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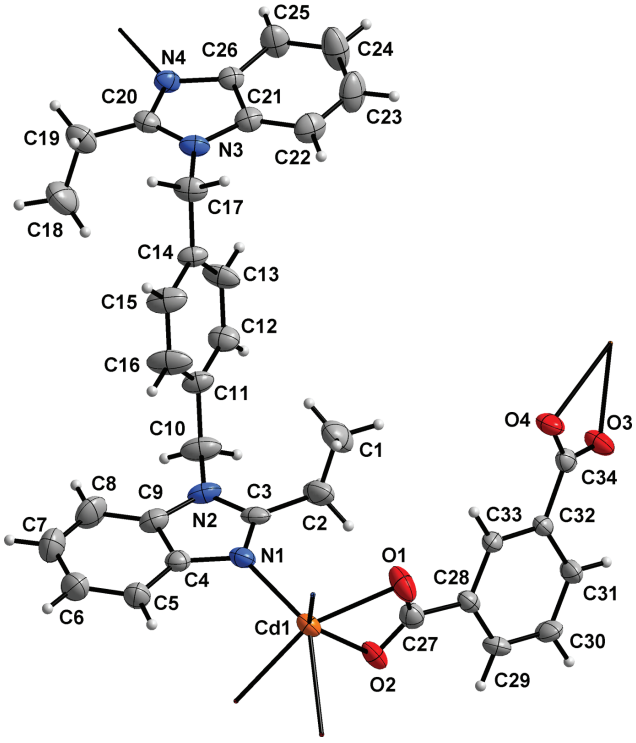
Crystal structure of poly[(μ_2-1,4-bis((2-ethyl-1*H*-benzo[*d*]imidazol-1-yl)methyl)benzene-κ^2*N*:*N*′)(μ_2-isophthalato-κ^4*O*,*O*′:*O*″,*O*‴)cadmium(II)], $C_{34}H_{30}N_4O_4Cd$



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Abstract

$C_{34}H_{30}N_4O_4Cd$, monoclinic, $P2_1/c$ (no. 14), $a = 10.382(2)$ Å, $b = 18.102(4)$ Å, $c = 18.449(5)$ Å, $\beta = 123.32(2)°$, $V = 2897.3(12)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0540$, $\omega R_{ref}(F^2) = 0.1069$, $T = 293(2)$ K.

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

Table 1: Data collection and handling.

Crystal:	Colourless prism
Size:	0.18 × 0.16 × 0.14 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.80 mm^{-1}
Diffractometer, scan mode:	Rigaku Saturn, 724 ω
θ_{max}:	25.0°
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	19414, 5093, 0.058
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4204
$N(param)_{refined}$:	390
Programs:	*CrystalClear* [9], SHELX [10]

Source of material

The title compound was prepared under the hydrothermal conditions. A mixture of 1,4-bis(2-ethylbenzimidazol-1-ylmethyl) benzene (beb) (39.4 mg, 0.1 mmol), $Cd(Ac)_2{\cdot}2H_2O$ (26.7 mg, 0.1 mmol), isophthalic acid (H_2ip) (33.2 mg, 0.2 mmol), and H_2O (10 mL) were placed in a Teflon-lined stainless steel vessel, heated to 130 °C for 5 day, and then cooled to room temperature for 24 h. Colorless block crystals of the title complex were obtained.

Experimenal details

Absorption corrections were applied by using multi-scan program. The hydrogen atoms were placed at calculated

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

Atom	x	y	z	U_{iso}*/U_{eq}
C1	0.1617(7)	0.3079(3)	0.1312(4)	0.0650(17)
H1A	0.2609	0.3314	0.1606	0.097*
H1B	0.1162	0.3096	0.0697	0.097*
H1C	0.1735	0.2573	0.1496	0.097*
C2	0.0594(6)	0.3475(3)	0.1525(3)	0.0534(15)
H2A	0.0472	0.3984	0.1332	0.064*
H2B	−0.0417	0.3246	0.1209	0.064*
C3	0.1205(5)	0.3468(3)	0.2467(3)	0.0378(12)
C4	0.1786(5)	0.3157(3)	0.3748(3)	0.0335(11)
C5	0.1963(6)	0.2834(3)	0.4482(3)	0.0447(13)
H5	0.1376	0.2426	0.4432	0.054*
C6	0.3012(6)	0.3128(4)	0.5277(4)	0.0586(17)
H6	0.3162	0.2905	0.5772	0.070*
C7	0.3859(7)	0.3753(4)	0.5363(4)	0.0674(18)
H7	0.4565	0.3942	0.5912	0.081*
C8	0.3670(6)	0.4091(3)	0.4653(4)	0.0638(18)
H8	0.4222	0.4515	0.4705	0.077*
C9	0.2626(5)	0.3783(3)	0.3848(3)	0.0415(13)
C10	0.2783(6)	0.4627(3)	0.2816(4)	0.0562(16)
H10A	0.2990	0.5012	0.3233	0.067*
H10B	0.1975	0.4804	0.2248	0.067*
C11	0.4218(5)	0.4501(3)	0.2817(3)	0.0394(12)
C12	0.4418(6)	0.4907(3)	0.2261(3)	0.0445(13)
H12	0.3662	0.5242	0.1887	0.053*
C13	0.5734(6)	0.4826(3)	0.2249(3)	0.0490(14)
H13	0.5845	0.5107	0.1865	0.059*
C14	0.6871(5)	0.4340(2)	0.2790(3)	0.0329(11)
C15	0.6666(6)	0.3932(3)	0.3346(4)	0.0555(16)
H15	0.7423	0.3598	0.3721	0.067*
C16	0.5356(6)	0.4009(3)	0.3357(4)	0.0640(18)
H16	0.5240	0.3723	0.3736	0.077*
C17	0.8295(6)	0.4221(3)	0.2777(3)	0.0423(13)
H17A	0.9147	0.4100	0.3359	0.051*
H17B	0.8125	0.3800	0.2409	0.051*
C18	0.9354(7)	0.5838(4)	0.4133(4)	0.076(2)
H18A	0.8998	0.6310	0.3852	0.115*
H18B	0.9910	0.5904	0.4750	0.115*
H18C	0.8486	0.5520	0.3947	0.115*
C19	1.0399(6)	0.5497(3)	0.3898(3)	0.0500(14)
H19A	1.1323	0.5796	0.4141	0.060*
H19B	1.0707	0.5011	0.4158	0.060*
C20	0.9673(5)	0.5427(3)	0.2942(3)	0.0353(12)
C21	0.8287(5)	0.4959(3)	0.1618(3)	0.0353(11)
C22	0.7331(6)	0.4546(3)	0.0871(4)	0.0480(14)
H22	0.6818	0.4127	0.0875	0.058*
C23	0.7193(7)	0.4795(3)	0.0133(4)	0.0648(18)
H23	0.6551	0.4542	−0.0384	0.078*
C24	0.7980(8)	0.5412(3)	0.0132(4)	0.0698(19)
H24	0.7876	0.5553	−0.0382	0.084*
C25	0.8912(6)	0.5822(3)	0.0870(3)	0.0507(14)
H25	0.9439	0.6235	0.0864	0.061*
C26	0.9033(5)	0.5594(3)	0.1623(3)	0.0335(11)
C27	−0.2840(6)	0.2519(3)	0.0628(3)	0.0380(12)
C28	−0.3656(5)	0.2783(2)	−0.0296(3)	0.0301(11)
C29	−0.5148(5)	0.3051(3)	−0.0733(3)	0.0367(12)
H29	−0.5673	0.3073	−0.0456	0.044*
C30	−0.5852(5)	0.3285(3)	−0.1577(3)	0.0427(13)
H30	−0.6874	0.3439	−0.1880	0.051*
C31	−0.5062(5)	0.3294(3)	−0.1979(3)	0.0367(12)
H31	−0.5548	0.3464	−0.2547	0.044*
C32	−0.3553(5)	0.3053(2)	−0.1548(3)	0.0280(10)
C33	−0.2876(5)	0.2781(2)	−0.0711(3)	0.0293(11)
H33	−0.1878	0.2595	−0.0423	0.035*
C34	−0.2667(5)	0.3080(3)	−0.1971(3)	0.0312(11)
Cd1	−0.10382(4)	0.20340(2)	0.22815(2)	0.03267(13)
N1	0.0884(4)	0.2963(2)	0.2870(2)	0.0347(9)
N2	0.2222(4)	0.3975(2)	0.3024(3)	0.0435(11)
N3	0.8729(4)	0.4857(2)	0.2467(3)	0.0365(10)
N4	0.9871(4)	0.5892(2)	0.2456(2)	0.0336(9)
O1	−0.1798(4)	0.2045(2)	0.0872(2)	0.0553(10)
O2	−0.3144(4)	0.27960(19)	0.1131(2)	0.0438(9)
O3	−0.3105(4)	0.3493(2)	−0.2605(2)	0.0449(9)
O4	−0.1471(4)	0.26831(19)	−0.1661(2)	0.0412(9)

positions and refined as riding atoms with fixed isotropic displacement parameters.

Results and discussion

Construction of coordination polymers based on assembly of metal ions and multi-functional organic ligands remains an interesting field of research [1–5]. The bis(ethylbenzimidazole) ligand with a long spacer are a good choice. The characteristics are as follows: (a) The longer spacers often causes the structural diversities. (b) The 2-position substituent ethyl may be conducive to enrich coordination ability of hbmb with metal ions [6, 7].

The asymmetric unit of the title structure consists of a 1,4-bis(2-ethylbenzimidazol-1-ylmethyl) benzene (beb), one isophthalate (ip^{2-}), and one Cd(II) ion. As shown in the figure, each Cd(II) is octahedrally coordinated by two N atoms from two beb ligands, and four oxygen atoms from two H_2ip. The bond lengths are Cd(1)–O(1) = 2.265(3) Å, Cd(1)–O(2) = 2.468(3) Å, Cd(1)–O(3) = 2.459(3) Å, Cd(1)–O(4) = 2.287(3) Å, Cd(1)–N(1) = 2.369(4) Å, and Cd(1)'–N(4) = 2.309(4) Å, respectively. They are in the normal range [8].

The beb ligand adopts asymmetric trans-conformation with the $N_{donor}\cdots N{-}C_{sp3}\cdots C$ torsion of 32.7° and 33.9°, respectively. Cd(II) metal centers link beb and ip^{2-} to form a 2D sheet structure.

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