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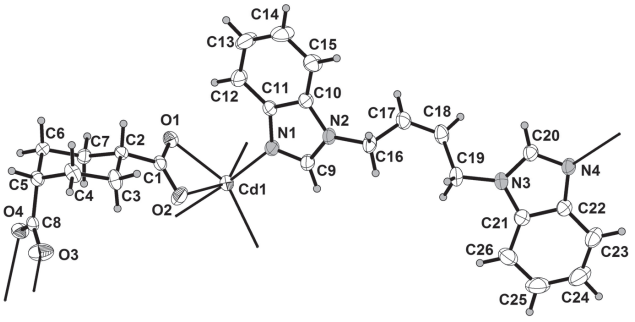
Crystal structure of poly{[μ_2-(*E*)-1,4-bis(1*H*-benzo[*d*]imidazol-1-yl)but-2-ene-κ^2*N*:*N*′][μ_3–cyclohexane-1,4-dicarboxylato-κ^4*O*,*O*′:*O*″:*O*‴] cadmium(II)}, $C_{26}H_{26}CdN_4O_4$



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Abstract

$C_{26}H_{26}CdN_4O_4$, monoclinic, $P2_1/c$ (no. 14), $a = 12.1676(8)$ Å, $b = 13.4592(9)$ Å, $c = 15.5782(10)$ Å, $\beta = 112.1310(10)$ Å, $V = 2363.2(3)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0244$, $wR_{ref}(F^2) = 0.0584$, $T = 293(2)$ K.

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A part of the title crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The synthesis was performed under hydrothermal conditions. A mixture of $Cd(NO_3)_2{\cdot}4H_2O$ (0.2 mmol, 0.0616 g), (*E*)-1,4-bis(1*H*-benzo[*d*]imidazol-1-yl)but-2-ene (0.2 mmol, 0.0576 g), cyclohexane-1,4-dicarboxylic acid (0.2 mmol, 0.0344 g) and H_2O (12 mL) was heated in a 20 mL stainless steel

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Table 1: Data collection and handling.

Crystal:	Block, colorless
Size:	0.24 × 0.22 × 0.18 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.97 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
θ_{max}, completeness:	28.4°, >96% (up to 54° > 99%)
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	14811, 5690, 0.021
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 4783
$N(param)_{refined}$:	316
Programs:	Bruker programs [1], SHELX [2]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.438745(11)	0.080470(9)	0.377390(9)	0.02272(5)
N1	0.33446(15)	−0.06435(12)	0.31825(12)	0.0319(4)
N2	0.30630(14)	−0.22484(12)	0.28049(12)	0.0302(4)
N3	0.53332(15)	−0.60292(12)	0.39735(12)	0.0303(4)
N4	0.53292(15)	−0.76377(12)	0.43337(12)	0.0329(4)
O1	0.26748(12)	0.17888(11)	0.29319(9)	0.0322(3)
O2	0.38873(13)	0.14797(12)	0.22171(10)	0.0406(4)
O3	0.39656(15)	0.43578(14)	0.00587(11)	0.0516(5)
O4	0.38324(12)	0.52239(11)	0.12008(10)	0.0355(3)
C1	0.29686(17)	0.18803(14)	0.22433(13)	0.0257(4)
C2	0.22114(16)	0.25431(14)	0.14447(13)	0.0260(4)
H2	0.1380	0.2345	0.1267	0.031*
C3	0.2533(2)	0.24742(15)	0.05891(14)	0.0345(5)
H3A	0.2330	0.1818	0.0318	0.041*
H3B	0.3383	0.2560	0.0775	0.041*
C4	0.1889(2)	0.32584(15)	−0.01435(13)	0.0349(5)
H4A	0.2164	0.3216	−0.0651	0.042*
H4B	0.1044	0.3120	−0.0389	0.042*
C5	0.21009(17)	0.43086(14)	0.02564(13)	0.0271(4)
H5	0.1601	0.4759	−0.0228	0.033*
C6	0.16891(18)	0.43760(15)	0.10681(15)	0.0314(4)
H6A	0.1838	0.5039	0.1330	0.038*
H6B	0.0842	0.4253	0.0849	0.038*
C7	0.23457(17)	0.36171(14)	0.18131(13)	0.0277(4)
H7A	0.2047	0.3654	0.2308	0.033*
H7B	0.3182	0.3788	0.2073	0.033*
C8	0.33896(16)	0.46495(14)	0.05222(12)	0.0247(4)
C9	0.38403(18)	−0.15050(15)	0.31621(15)	0.0338(5)
H9	0.4658	−0.1594	0.3376	0.041*
C10	0.19436(17)	−0.18424(15)	0.25746(13)	0.0286(4)
C11	0.21248(17)	−0.08339(14)	0.2800(14)	0.0278(4)
C12	0.11589(19)	−0.02023(17)	0.26475(16)	0.0392(5)

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Table 2 (continued)

Atom	x	y	z	U_{iso}*/U_{eq}
H12	0.1263	0.0471	0.2791	0.047*
C13	0.0041(2)	−0.06201(19)	0.2268(2)	0.0523(7)
H13	−0.0620	−0.0218	0.2155	0.063*
C14	−0.0125(2)	−0.1629(2)	0.2048(2)	0.0534(7)
H14	−0.0893	−0.1880	0.1798	0.064*
C15	0.08141(19)	−0.22599(17)	0.21909(16)	0.0413(5)
H15	0.0702	−0.2931	0.2040	0.050*
C16	0.3348(2)	−0.32839(15)	0.26869(15)	0.0354(5)
H16A	0.4172	−0.3328	0.2751	0.042*
H16B	0.2859	−0.3504	0.2067	0.042*
C17	0.3150(2)	−0.39570(15)	0.33842(15)	0.0355(5)
H17	0.2513	−0.3815	0.3555	0.043*
C18	0.3811(2)	−0.47340(15)	0.37732(15)	0.0356(5)
H18	0.3590	−0.5116	0.4179	0.043*
C19	0.4897(2)	−0.50418(15)	0.36024(15)	0.0360(5)
H19A	0.4716	−0.5040	0.2940	0.043*
H19B	0.5520	−0.4558	0.3884	0.043*
C20	0.46911(18)	−0.68368(15)	0.40076(14)	0.0328(5)
H20	0.3869	−0.6827	0.3817	0.039*
C21	0.65079(18)	−0.63290(15)	0.43087(13)	0.0299(4)
C22	0.64981(17)	−0.73309(15)	0.45513(13)	0.0296(4)
C23	0.7566(2)	−0.78356(17)	0.49773(17)	0.0436(6)
H23	0.7581	−0.8495	0.5160	0.052*
C24	0.8594(2)	−0.7325(2)	0.5118(2)	0.0603(8)
H24	0.9317	−0.7648	0.5398	0.072*
C25	0.8588(2)	−0.6336(2)	0.4855(2)	0.0644(8)
H25	0.9307	−0.6019	0.4963	0.077*
C26	0.7550(2)	−0.58169(18)	0.44399(19)	0.0471(6)
H26	0.7546	−0.5159	0.4257	0.057*

reactor with a Teflon liner from 298 to 433 K in 6 h and maintained at 433 K for 72 h, after which the mixture was cooled to 298 K. Colorless crystals of the title compound were obtained (yield 67% based on the amount of $Cd(NO_3)_2{\cdot}4H_2O$).

Experimental details

H atoms were positioned in accord with the chemical needs. The U_{iso} values of the hydrogen atoms were set to $1.2U_{eq}$(C) and $1.5U_{eq}$(C) respectively.

Discussion

Coordination polymers are a class of materials with unique electronic, optical and catalytic properties [3–6]. They are unparalleled for their diversified, designable and tailorable structures as well as unique chemical and physical properties [7–10]. Herein, we present a new cadmium-carboxylate coordination polymer. In the title two-dimensional coordination polymer the Cd atom lies in a general position and displays a slightly distorted octahedral coordination geometry. Three cyclohexane-1,4-dicarboxylate ligands connect two cadmium atoms to form an eight-member ring. The (*E*)-1,4-bis(1*H*-benzo[*d*]imidazol-1-yl)but-2-ene ligands link adjacent metal atoms into polymeric chains parallel to the *b* axis. The bond lengths and angles are normal. The N-contained neutral ligands and carboxylate ligands result in the formation of a two-dimensional network.

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