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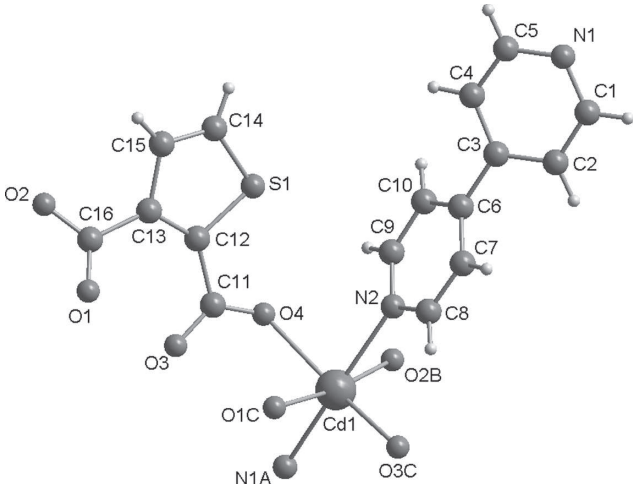
Crystal structure of poly-[μ_2-4,4′-bipyridine-κ^2 *N*:*N*′-μ_3-thiophene-2,3-di-carboxylato-κ^4 *O*,*O*′, *O*″:*O*‴-cadmium(II)]



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Abstract

$C_{16}H_{10}N_2O_4S_1Cd$, orthorhombic, P2(1)2(1)2(1), $a = 8.977(2)$ Å, $b = 11.751(3)$ Å, $c = 14.224(4)$ Å, $\alpha = 90°$, $\beta = 90°$, $\gamma = 90°$, $V = 1500.6(6)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0188$, $wR_{ref}(F^2) = 0.0431$, $T = 296(2)$ K.

CCDC no.: 966307

Source of material

A mixture of $Cd(OAc)_2{\cdot}2H_2O$ (0.1 mmol, 0.0267 g), 4,4′-bipyridine (0.1 mmol, 0.015 g), thiophene-2,3-dicarboxylic acid (0.25 mmol, 0.043 g) was dissolved in 10 mL H_2O. Then the solution was heated in a 25 mL Teflon-lined autoclave under autogenous pressure at 413 K for four days. After cooling to room temperature, The colourless block crystals that formed were collected.

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Table 1: Data collection and handling.

Crystal:	Colourless, block, size 0.20×0.30×0.40 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	16.15 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω scans
$2\theta_{max}$:	50.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	11030, 2776
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2669
$N(param)_{refined}$:	233
Programs:	SHELX [15]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(14)	4*a*	0.4754	0.1198	0.277	0.043
H(15)	4*a*	0.6845	0.0305	0.2024	0.031
H(14′)	4*a*	0.4172	0.0977	0.3011	0.043
H(15′)	4*a*	0.2227	−0.0384	0.2685	0.031
H(1)	4*a*	−0.2472	0.5584	−0.006	0.035
H(2)	4*a*	−0.2454	0.3639	−0.0145	0.035
H(4)	4*a*	0.1144	0.3643	0.1519	0.034
H(5)	4*a*	0.1155	0.5595	0.1433	0.034
H(7)	4*a*	−0.1119	0.1976	−0.0744	0.045
H(8)	4*a*	−0.1051	0.0036	−0.0787	0.047
H(9)	4*a*	−0.0053	−0.0113	0.1868	0.031
H(10)	4*a*	−0.0066	0.1831	0.1987	0.034

Experimental details

There is a positional disorder concerning the sulfur position in the thiophene ring.

Discussion

Great interest has been focused on the rapidly expanding field of metal-organic frameworks (MOFs) due to their structural and topological diversity as well as their potential applications as functional materials [1–3]. In recent years, organic carboxylate ligands have been widely used in synthesizing MOFs due to the rich coordination modes and strong coordination ability of the carboxyl group [4, 5]. Among them, thiophenedicarboxylic acids are useful and important

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Table 3: Atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S(1)	4*a*	0.3057(2)	−0.0192(2)	0.2348(2)	0.0323(7)	0.0359(8)	0.0393(8)	0.0028(6)	−0.0011(6)	−0.0117(7)
C(12)	4*a*	0.3899(9)	−0.1321(9)	0.1794(8)	0.021(2)	0.021(2)	0.021(2)	−0.001(1)	0.001(1)	−0.001(1)
C(13)	4*a*	0.5417(9)	−0.1166(6)	0.1733(8)	0.021(2)	0.022(2)	0.022(2)	−0.001(1)	0.001(1)	0.000(1)
C(14)	4*a*	0.4686(8)	0.0503(6)	0.2460(5)	0.037(2)	0.034(2)	0.036(2)	−0.002(1)	0.001(1)	−0.003(1)
C(15)	4*a*	0.5895(7)	−0.0005(7)	0.2072(5)	0.026(2)	0.026(2)	0.025(2)	0.001(1)	−0.002(1)	−0.000(1)
S(1')	4*a*	0.6043(3)	−0.0104(3)	0.2308(2)	0.0323(7)	0.0359(8)	0.0393(8)	0.0028(6)	−0.0011(6)	−0.0117(7)
C(12')	4*a*	0.533(1)	−0.1308(9)	0.179(1)	0.021(2)	0.021(2)	0.021(2)	−0.001(1)	0.001(1)	−0.001(1)
C(13')	4*a*	0.381(1)	−0.136(1)	0.188(1)	0.021(2)	0.022(2)	0.022(2)	−0.001(1)	0.001(1)	0.000(1)
C(14')	4*a*	0.433(1)	0.0301(7)	0.2687(6)	0.037(2)	0.034(2)	0.036(2)	−0.002(1)	0.001(1)	−0.003(1)
C(15')	4*a*	0.3208(9)	−0.0445(8)	0.2481(8)	0.026(2)	0.026(2)	0.025(2)	0.001(1)	−0.002(1)	−0.000(1)
Cd(1)	4*a*	−0.04930(2)	−0.22545(2)	0.05035(2)	0.0239(1)	0.0128(1)	0.0260(1)	−0.0005(1)	0.0024(1)	−0.00138(9)
N(1)	4*a*	−0.0641(3)	0.5785(2)	0.0665(2)	0.025(1)	0.015(1)	0.028(1)	−0.002(1)	0.002(1)	0.001(1)
N(2)	4*a*	−0.0526(3)	−0.0235(2)	0.0532(2)	0.034(1)	0.016(1)	0.029(1)	0.001(1)	−0.003(2)	−0.002(1)
O(1)	4*a*	0.6379(2)	−0.2524(2)	0.0589(2)	0.031(1)	0.049(2)	0.028(1)	0.012(1)	−0.003(1)	−0.012(1)
O(2)	4*a*	0.7828(2)	−0.1924(2)	0.1732(2)	0.021(1)	0.036(2)	0.036(1)	0.000(1)	−0.003(1)	−0.007(1)
O(3)	4*a*	0.3351(2)	−0.3042(2)	0.0988(2)	0.031(1)	0.022(1)	0.036(1)	−0.000(1)	0.003(1)	−0.006(1)
O(4)	4*a*	0.1452(2)	−0.2062(2)	0.1588(2)	0.019(1)	0.035(2)	0.032(1)	−0.002(1)	0.0006(9)	−0.005(1)
C(1)	4*a*	−0.1702(4)	0.5189(3)	0.0232(2)	0.029(2)	0.021(2)	0.037(2)	0.003(1)	−0.004(1)	0.002(1)
C(2)	4*a*	−0.1718(4)	0.4016(3)	0.0193(2)	0.029(2)	0.018(2)	0.040(2)	−0.005(1)	−0.009(2)	−0.002(1)
C(3)	4*a*	−0.0623(4)	0.3402(2)	0.0665(2)	0.028(2)	0.017(2)	0.030(2)	−0.001(1)	0.002(2)	0.000(1)
C(4)	4*a*	0.0428(4)	0.4017(3)	0.1162(2)	0.026(2)	0.021(2)	0.037(2)	0.002(2)	−0.006(2)	0.002(1)
C(5)	4*a*	0.0406(4)	0.5195(3)	0.1124(2)	0.025(2)	0.024(2)	0.036(2)	−0.005(2)	−0.004(2)	−0.004(1)
C(6)	4*a*	−0.0606(3)	0.2144(2)	0.0630(2)	0.027(2)	0.017(2)	0.034(2)	0.001(2)	−0.003(2)	−0.002(1)
C(7)	4*a*	−0.0895(4)	0.1571(3)	−0.0201(2)	0.054(3)	0.021(2)	0.036(2)	−0.001(2)	−0.015(2)	0.002(1)
C(8)	4*a*	−0.0848(4)	0.0402(3)	−0.0222(2)	0.059(3)	0.024(2)	0.035(2)	−0.002(2)	−0.013(2)	−0.005(1)
C(9)	4*a*	−0.0260(4)	0.0314(3)	0.1333(2)	0.031(2)	0.020(2)	0.027(2)	0.002(2)	−0.001(2)	0.002(1)
C(10)	4*a*	−0.0275(4)	0.1486(3)	0.1413(2)	0.040(2)	0.019(2)	0.027(2)	0.003(2)	−0.004(2)	−0.006(1)
C(11)	4*a*	0.2819(3)	−0.2228(3)	0.1434(2)	0.025(2)	0.020(1)	0.020(2)	0.002(2)	−0.001(1)	0.005(2)
C(16)	4*a*	0.6583(3)	−0.1963(2)	0.1322(2)	0.022(2)	0.017(2)	0.022(2)	−0.002(1)	0.004(1)	0.003(1)

organic moieties in preparing electronic and optical materials owing to their good electron-transferring ability and structural rigidity [6–9]. However, MOFs constructed from thiophenedicarboxylic acids are rather limited and most of the work has been devoted on MOFs built from commercially available thiophene-2,5-dicarboxylic acid [10]. On the other hand, a number of bis(imidazole)-containing ligands have been widely employed as the secondary ligands meeting the requirement of coordination geometries of metal ions or tuning the fine structure [11, 12]. As the most widely used flexible bidentate 1,10-(1,4-butanediyl)bis(imidazole) ligands, it possesses an excellent coordination ability and has been widely used to construct MOFs [13, 14].

The asymmetric unit of the title structure contains one Cd(II) ion, one 4,4′-bipyridine ligand and one thiophene-2,3-di-carboxylate dianion as bridging ligand to construct a new coordination polymer. The cadmium atom is six-coordinated by four atoms of three anionic ligands and two nitrogen atoms in a trans-arrangment from two bipyridine ligands. The O—Cd—O are in the range of 74.60(8)° to 172.90(8)°. The O4—Cd—N2 angle is 84.32(9)° (Tables 1–3). These interactions result in the infinite three dimensional architecture.

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