S, 16.05.

2 Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

3 Comment

In recent years, metal coordination polymers have provoked great interest for their promising applications.[3,4] Carboxylate compounds are among the most well-represented and are probably one of the most studied classes of coordination chemistry because of their structural diversity and numerous useful physical features.[5,6]

As shown in Figure, each Cd(II) ion exhibits a different coordination geometry. The Cd1 is six-coordinated in an octahedral environment with two oxygen atoms from two coordinated methanol molecules and four oxygen atoms

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*X*	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.5000	0.5000	0.5000	0.02689 (7)
Cd2	0.5000	0.35303 (2)	0.7500	0.02604 (7)
S1	0.73673 (4)	0.80080 (6)	0.63262 (5)	0.05104 (17)
S2[a]	0.5875 (3)	0.0649 (4)	0.33786 (18)	0.0679 (8)
S2A[b]	0.6238 (5)	−0.0315 (8)	0.4271 (6)	0.0605 (14)
O1	0.54400 (8)	0.53915 (15)	0.65481 (10)	0.0355 (3)
O2	0.61093 (8)	0.45839 (14)	0.77863 (10)	0.0319 (3)
O3	0.48317 (9)	0.30794 (14)	0.55676 (12)	0.0399 (4)
O4	0.55455 (9)	0.20567 (15)	0.66549 (11)	0.0409 (4)
O5	0.38334 (9)	0.53959 (18)	0.53719 (12)	0.0481 (4)
H5	0.3724	0.5108	0.5961	0.058*
C1	0.60248 (11)	0.53665 (19)	0.71043 (14)	0.0273 (4)
C2	0.66202 (11)	0.62649 (18)	0.69769 (14)	0.0288 (4)
C3	0.65882 (13)	0.7147 (2)	0.62719 (17)	0.0405 (5)
H3	0.6189	0.7263	0.5817	0.049*
C4	0.77565 (13)	0.7208 (2)	0.72975 (17)	0.0424 (5)
H4	0.8219	0.7370	0.7606	0.051*
C5	0.72986 (12)	0.6296 (2)	0.75619 (17)	0.0386 (5)
H5A	0.7418	0.5752	0.8072	0.046*
C6	0.53047 (11)	0.22444 (18)	0.57966 (15)	0.0306 (4)
C7	0.55813 (12)	0.14591 (19)	0.50292 (16)	0.0328 (4)
C8	0.54482 (16)	0.1668 (3)	0.40432 (18)	0.0510 (6)
H8	0.5130	0.2296	0.3757	0.061*
C9[a]	0.6247 (10)	−0.0124 (14)	0.4390 (10)	0.057 (3)
H9[a]	0.6555	−0.0808	0.4378	0.068*
C9A[b]	0.5755 (17)	0.071 (3)	0.3500 (11)	0.067 (4)
H9A[b]	0.5703	0.0649	0.2828	0.080*
C10	0.60234 (14)	0.0418 (2)	0.52309 (19)	0.0450 (6)
H10	0.6188	0.0119	0.5871	0.054*
C11	0.32147 (13)	0.5999 (3)	0.4912 (2)	0.0504 (6)
H11A	0.3324	0.6280	0.4284	0.076*
H11B	0.3090	0.6695	0.5296	0.076*
H11C	0.2809	0.5433	0.4844	0.076*

[a]Occupancy: 0.651 (4), [b]Occupancy: 0.349 (4).

from four 3-thiophenecarboxylato molecules. Meanwhile, the Cd2 is six-coordinated in a distorted octahedral environment with six oxygen atoms from four 3-thiophenecarboxylato molecules as a bidentate ligand bridging adjacent above-mentioned crystallographically independent Cd(II) ions to form a 1D chain. A three-dimensional network is assembled through intermolecular hydrogen bonding and intermolecular π-π interactions. The bond distances of Cd–O are 2.2503(16) and 2.5734 (15) Å, which are similar with the refs.[7,8]

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Conflict of interest: The authors declare no conflicts of interest regarding this article.

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