Crystal structure of *poly*-[bis{ μ_2 -*N*-(4-(1*H*-imidazol-1-yl)phenyl)-4-(1*H*-imidazol-1-yl)-*N*-phenylaniline- $\kappa^2 N:N'$ }-(μ_2 -naphthalene-2,6-dicarboxylato)-(μ_4 -naphthalene-2,6-dicarboxylato)dicadmium(II)], $C_{36}H_{25}N_5O_4Cd$

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$\text{C}_{36}\text{H}_{25}\text{N}_5\text{O}_4\text{Cd}$, monoclinic, $P\bar{1}$ (No. 2), $a = 9.708(5)$ Å, $b = 10.954(5)$ Å, $c = 15.014(5)$ Å, $\alpha = 97.858(5)^\circ$, $\beta = 98.584(5)^\circ$, $\gamma = 104.798(5)^\circ$, $V = 1500.6(11)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0297$, $wR_{\text{ref}}(F^2) = 0.0904$, $T = 293(2)$ K.

A part of the 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.

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Crystal:	Colorless blocks
	Size 0.28 × 0.22 × 0.21 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	7.8 cm ⁻¹
Diffractometer, scan mode:	Bruker CCD, φ and ω
2 $\theta_{\max}$, completeness:	56.6°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	11248, 7455, 0.015
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 6339
$N(\text{param})_{\text{refined}}$:	416
Programs:	SHELX [11]

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.0799(4)	0.1418(3)	−0.04865(19)	0.0551(8)
H1	0.1130	0.1115	0.0030	0.066*
C2	0.0235(4)	0.0687(3)	−0.13296(19)	0.0521(7)
H2	0.0106	−0.0189	−0.1498	0.063*
C3	0.0253(3)	0.2685(2)	−0.13553(16)	0.0371(5)
H3	0.0122	0.3416	−0.1566	0.044*
C4	−0.0751(3)	0.1157(2)	−0.28399(16)	0.0339(5)
C5	−0.0546(3)	0.0095(3)	−0.33598(18)	0.0428(6)
H5	0.0045	−0.0359	−0.3096	0.051*
C6	−0.1217(3)	−0.0288(3)	−0.42687(17)	0.0426(6)
H6	−0.1057	−0.0991	−0.4617	0.051*
C7	−0.2132(3)	0.0362(2)	−0.46752(16)	0.0364(5)
C8	−0.2271(3)	0.1458(2)	−0.41577(17)	0.0384(5)
H8	−0.2826	0.1935	−0.4428	0.046*
C9	−0.1597(3)	0.1856(2)	−0.32440(17)	0.0362(5)
H9	−0.1711	0.2587	−0.2904	0.043*
C10	−0.3456(3)	0.0594(2)	−0.61679(17)	0.0373(5)
C11	−0.4800(3)	0.0095(3)	−0.67544(18)	0.0414(6)
H11	−0.5358	−0.0730	−0.6746	0.050*
C12	−0.5320(3)	0.0805(3)	−0.73488(18)	0.0422(6)
H12	−0.6213	0.0453	−0.7743	0.051*
C13	−0.4516(3)	0.2032(2)	−0.73568(17)	0.0375(5)

Table 2: (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C14	−0.3189(3)	0.2542(3)	−0.6772(2)	0.0499(7)
H14	−0.2650	0.3378	−0.6768	0.060*
C15	−0.2652(3)	0.1824(3)	−0.6192(2)	0.0490(7)
H15	−0.1742	0.2171	−0.5816	0.059*
C16	−0.6427(3)	0.2793(3)	−0.81927(19)	0.0423(6)
H16	−0.7197	0.2295	−0.7982	0.051*
C17	−0.4229(3)	0.3644(3)	−0.84062(19)	0.0450(6)
H17	−0.3231	0.3849	−0.8380	0.054*
C19	−0.3521(3)	−0.1526(3)	−0.58199(19)	0.0487(7)
C20	−0.4267(3)	−0.2204(3)	−0.5248(3)	0.0589(8)
H20	−0.4321	−0.1794	−0.4675	0.071*
C21	−0.4940(5)	−0.3515(3)	−0.5541(4)	0.0926(15)
H21	−0.5453	−0.3981	−0.5162	0.111*
C22	−0.4852(7)	−0.4119(4)	−0.6377(5)	0.135(3)
H22	−0.5311	−0.4992	−0.6569	0.162*
C23	−0.4090(8)	−0.3444(5)	−0.6932(4)	0.134(3)
H23	−0.4038	−0.3862	−0.7503	0.161*
C24	−0.3394(5)	−0.2145(4)	−0.6656(3)	0.0845(13)
H24	−0.2849	−0.1696	−0.7028	0.101*
C25	0.2467(3)	0.6620(2)	0.0281(2)	0.0409(6)
C26	0.3200(3)	0.7923(2)	0.00886(17)	0.0353(5)
C27	0.2563(3)	0.8399(2)	−0.06475(19)	0.0423(6)
H27	0.1643	0.7948	−0.0979	0.051*
C28	0.3287(3)	0.9513(2)	−0.08747(19)	0.0428(6)
H28	0.2860	0.9808	−0.1367	0.051*
C29	0.4684(3)	1.0234(2)	−0.03752(17)	0.0332(5)
C30	0.5460(3)	1.1405(2)	−0.05870(18)	0.0378(5)
H30	0.5051	1.1721	−0.1074	0.045*
C31	0.0700(3)	0.4015(3)	0.24761(17)	0.0408(6)
C32	0.0587(3)	0.4275(2)	0.34662(16)	0.0347(5)
C33	0.1196(3)	0.3609(3)	0.40927(17)	0.0394(6)
H33	0.1683	0.3028	0.3889	0.047*
C34	0.1075(3)	0.3809(2)	0.49900(17)	0.0381(5)
H34	0.1504	0.3383	0.5396	0.046*
C35	−0.0110(3)	0.5140(2)	0.37699(16)	0.0333(5)
H35	−0.0466	0.5608	0.3364	0.040*
C36	−0.0304(2)	0.5341(2)	0.46909(16)	0.0311(5)
C18	−0.5183(3)	0.4134(3)	−0.88838(19)	0.0480(7)
H18	−0.4937	0.4745	−0.9250	0.058*
N1	0.0813(2)	0.2671(2)	−0.05055(14)	0.0402(5)
N2	−0.0109(2)	0.15086(19)	−0.18854(13)	0.0357(4)
N3	−0.2916(3)	−0.0159(2)	−0.55801(15)	0.0443(5)
N4	−0.5037(2)	0.2778(2)	−0.79655(14)	0.0387(5)
N5	−0.6557(3)	0.3610(2)	−0.87553(16)	0.0452(5)
O1	0.3063(3)	0.6245(2)	0.09341(19)	0.0816(9)
O2	0.1322(2)	0.59283(18)	−0.02259(16)	0.0529(5)
O3	0.0705(2)	0.2928(2)	0.21219(13)	0.0524(5)
O4	0.0782(3)	0.4951(2)	0.20553(13)	0.0572(6)
Cd1	0.135574(19)	0.425080(15)	0.073588(11)	0.03183(7)

Source of material

A mixture of naphthalene-2,6-dicarboxylic acid (0.2 mmol, 0.043 g), *N*-(4-(1*H*-imidazol-1-yl)phenyl)-4-(1*H*-imidazol-1-yl)-*N*-phenylaniline (0.2 mmol, 0.076 g), Cd(CH₃COO)₂·

(H₂O), (0.2 mmol, 0.053 g), and H₂O (20 mL) was stirred for 20 min. The mixtures were transferred in a 30 mL stainless steel reactor with a Teflon liner and heated from 293 to 463 K in 4 h and a constant temperature was maintained for 72 h. After cooling to room temperature colorless block crystals were collected in 56.8 % yield based on Cd(CH₃COO)₂·2(H₂O).

Experimental details

The C-bound H atoms were positioned with idealized geometry and were refined with *U*_{iso}(H) = 1.2*U*_{eq}(C) using a riding model with C–H = 0.93 Å for aromatic H atoms.

Discussion

Recently, many efforts have been devoted to design and synthesize coordination polymers, not only due to their potential applications in the realm of gas adsorption and separation, catalysis, magnetism, luminescence, host-guest chemistry etc, but also for their aesthetic and often complicated architectures and topologies [1–4]. It is well known that carboxylates are excellent building blocks for the construction of coordination polymers because the carboxylate groups may induce core aggregation and link these discrete clusters into an extended framework by virtue of its bridging ability [5–10]. Taking these into account, we chose naphthalene-2,6-dicarboxylate and *N*-(4-(1*H*-imidazol-1-yl)phenyl)-4-(1*H*-imidazol-1-yl)-*N*-phenylaniline as neutral ligand, generating the title compound.

In the title compound, Cd(II) displays a slightly distorted octahedral geometry defined by two N atoms from two *N*-(4-(1*H*-imidazol-1-yl)phenyl)-4-(1*H*-imidazol-1-yl)-*N*-phenylaniline ligands and four O atoms from three naphthalene-2,6-dicarboxylate ligands. The bond lengths and angles are in a normal range. In the crystal, the Cd(II) ions are bridged by naphthalene-2,6-dicarboxylate and neutral ligands forming a three-dimensional supramolecular network.

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