Crystal structure of bis{(4,4′-biphenyldicarboxylato-κ^2O:O')-[μ-2,2′-bis(1*H*-imidazolyl)ether-κ^2N:N']}dizinc(II) tetrahydrate, $Zn_2(C_{14}H_8O_4)_2(C_{10}H_{14}N_4)_2 \cdot 4H_2O$

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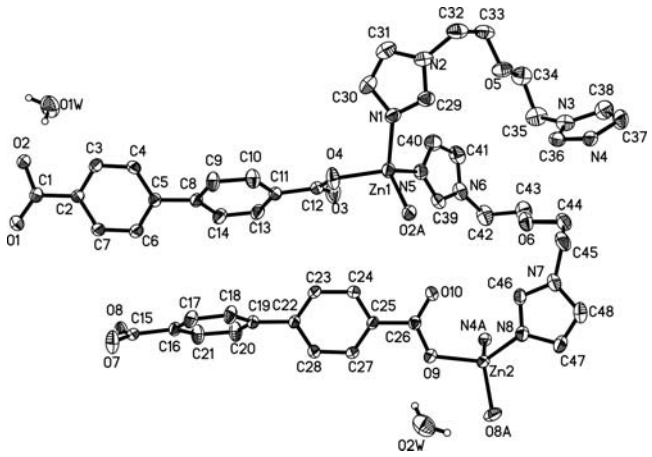

Abstract

$C_{48}H_{48}N_8O_{12}Zn_2$, monoclinic, $P2_1/n$ (no. 14), a = 9.716(3) Å, b = 25.147(6) Å, c = 20.340(4) Å, β = 102.824(9)°, V = 4845.7 Å^3, Z = 4, $R_{gt}(F)$ = 0.063, $wR_{ref}(F^2)$ = 0.127, T = 293 K.

Source of material

A mixture of $Zn(CH_3COO)_2 \cdot 2H_2O$ (43.9 mg, 0.2 mmol), 4,4′-biphenyldicarboxylic acid (H_2L, 48.4 mg, 0.2 mmol) and bis-(imidazole) (BIE, 41.2 mg, 0.2 mmol) was added to water (7 ml). After stirring for 15 min, the precipitate was dissolved by dropwise addition of an aqueous solution of NH_3 (14 M, 3 ml). Colorless crystals were obtained after allowing the solution to stand at room temperature for several days.

Experimental details

All H atoms on C atoms were generated geometrically and refined as riding with d(C—H) = 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C). The hydrogen atoms of water molecules were located in a difference Fourier map and refined isotropically with U_{iso}(H) = 1.5 U_{eq}(O).

Discussion

Bis(imidazole) ligands (BIE), as an important family of flexible N-donor ligands, have attracted chemists' great interest because of their flexible nature of –CH_2– spacers [1]. The flexible nature of –CH_2– spacers allows the backbones to bend and rotate freely when coordinating to metal centers so as to conform to the coordination of metal ions [2]. Up to now, coordination polymers containing 1,1′-(1,4-butanediyl)bis(imidazole) have been widely studied [3]. However, BIE, as a representatively flexible ligand, is rarely investigated in this field [4].

In the title crystal structure, each zinc(II) cation is four-coordinated by two N atoms from two BIE ligands and two O atoms from two 4,4′-biphenyldicarboxylate anions in a slightly distorted tetrahedral manner. The bond lengths of Zn—O and Zn—N are similar to the reported values [4]. The BIE ligands, acting in *trans*-conformation coordination modes, connect the zinc cations to form chains, which are further interconnected by the L^{2-} anions to give layers.

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.15 × 0.18 × 0.27 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	10.61 cm^{-1}
Diffractometer, scan mode:	Bruker APEX CCD, ω
$2\theta_{max}$:	54.92°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	45654, 1098
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 5458
$N(param)_{refined}$:	643
Programs:	SHELXS-97, SHELXL-97 [5]

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

Atom	Site	x	y	z	U_{iso}
H(3)	4*e*	0.2490	0.7440	0.8268	0.052
H(4)	4*e*	0.2974	0.6664	0.7781	0.050
H(6)	4*e*	–0.0630	0.6037	0.8065	0.057
H(7)	4*e*	–0.1015	0.6792	0.8645	0.053
H(9)	4*e*	0.3575	0.5741	0.7854	0.063
H(10)	4*e*	0.4015	0.5055	0.7182	0.062
H(13)	4*e*	–0.0054	0.5002	0.6277	0.061
H(14)	4*e*	–0.0522	0.5657	0.6985	0.059
H(17)	4*e*	0.0080	0.4946	0.9052	0.060
H(18)	4*e*	0.0571	0.4300	0.8335	0.063
H(20)	4*e*	–0.3354	0.4416	0.7230	0.066
H(21)	4*e*	–0.3775	0.5103	0.7908	0.065
H(23)	4*e*	0.0760	0.4029	0.7125	0.049
H(24)	4*e*	0.1062	0.3311	0.6462	0.049
H(27)	4*e*	–0.2504	0.2669	0.6782	0.048
H(28)	4*e*	–0.2907	0.3425	0.7353	0.051
H(29)	4*e*	0.6752	0.3375	0.5402	0.062
H(30)	4*e*	0.5768	0.4853	0.5664	0.079
H(31)	4*e*	0.7871	0.4862	0.5204	0.081
H(32A)	4*e*	0.9285	0.3545	0.5131	0.081
H(32B)	4*e*	0.9494	0.4118	0.4864	0.081
H(33A)	4*e*	0.7575	0.3946	0.3924	0.073
H(33B)	4*e*	0.8888	0.3577	0.3932	0.073
H(34A)	4*e*	0.7054	0.2948	0.3289	0.081

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Table 2. Continued.

Atom	Site	x	y	z	U_{iso}
H(34B)	4*e*	0.5869	0.3345	0.3395	0.081
H(35A)	4*e*	0.5008	0.2699	0.4041	0.088
H(35B)	4*e*	0.4953	0.2481	0.3312	0.088
H(36)	4*e*	0.6543	0.2216	0.5009	0.058
H(37)	4*e*	0.8519	0.1212	0.4078	0.076
H(38)	4*e*	0.7097	0.1787	0.3223	0.079
H(39)	4*e*	0.1602	0.2984	0.5046	0.061
H(40)	4*e*	0.3745	0.3971	0.4166	0.075
H(41)	4*e*	0.2307	0.3423	0.3287	0.077
H(42A)	4*e*	0.0022	0.2772	0.3326	0.087
H(42B)	4*e*	0.0045	0.2528	0.4039	0.087
H(43A)	4*e*	0.0807	0.1895	0.3355	0.086

Table 2. Continued.

Atom	Site	x	y	z	U_{iso}
H(43B)	4*e*	0.2039	0.2275	0.3265	0.086
H(44A)	4*e*	0.3823	0.1593	0.3890	0.072
H(44B)	4*e*	0.2457	0.1247	0.3858	0.072
H(45A)	4*e*	0.4343	0.1026	0.4797	0.076
H(45B)	4*e*	0.4176	0.1594	0.5092	0.076
H(46)	4*e*	0.1603	0.1773	0.5338	0.060
H(47)	4*e*	0.0614	0.0285	0.5560	0.072
H(48)	4*e*	0.2724	0.0297	0.5103	0.079
H(1A)	4*e*	0.101(8)	0.8953(6)	0.753(3)	0.164
H(1B)	4*e*	0.115(8)	0.842(2)	0.781(2)	0.164
H(2A)	4*e*	–0.143(7)	0.116(1)	0.722(2)	0.141
H(2B)	4*e*	–0.132(7)	0.173(1)	0.720(2)	0.141

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}
Zn(1)	4*e*	0.39847(5)	0.37644(2)	0.57634(2)	0.0559(3)	0.0352(3)	0.0430(3)	0.0045(2)	0.0154(2)	–0.0001(2)
Zn(2)	4*e*	–0.11776(5)	0.13823(2)	0.56848(2)	0.0524(3)	0.0311(2)	0.0411(3)	–0.0057(2)	0.0160(2)	–0.0022(2)
C(1)	4*e*	0.0435(4)	0.7691(2)	0.8887(2)	0.044(3)	0.037(2)	0.046(2)	0.003(2)	0.007(2)	–0.002(2)
C(2)	4*e*	0.0695(4)	0.7201(1)	0.8512(2)	0.041(3)	0.032(2)	0.038(2)	0.001(2)	0.010(2)	0.002(2)
C(3)	4*e*	0.1873(4)	0.7154(1)	0.8242(2)	0.043(3)	0.036(2)	0.053(2)	–0.006(2)	0.012(2)	–0.005(2)
C(4)	4*e*	0.2148(4)	0.6693(1)	0.7937(2)	0.039(3)	0.044(2)	0.047(2)	0.001(2)	0.020(2)	–0.001(2)
C(5)	4*e*	0.1210(4)	0.6266(1)	0.7857(2)	0.035(2)	0.034(2)	0.044(2)	0.005(2)	0.010(2)	–0.002(2)
C(6)	4*e*	0.0017(5)	0.6315(1)	0.8118(2)	0.052(3)	0.034(2)	0.061(3)	–0.003(2)	0.022(2)	–0.001(2)
C(7)	4*e*	–0.0229(4)	0.6772(1)	0.8456(2)	0.042(3)	0.039(2)	0.056(2)	0.001(2)	0.022(2)	–0.002(2)
C(8)	4*e*	0.1486(4)	0.5789(1)	0.7475(2)	0.045(3)	0.032(2)	0.039(2)	–0.001(2)	0.010(2)	–0.001(2)
C(9)	4*e*	0.2835(5)	0.5594(2)	0.7536(2)	0.046(3)	0.053(3)	0.052(2)	0.011(2)	–0.005(2)	–0.017(2)
C(10)	4*e*	0.3099(5)	0.5184(2)	0.7129(2)	0.043(3)	0.053(3)	0.055(3)	0.018(2)	0.001(2)	–0.007(2)
C(11)	4*e*	0.2032(4)	0.4961(1)	0.6647(2)	0.047(3)	0.032(2)	0.045(2)	0.003(2)	0.016(2)	0.002(2)
C(12)	4*e*	0.2333(5)	0.4544(2)	0.6170(2)	0.061(3)	0.035(2)	0.051(3)	–0.005(2)	0.027(2)	–0.002(2)
C(13)	4*e*	0.0684(5)	0.5147(2)	0.6597(2)	0.047(3)	0.043(2)	0.062(3)	–0.010(2)	0.009(2)	–0.014(2)
C(14)	4*e*	0.0404(4)	0.5548(1)	0.7015(2)	0.038(3)	0.038(2)	0.070(3)	–0.001(2)	0.012(2)	–0.006(2)
C(15)	4*e*	–0.2206(5)	0.5523(1)	0.9020(2)	0.054(3)	0.031(2)	0.047(2)	–0.008(2)	0.022(2)	–0.003(2)
C(16)	4*e*	–0.1900(4)	0.5097(1)	0.8553(2)	0.045(3)	0.028(2)	0.041(2)	0.003(2)	0.010(2)	–0.002(2)
C(17)	4*e*	–0.0611(4)	0.4847(2)	0.8678(2)	0.043(3)	0.043(2)	0.058(3)	–0.002(2)	–0.001(2)	–0.013(2)
C(18)	4*e*	–0.0325(4)	0.4450(2)	0.8255(2)	0.042(3)	0.039(2)	0.075(3)	0.010(2)	0.009(2)	–0.015(2)
C(19)	4*e*	–0.1353(4)	0.4274(1)	0.7715(2)	0.046(3)	0.031(2)	0.039(2)	0.001(2)	0.013(2)	–0.002(2)
C(20)	4*e*	–0.2646(5)	0.4523(2)	0.7593(2)	0.050(3)	0.058(3)	0.049(2)	0.015(2)	–0.006(2)	–0.017(2)
C(21)	4*e*	–0.2901(4)	0.4934(2)	0.8006(2)	0.045(3)	0.055(3)	0.058(3)	0.018(2)	–0.003(2)	–0.016(2)
C(22)	4*e*	–0.1114(4)	0.3808(1)	0.7305(2)	0.047(3)	0.026(2)	0.038(2)	0.001(2)	0.012(2)	–0.002(2)
C(23)	4*e*	0.0080(4)	0.3763(1)	0.7041(2)	0.044(3)	0.030(2)	0.053(2)	–0.008(2)	0.017(2)	–0.005(2)
C(24)	4*e*	0.0279(4)	0.3326(1)	0.6655(2)	0.043(3)	0.036(2)	0.048(2)	–0.003(2)	0.020(2)	–0.002(2)
C(25)	4*e*	–0.0687(4)	0.2914(1)	0.6555(2)	0.043(3)	0.027(2)	0.035(2)	0.001(2)	0.007(2)	0.000(2)
C(26)	4*e*	–0.0506(4)	0.2443(1)	0.6121(2)	0.034(2)	0.035(2)	0.041(2)	–0.000(2)	0.007(2)	–0.004(2)
C(27)	4*e*	–0.1863(4)	0.2949(1)	0.6834(2)	0.041(3)	0.034(2)	0.048(2)	–0.009(2)	0.016(2)	–0.005(2)
C(28)	4*e*	–0.2089(4)	0.3398(1)	0.7189(2)	0.042(3)	0.039(2)	0.050(2)	–0.002(2)	0.019(2)	–0.007(2)
C(29)	4*e*	0.6761(5)	0.3745(2)	0.5410(2)	0.051(3)	0.047(3)	0.058(3)	0.001(2)	0.015(2)	0.011(2)
C(30)	4*e*	0.6230(6)	0.4554(2)	0.5552(2)	0.076(4)	0.041(3)	0.078(3)	–0.005(2)	0.011(3)	0.001(2)
C(31)	4*e*	0.7390(6)	0.4562(2)	0.5299(2)	0.075(4)	0.057(3)	0.066(3)	–0.017(3)	0.008(3)	0.007(2)
C(32)	4*e*	0.8802(5)	0.3842(2)	0.4876(2)	0.046(3)	0.074(3)	0.084(3)	–0.011(3)	0.015(3)	0.011(3)
C(33)	4*e*	0.8155(5)	0.3665(2)	0.4169(2)	0.050(3)	0.066(3)	0.071(3)	–0.001(2)	0.025(3)	0.021(2)
C(34)	4*e*	0.6470(5)	0.3053(2)	0.3596(2)	0.066(3)	0.072(3)	0.060(3)	0.010(3)	0.005(3)	0.024(3)
C(35)	4*e*	0.5582(5)	0.2590(2)	0.3731(2)	0.061(3)	0.081(4)	0.071(3)	–0.001(3)	–0.001(3)	0.015(3)
C(36)	4*e*	0.6858(4)	0.2033(2)	0.4674(2)	0.048(3)	0.053(3)	0.045(2)	–0.009(2)	0.015(2)	–0.004(2)
C(37)	4*e*	0.7939(5)	0.1487(2)	0.4160(2)	0.086(4)	0.057(3)	0.049(3)	–0.002(3)	0.022(3)	–0.018(2)
C(38)	4*e*	0.7154(5)	0.1801(2)	0.3686(2)	0.090(4)	0.069(3)	0.036(2)	–0.013(3)	0.010(3)	–0.010(2)
C(39)	4*e*	0.1954(4)	0.3165(2)	0.4719(2)	0.048(3)	0.057(3)	0.051(3)	0.008(2)	0.019(2)	–0.002(2)
C(40)	4*e*	0.3132(5)	0.3703(2)	0.4234(2)	0.080(4)	0.060(3)	0.050(3)	0.002(3)	0.018(3)	0.013(2)
C(41)	4*e*	0.2333(5)	0.3404(2)	0.3747(2)	0.079(4)	0.073(3)	0.042(2)	0.017(3)	0.014(3)	0.007(2)
C(42)	4*e*	0.0635(5)	0.2640(2)	0.3737(2)	0.051(3)	0.092(4)	0.068(3)	0.001(3)	0.000(3)	–0.024(3)
C(43)	4*e*	0.1449(5)	0.2171(2)	0.3570(2)	0.067(4)	0.084(4)	0.058(3)	–0.001(3)	0.000(3)	–0.025(3)
C(44)	4*e*	0.3070(5)	0.1513(2)	0.4118(2)	0.050(3)	0.069(3)	0.066(3)	–0.005(2)	0.024(2)	–0.021(2)
C(45)	4*e*	0.3674(5)	0.1309(2)	0.4818(2)	0.040(3)	0.078(3)	0.074(3)	0.004(2)	0.018(3)	–0.024(3)
C(46)	4*e*	0.1602(5)	0.1403(2)	0.5334(2)	0.051(3)	0.041(2)	0.060(3)	0.001(2)	0.019(2)	–0.015(2)
C(47)	4*e*	0.1068(5)	0.0588(2)	0.5455(2)	0.080(4)	0.034(2)	0.070(3)	0.006(2)	0.022(3)	–0.002(2)
C(48)	4*e*	0.2236(5)	0.0592(2)	0.5205(2)	0.072(4)	0.054(3)	0.071(3)	0.020(3)	0.018(3)	–0.012(2)

Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	4*e*	0.5826(4)	0.4037(1)	0.5623(2)	0.057(3)	0.040(2)	0.050(2)	–0.006(2)	0.014(2)	0.004(2)
N(2)	4*e*	0.7727(4)	0.4045(1)	0.5207(2)	0.047(3)	0.056(2)	0.058(2)	–0.009(2)	0.008(2)	0.011(2)
N(3)	4*e*	0.6463(4)	0.2141(1)	0.4017(2)	0.047(2)	0.064(2)	0.047(2)	–0.005(2)	0.004(2)	0.005(2)
N(4)	4*e*	0.7753(4)	0.1634(1)	0.4786(2)	0.055(2)	0.040(2)	0.043(2)	–0.008(2)	0.017(2)	–0.007(2)
N(5)	4*e*	0.2901(4)	0.3550(1)	0.4850(2)	0.059(3)	0.045(2)	0.046(2)	0.006(2)	0.016(2)	0.001(2)
N(6)	4*e*	0.1566(4)	0.3068(1)	0.4054(2)	0.049(3)	0.069(3)	0.047(2)	0.011(2)	0.004(2)	–0.010(2)
N(7)	4*e*	0.2567(4)	0.1108(1)	0.5130(2)	0.046(2)	0.055(2)	0.053(2)	0.007(2)	0.013(2)	–0.012(2)
N(8)	4*e*	0.0645(4)	0.1107(1)	0.5530(2)	0.064(3)	0.040(2)	0.048(2)	0.001(2)	0.018(2)	–0.004(2)
O(1)	4*e*	–0.0223(3)	0.7678(1)	0.9327(1)	0.058(2)	0.052(2)	0.062(2)	–0.004(1)	0.031(2)	–0.012(1)
O(2)	4*e*	0.1014(3)	0.8121(1)	0.8706(1)	0.066(2)	0.035(2)	0.055(2)	–0.005(1)	0.024(2)	–0.004(1)
O(3)	4*e*	0.1495(4)	0.4455(1)	0.5648(2)	0.074(3)	0.094(3)	0.085(2)	–0.006(2)	0.005(2)	–0.052(2)
O(4)	4*e*	0.3509(4)	0.4308(1)	0.6357(1)	0.085(3)	0.058(2)	0.063(2)	0.029(2)	0.016(2)	–0.012(2)
O(5)	4*e*	0.7319(3)	0.3211(1)	0.4216(1)	0.063(2)	0.065(2)	0.050(2)	–0.010(2)	0.009(2)	0.019(2)
O(6)	4*e*	0.2290(3)	0.1982(1)	0.4182(1)	0.066(2)	0.065(2)	0.056(2)	0.004(2)	0.016(2)	–0.017(2)
O(7)	4*e*	–0.1542(3)	0.5542(1)	0.9606(1)	0.092(3)	0.061(2)	0.053(2)	0.017(2)	–0.003(2)	–0.022(2)
O(8)	4*e*	–0.3205(3)	0.5842(1)	0.8767(1)	0.076(2)	0.046(2)	0.051(2)	0.026(2)	0.011(2)	–0.003(1)
O(9)	4*e*	–0.1100(3)	0.20066(9)	0.6262(1)	0.066(2)	0.034(2)	0.052(2)	–0.007(1)	0.022(2)	–0.006(1)
O(10)	4*e*	0.0151(3)	0.2487(1)	0.5676(1)	0.055(2)	0.047(2)	0.059(2)	–0.004(1)	0.029(2)	–0.013(1)
O(1W)	4*e*	0.1008(5)	0.8608(2)	0.7425(2)	0.119(4)	0.138(4)	0.072(2)	–0.013(3)	0.024(3)	–0.023(2)
O(2W)	4*e*	–0.1196(5)	0.1449(2)	0.7467(2)	0.099(3)	0.131(3)	0.051(2)	–0.006(3)	0.012(2)	–0.010(2)

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