Crystal structure of catena-bis[(4-chlorobenzoate-κ*O*)-(1,4-bis(2-methylbenzimidazol-1-ylmethyl)benzene-κ^2*N*:*N*′)zinc(II)], $C_{38}H_{30}Cl_2N_4O_4Zn$

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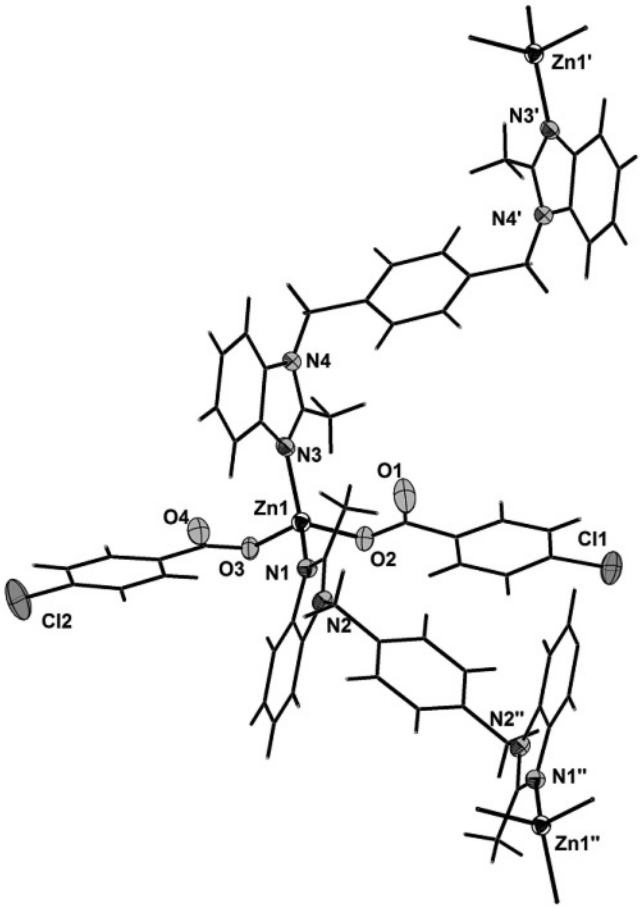

Abstract

$C_{38}H_{30}Cl_2N_4O_4Zn$, monoclinic, $P2_1/c$ (no. 14), a = 11.5694(8) Å, b = 14.143(1) Å, c = 21.969(2) Å, β = 100.856(2)°, V = 3530.5 Å^3, Z = 4, $R_{gt}(F)$ = 0.0499, $wR_{ref}(F^2)$ = 0.1282, T = 296 K.

Source of material

The title compound was prepared under the hydrothermal conditions. A mixture of 1,4-bis(2-methylbenzimidazol-1-ylmethyl) benzene (73.2 mg, 0.2 mmol), $Zn(Ac)_2{\cdot}2H_2O$ (22.0 mg, 0.1 mmol), 4-chlorobenzoicacid (31.3 mg, 0.2 mmol) and H_2O (10 mL) were placed in a Teflon-lined stainless steel vessel, heated to 130 °C for 4 days, and then cooled to room temperature for 24 h. Colourless block crystals of the title complex were obtained.

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Experimental details

The data of the title complex was collected on a Bruker Smart APEX II CCD diffractomer [15]. Absorption corrections were applied by using multi-scan program [15]. The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.20×0.24×0.26 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	8.93 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{max}$:	52°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	19812, 6913
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4072
$N(param)_{refined}$:	444
Programs:	SHELX [14], SADABS [15], DIAMOND [16]

Discussion

During the past decades, intense interest has been focused on the design and synthesis of functional metal-organic frameworks (MOFs) owing to their variety of intriguing topologies [1] and potential applications in the areas of anion/guest exchange, catalysis, magnetism, luminescence and gas storage [2-6]. Up to now, many researches demonstrate that using mixed organic ligands, especially the mixed polycarboxylate and N-containing ones, with more tunable factors, are good candidates for the construction of novel MOFs [7]. According to our recent research, we selected 4-chlorobenzoicacid (H*cbc*) as O-donor ligand and 1,4-bis(2-methylbenzimidazol-1-ylmethyl)benzene (*bmb*) as N-donor ligands for several reasons: (1) 4-chlorobenzoic acid and its deprotonated anion has been proved to be excellent structural constructors due to its various coordination modes to metal ions, which often generate interesting structure [8]; (2) the 2-position substituent methyl of *bmb* effectively enhances the donated electrons abilityof benzimidazole ring, and makes *bmb* exhibit strong collaborative coordination ability with organic carboxylate ligands [9-12]. There are two half *bmb*, two *cbc*$^-$ and one Zn(II) ion in the asymmetric unit. As shown in the figure (' =1–*x*, 1–*y*, 1–*z*; " =–*x*, 1–*y*, 1–*z*), the Zn(II) ion is four-coordinated in a tetrahedral geometry, ligated by two oxygen atoms (O2 and O3) from two unsymmetry-related *cbc*$^-$, two nitrogen atoms (N1 and N3) from two distinct *bmb*. The bond lengths are Zn1–O2 = 1.982(2) Å, Zn1–O3 = 1.992(2) Å, Zn1–N1 = 2.009(3) Å and Zn1–N3 = 2.011(3) Å, respectively. They are in the normal range [13]. In the title complex, there are two kinds of *bmb* ligands. Both of them adopt a symmetric *trans*-conformation with the N_{donor}···N–C_{sp3}···C torsion of 66.449° and 125.798°, respectively. The two methylbenz-imidazol arms of *bmb* bend in opposite di-

rections to bridge two adjacent Zn^{2+} ions to form a zigzag chain. The *cbc*$^-$ anion is coordinated in a monodentate mode. The 1D Zn-*bmb* motif is decorated with *cbc*$^-$ anions at both sides in an approximately parallel fashion.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1A)	4*e*	0.1136	0.4955	0.2779	0.074
H(1B)	4*e*	0.1206	0.4555	0.2121	0.074
H(1C)	4*e*	0.0333	0.4105	0.2505	0.074
H(4)	4*e*	–0.1920	0.7765	0.2322	0.052
H(5)	4*e*	–0.3289	0.8181	0.1458	0.067
H(6)	4*e*	–0.3587	0.7268	0.0580	0.070
H(7)	4*e*	–0.2579	0.5866	0.0543	0.063
H(9A)	4*e*	–0.1593	0.4170	0.1009	0.053
H(9B)	4*e*	–0.0286	0.3969	0.1329	0.053
H(11)	4*e*	–0.1630	0.4048	–0.0058	0.050
H(12)	4*e*	0.0967	0.5552	0.0948	0.054
H(13A)	4*e*	0.1630	0.7397	0.4252	0.078
H(13B)	4*e*	0.2827	0.6895	0.4515	0.078
H(13C)	4*e*	0.1959	0.7149	0.4959	0.078
H(16)	4*e*	–0.1072	0.4554	0.3338	0.053
H(17)	4*e*	–0.1179	0.2989	0.3629	0.066
H(18)	4*e*	0.0054	0.2402	0.4480	0.070
H(19)	4*e*	0.1418	0.3350	0.5095	0.060
H(21A)	4*e*	0.2565	0.4699	0.5594	0.053
H(21B)	4*e*	0.2693	0.5801	0.5573	0.053
H(23)	4*e*	0.4815	0.5573	0.5946	0.072
H(24)	4*e*	0.3359	0.4634	0.4286	0.075
H(27)	4*e*	0.2184	0.9159	0.2848	0.058
H(28)	4*e*	0.3594	1.0146	0.2591	0.074
H(30)	4*e*	0.5529	0.7920	0.2326	0.080
H(31)	4*e*	0.4095	0.6934	0.2563	0.077
H(34)	4*e*	–0.2249	0.8878	0.3898	0.064
H(35)	4*e*	–0.3777	0.9604	0.4262	0.075
H(37)	4*e*	–0.5457	0.7146	0.4213	0.078
H(38)	4*e*	–0.3984	0.6429	0.3808	0.065

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	4*e*	0.0691(3)	0.4683(3)	0.2407(2)	0.054(3)	0.042(2)	0.053(3)	0.016(2)	0.013(2)	0.002(2)
C(2)	4*e*	–0.0230(3)	0.5351(2)	0.2123(2)	0.043(2)	0.036(2)	0.034(2)	–0.004(2)	0.018(2)	0.002(2)
C(3)	4*e*	–0.1428(3)	0.6556(2)	0.1947(2)	0.038(2)	0.035(2)	0.033(2)	0.001(2)	0.013(2)	0.005(2)
C(4)	4*e*	–0.2046(3)	0.7386(3)	0.1970(2)	0.051(2)	0.046(2)	0.034(2)	0.007(2)	0.013(2)	–0.001(2)
C(5)	4*e*	–0.2854(4)	0.7628(3)	0.1453(2)	0.059(3)	0.055(3)	0.055(3)	0.020(2)	0.012(2)	0.007(2)
C(6)	4*e*	–0.3041(4)	0.7073(3)	0.0924(2)	0.062(3)	0.068(3)	0.040(3)	0.018(2)	–0.004(2)	0.007(2)
C(7)	4*e*	–0.2443(4)	0.6246(3)	0.0895(2)	0.066(3)	0.052(3)	0.039(2)	0.004(2)	0.007(2)	–0.001(2)
C(8)	4*e*	–0.1624(3)	0.6003(2)	0.1415(2)	0.046(2)	0.033(2)	0.032(2)	0.000(2)	0.012(2)	0.003(2)
C(9)	4*e*	–0.0815(4)	0.4448(2)	0.1119(2)	0.068(3)	0.031(2)	0.039(2)	–0.004(2)	0.023(2)	–0.005(2)
C(10)	4*e*	–0.0404(3)	0.4753(2)	0.0538(2)	0.053(2)	0.024(2)	0.036(2)	0.004(2)	0.017(2)	–0.003(2)
C(11)	4*e*	–0.0970(3)	0.4433(2)	–0.0033(2)	0.052(2)	0.035(2)	0.042(2)	–0.005(2)	0.017(2)	–0.007(2)
C(12)	4*e*	0.0574(4)	0.5327(2)	0.0567(2)	0.060(3)	0.038(2)	0.037(2)	–0.003(2)	0.010(2)	–0.005(2)
C(13)	4*e*	0.2014(4)	0.6945(3)	0.4548(2)	0.050(3)	0.052(3)	0.052(3)	–0.015(2)	0.003(2)	–0.001(2)
C(14)	4*e*	0.1439(3)	0.6015(3)	0.4424(2)	0.029(2)	0.042(2)	0.041(2)	–0.001(2)	0.011(2)	0.001(2)
C(15)	4*e*	0.0284(3)	0.4878(2)	0.4032(2)	0.032(2)	0.033(2)	0.039(2)	0.000(2)	0.010(2)	0.000(2)
C(16)	4*e*	–0.0562(3)	0.4316(3)	0.3682(2)	0.043(2)	0.044(2)	0.046(2)	–0.003(2)	0.007(2)	–0.002(2)
C(17)	4*e*	–0.0625(4)	0.3388(3)	0.3861(2)	0.054(3)	0.050(3)	0.061(3)	–0.017(2)	0.016(2)	–0.011(2)
C(18)	4*e*	0.0115(4)	0.3036(3)	0.4377(2)	0.064(3)	0.037(2)	0.079(3)	–0.007(2)	0.025(3)	0.004(2)
C(19)	4*e*	0.0933(4)	0.3587(3)	0.4742(2)	0.048(3)	0.050(3)	0.056(3)	0.009(2)	0.017(2)	0.012(2)
C(20)	4*e*	0.1005(3)	0.4524(3)	0.4557(2)	0.034(2)	0.040(2)	0.040(2)	0.002(2)	0.013(2)	0.003(2)
C(21)	4*e*	0.2692(3)	0.5226(3)	0.5332(2)	0.034(2)	0.058(3)	0.039(2)	0.001(2)	0.006(2)	0.006(2)
C(22)	4*e*	0.3882(3)	0.5115(2)	0.5149(2)	0.034(2)	0.041(2)	0.034(2)	0.000(2)	0.002(2)	0.002(2)
C(23)	4*e*	0.4878(4)	0.5335(3)	0.5559(2)	0.041(2)	0.096(4)	0.042(2)	–0.003(2)	0.006(2)	–0.028(2)
C(24)	4*e*	0.4021(3)	0.4783(3)	0.4582(2)	0.034(2)	0.102(4)	0.048(3)	–0.005(2)	0.000(2)	–0.028(3)
C(25)	4*e*	0.2094(3)	0.7277(3)	0.2922(2)	0.041(2)	0.044(2)	0.052(3)	0.001(2)	0.015(2)	–0.001(2)
C(26)	4*e*	0.2979(3)	0.7941(3)	0.2732(2)	0.036(2)	0.042(2)	0.043(2)	0.001(2)	0.011(2)	–0.001(2)
C(27)	4*e*	0.2857(3)	0.8901(3)	0.2740(2)	0.040(2)	0.046(3)	0.063(3)	0.003(2)	0.020(2)	0.000(2)
C(28)	4*e*	0.3701(4)	0.9495(3)	0.2593(2)	0.065(3)	0.041(2)	0.087(4)	0.002(2)	0.033(3)	0.003(2)
C(29)	4*e*	0.4695(4)	0.9117(3)	0.2450(2)	0.045(3)	0.053(3)	0.059(3)	–0.009(2)	0.018(2)	0.005(2)
C(30)	4*e*	0.4851(4)	0.8171(3)	0.2432(2)	0.053(3)	0.061(3)	0.096(4)	0.005(2)	0.040(3)	0.005(3)
C(31)	4*e*	0.3991(4)	0.7585(3)	0.2574(2)	0.059(3)	0.043(2)	0.100(4)	0.008(2)	0.042(3)	0.004(2)
C(32)	4*e*	–0.1995(3)	0.7080(3)	0.3569(2)	0.035(2)	0.048(2)	0.035(2)	0.002(2)	0.008(2)	0.005(2)
C(33)	4*e*	–0.2959(3)	0.7568(3)	0.3814(2)	0.035(2)	0.047(2)	0.036(2)	0.005(2)	0.009(2)	0.005(2)
C(34)	4*e*	–0.2901(4)	0.8526(3)	0.3954(2)	0.042(2)	0.054(3)	0.067(3)	–0.001(2)	0.021(2)	–0.011(2)
C(35)	4*e*	–0.3808(4)	0.8960(3)	0.4177(2)	0.056(3)	0.053(3)	0.081(3)	0.009(2)	0.018(3)	–0.019(2)
C(36)	4*e*	–0.4744(4)	0.8438(3)	0.4270(2)	0.038(2)	0.077(3)	0.065(3)	0.014(2)	0.016(2)	–0.013(3)
C(37)	4*e*	–0.4816(4)	0.7496(3)	0.4142(2)	0.041(3)	0.071(3)	0.090(4)	0.000(2)	0.028(3)	–0.001(3)
C(38)	4*e*	–0.3927(3)	0.7069(3)	0.3906(2)	0.045(3)	0.050(2)	0.072(3)	–0.001(2)	0.020(2)	0.005(2)
Cl(1)	4*e*	0.5814(1)	0.98538(9)	0.22884(6)	0.0704(8)	0.0769(8)	0.101(1)	–0.0248(7)	0.0398(8)	0.0033(7)
Cl(2)	4*e*	–0.5874(1)	0.8974(1)	0.45641(8)	0.0587(8)	0.122(1)	0.145(1)	0.0126(8)	0.0425(9)	–0.050(1)
N(1)	4*e*	–0.0556(3)	0.6127(2)	0.2385(1)	0.038(2)	0.035(2)	0.034(2)	0.006(2)	0.008(1)	–0.002(1)
N(2)	4*e*	–0.0857(3)	0.5241(2)	0.1540(1)	0.048(2)	0.032(2)	0.033(2)	0.000(2)	0.014(2)	–0.002(1)
N(3)	4*e*	0.0585(2)	0.5820(2)	0.3949(1)	0.029(2)	0.039(2)	0.038(2)	0.001(1)	0.003(1)	0.001(1)
N(4)	4*e*	0.1726(3)	0.5268(2)	0.4805(1)	0.031(2)	0.043(2)	0.039(2)	0.001(2)	0.005(1)	0.005(2)
O(1)	4*e*	0.2280(3)	0.6430(2)	0.2942(2)	0.064(2)	0.044(2)	0.153(3)	0.004(2)	0.052(2)	0.007(2)
O(2)	4*e*	0.1181(2)	0.7656(2)	0.3069(1)	0.042(2)	0.048(2)	0.051(2)	–0.002(1)	0.021(1)	–0.004(1)
O(3)	4*e*	–0.1107(2)	0.7572(2)	0.3497(1)	0.036(2)	0.044(2)	0.050(2)	0.000(1)	0.018(1)	0.001(1)

Table 3. continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(4)	4*e*	–0.2087(2)	0.6227(2)	0.3457(1)	0.050(2)	0.040(2)	0.077(2)	–0.000(1)	0.021(2)	–0.007(2)
Zn(1)	4*e*	0.00367(4)	0.66858(3)	0.32262(2)	0.0355(2)	0.0358(2)	0.0367(3)	0.0012(2)	0.0086(2)	–0.0006(2)

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