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Crystal structure of bis(2-(3-(carboxylatomethyl-κ*O,O'*)-4-(phenylthio)-phenyl)propanoate-κ*O,O'*)bis(2,2'-dipyridyl-κ*N,N'*)dizinc(II), $C_{54}H_{44}N_4O_8S_2Zn_2$

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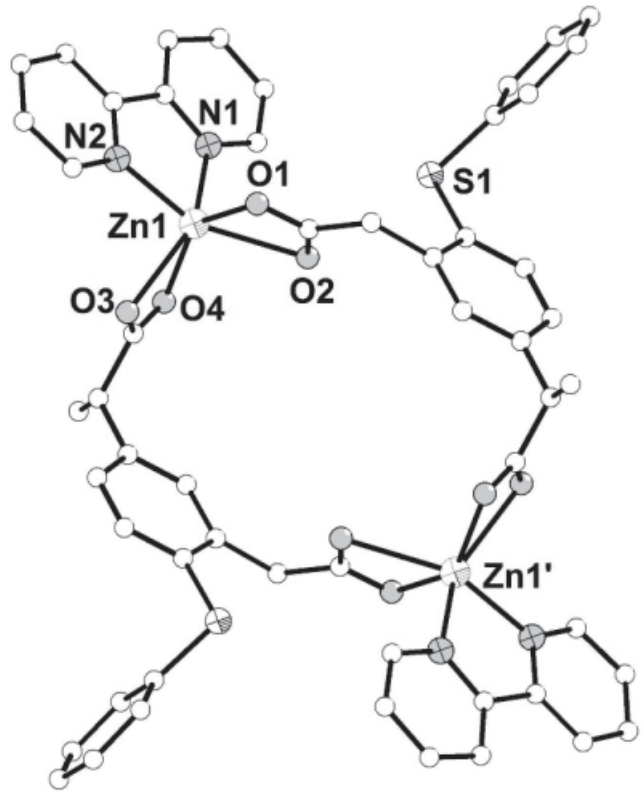

Abstract

$C_{54}H_{44}N_4O_8S_2Zn_2$, monoclinic, $P2_1/c$ (no. 14), a = 13.299(4) Å, b = 12.019(3) Å, c = 15.320(4) Å, β = 93.256(4)°, V = 2444.8 Å^3, Z = 2, $R_{gt}(F)$ = 0.0502, $wR_{ref}(F^2)$ = 0.1430, T = 296 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.19×0.24×0.28 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	11.27 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	12811, 4298
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2416
$N(param)_{refined}$:	317
Programs:	SHELX [5]

Source of material

A mixture of 2-(3-(carboxymethyl)-4-(phenylthio)phenyl) propanoic acid (0.3158 g, 1 mmol), 2,2'-bipyridine (0.1584 g, 1 mmol), $ZnCl_2$ (0.1372 g, 1 mmol), water (10 ml), ethanol (5 ml) and DMF (5 ml) was placed in a Parr Teflon-lined stainless steel vessel (25 ml). Then an aqueous solution of sodium hydroxide was added dropwise until the pH value reached 6.0. The sealed reactor was kept under autogenous pressure at 403K for 72 h and then slowly cooled to room temperature at a rate of 10K per hour. Colourless needles of the title complex were obtained. Elemental analysis cald (%): C, 60.46; H, 4.11; N, 5.23; O, 11.94; S, 5.97; Zn, 12.20. found (%): C, 60.12; H, 4.34; N, 5.57; O, 11.41; S, 6.08; Zn, 12.35.

Experimental details

The positions of all H atoms were fixed geometrically using a riding model, in the later stages the U_{iso} value was fixed. The bond lengths for C–H are about 0.93Å in benzene ring and pyridine ring.

Discussion

Zaltoprofen aroused considerable interest in biology and medicine due to its antiproliferative activities. It is an antimicrobial drug belonging to the carboxylic acid derivatives, and has exhibited wide applications in human and veterinary medicine. The ligand used in this investigation shows some similarities to zaltoprofen. Metal complexes containing carboxylato ligands are of general interest [e.g. 1-4]. In the title compound the Zn metal atom resides in an slightly distorted cis-octahedral geometry. The Zn(II) atom is coordinated by two N atoms from a 2,2'-bipyridine ligand and four carboxylate O atoms (O1, O2, O3a, O4a) from two dicarboxylate ligands. The lengths of the Zn–O bonds range from 2.022(4) to 2.372(4) Å. The Zn–N1 and Zn–N2 bond legnths are 2.067(4) and 2.091(4) Å, respectively. Two Zn metal centres are centrosymmetrically bridged by two dicarboxylic ligands giving a cyclic dimer. The phenylsulfide bases are located outside of the dimeric unit (Fig.).

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

Atom	Site	x	y	z	U_{iso}
H(1)	4*e*	0.9250	0.7582	0.2062	0.079
H(2)	4*e*	0.8576	0.8741	0.0995	0.100
H(3)	4*e*	0.9104	0.8579	–0.0403	0.111
H(4)	4*e*	1.0298	0.7244	–0.0719	0.090
H(7)	4*e*	1.1324	0.5863	–0.0913	0.099
H(8)	4*e*	1.2464	0.4436	–0.1006	0.115
H(9)	4*e*	1.2927	0.3418	0.0220	0.116
H(10)	4*e*	1.2288	0.3898	0.1536	0.097
H(12A)	4*e*	0.8489	0.3465	0.3242	0.086
H(12B)	4*e*	0.7853	0.4131	0.2529	0.086
H(15)	4*e*	0.6095	0.6646	0.4201	0.078
H(16)	4*e*	0.5942	0.5654	0.5443	0.087

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Table 2. continued.

Atom	Site	*x*	*y*	*z*	U_{iso}
H(18)	4*e*	0.7922	0.3477	0.4672	0.079
H(19)	4*e*	0.3982	0.5165	0.1703	0.147
H(20)	4*e*	0.5592	0.4986	0.2356	0.110
H(22)	4*e*	0.6040	0.8231	0.1991	0.102
H(23)	4*e*	0.4454	0.8357	0.1310	0.139

Table 2. continued.

Atom	Site	*x*	*y*	*z*	U_{iso}
H(24)	4*e*	0.3427	0.6868	0.1205	0.163
H(25A)	4*e*	0.5892	0.2733	0.5572	0.197
H(25B)	4*e*	0.6271	0.2518	0.6545	0.197
H(25C)	4*e*	0.6977	0.2260	0.5786	0.197
H(26)	4*e*	0.6288	0.4206	0.6303	0.135

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*	1.07741(4)	0.56504(5)	0.22473(3)	0.0625(4)	0.0723(5)	0.0423(3)	–0.0091(3)	–0.0065(3)	0.0037(3)
S(1)	4*e*	0.7220(1)	0.6492(1)	0.26999(9)	0.0620(8)	0.077(1)	0.0633(8)	–0.0020(7)	–0.0061(7)	0.0191(7)
O(1)	4*e*	0.9759(3)	0.4404(3)	0.2310(2)	0.062(2)	0.077(3)	0.063(2)	0.009(2)	0.008(2)	0.014(2)
O(2)	4*e*	0.9409(3)	0.5763(3)	0.3175(2)	0.073(2)	0.080(3)	0.070(2)	–0.023(2)	0.006(2)	–0.009(2)
O(3)	4*e*	0.7786(4)	0.5028(5)	0.6944(3)	0.142(4)	0.128(4)	0.065(3)	–0.046(4)	–0.022(3)	0.015(3)
O(4)	4*e*	0.8320(3)	0.3359(4)	0.6939(3)	0.085(3)	0.141(4)	0.062(2)	–0.009(3)	–0.015(2)	0.021(3)
N(1)	4*e*	1.0131(3)	0.6735(3)	0.1329(2)	0.060(3)	0.052(3)	0.044(2)	–0.010(2)	–0.004(2)	–0.005(2)
N(2)	4*e*	1.1442(3)	0.5149(4)	0.1109(3)	0.057(3)	0.059(3)	0.057(2)	–0.005(2)	–0.005(2)	0.001(2)
C(1)	4*e*	0.9456(4)	0.7511(5)	0.1495(3)	0.079(4)	0.059(4)	0.060(3)	–0.005(3)	0.001(3)	–0.009(3)
C(2)	4*e*	0.9053(5)	0.8210(5)	0.0862(4)	0.093(5)	0.067(4)	0.089(4)	0.010(3)	–0.008(4)	–0.002(4)
C(3)	4*e*	0.9365(5)	0.8109(6)	0.0035(4)	0.102(5)	0.090(5)	0.083(4)	0.005(4)	–0.026(4)	0.030(4)
C(4)	4*e*	1.0071(4)	0.7310(5)	–0.0158(3)	0.078(4)	0.091(5)	0.055(3)	–0.010(4)	–0.014(3)	0.020(3)
C(5)	4*e*	1.0424(4)	0.6621(4)	0.0505(3)	0.056(3)	0.059(3)	0.041(3)	–0.015(3)	–0.010(2)	0.002(2)
C(6)	4*e*	1.1168(4)	0.5725(4)	0.0383(3)	0.059(3)	0.067(4)	0.047(3)	–0.010(3)	–0.005(2)	–0.004(3)
C(7)	4*e*	1.1533(5)	0.5461(6)	–0.0417(3)	0.088(4)	0.115(6)	0.043(3)	–0.011(4)	–0.002(3)	–0.015(3)
C(8)	4*e*	1.2201(5)	0.4608(7)	–0.0472(4)	0.104(5)	0.117(6)	0.069(4)	0.002(5)	0.017(4)	–0.028(4)
C(9)	4*e*	1.2482(5)	0.4011(6)	0.0251(5)	0.093(5)	0.091(5)	0.106(5)	0.009(4)	0.008(4)	–0.040(4)
C(10)	4*e*	1.2093(5)	0.4303(5)	0.1038(4)	0.078(4)	0.074(4)	0.089(4)	–0.001(4)	–0.014(3)	0.004(3)
C(11)	4*e*	0.9203(4)	0.4856(5)	0.2850(3)	0.047(3)	0.068(4)	0.048(3)	0.005(3)	0.001(2)	0.012(3)
C(12)	4*e*	0.8278(4)	0.4207(4)	0.3062(4)	0.061(3)	0.060(4)	0.096(4)	–0.001(3)	0.013(3)	–0.010(3)
C(13)	4*e*	0.7645(3)	0.4686(4)	0.3763(3)	0.038(3)	0.056(3)	0.063(3)	–0.004(2)	–0.005(2)	–0.005(2)
C(14)	4*e*	0.7091(3)	0.5654(4)	0.3647(3)	0.048(3)	0.058(3)	0.045(3)	–0.003(3)	–0.010(2)	–0.001(2)
C(15)	4*e*	0.6467(4)	0.5996(5)	0.4285(3)	0.065(4)	0.068(4)	0.062(3)	0.009(3)	0.002(3)	–0.009(3)
C(16)	4*e*	0.6381(4)	0.5407(5)	0.5033(3)	0.070(4)	0.101(5)	0.045(3)	–0.011(4)	0.002(3)	–0.010(3)
C(17)	4*e*	0.6924(4)	0.4463(5)	0.5196(3)	0.057(3)	0.094(5)	0.044(3)	–0.027(3)	–0.012(3)	0.011(3)
C(18)	4*e*	0.7544(4)	0.4119(4)	0.4567(4)	0.048(3)	0.061(4)	0.085(4)	–0.007(3)	–0.027(3)	0.022(3)
C(19)	4*e*	0.4401(6)	0.5783(8)	0.1762(5)	0.104(6)	0.152(8)	0.106(5)	–0.054(5)	–0.038(5)	0.039(5)
C(20)	4*e*	0.5365(5)	0.5678(6)	0.2157(4)	0.091(5)	0.102(5)	0.080(4)	–0.014(4)	–0.024(3)	0.023(4)
C(21)	4*e*	0.5975(4)	0.6583(5)	0.2254(3)	0.060(3)	0.071(4)	0.046(3)	–0.002(3)	–0.004(2)	0.004(3)
C(22)	4*e*	0.5632(4)	0.7603(5)	0.1935(4)	0.086(4)	0.087(5)	0.079(4)	0.011(4)	–0.014(3)	0.024(3)
C(23)	4*e*	0.4679(6)	0.7676(7)	0.1534(5)	0.093(5)	0.138(7)	0.114(6)	0.018(5)	–0.026(5)	0.048(5)
C(24)	4*e*	0.4074(6)	0.679(1)	0.1461(5)	0.084(5)	0.20(1)	0.119(6)	–0.023(6)	–0.040(5)	0.075(7)
C(25)	4*e*	0.6467(6)	0.2752(6)	0.5981(4)	0.176(8)	0.126(7)	0.087(4)	–0.080(6)	–0.034(5)	0.037(4)
C(26)	4*e*	0.6838(6)	0.3812(7)	0.6035(4)	0.122(6)	0.147(7)	0.064(4)	–0.075(5)	–0.042(4)	0.042(4)
C(27)	4*e*	0.7720(5)	0.4071(7)	0.6673(3)	0.091(5)	0.108(6)	0.042(3)	–0.047(4)	–0.007(3)	0.022(3)

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