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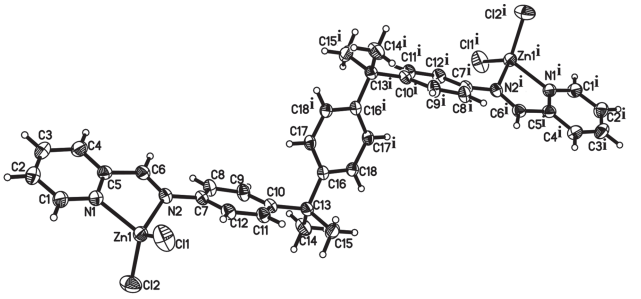
Crystal structure of tetrachlorido(1*E*,1′*E*)-*N*,*N*′-((1,4-phenylenebis(propane-2,2-diyl))bis(4,1-phenylene))bis(1-(pyridin-2-yl-κ*N*)methanimine-κ*N*)dizinc(II), $C_{36}H_{34}N_4Zn_2Cl_4$



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Abstract

$C_{36}H_{34}N_4Zn_2Cl_4$, monoclinic, $P2_1/n$, $a = 7.4932(15)$ Å, $b = 18.4540(37)$ Å, $c = 12.9670(26)$ Å, $\beta = 99.862(30)°$, $V = 1766.57(59)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0400$, $wR_{ref}(F^2) = 0.1184$, $T = 293$ K.

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The crystal structure is shown in the figure (symmetry code i: $-x$, $1-y$, $1-z$). Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

All reagents for synthesis were purchased commercially and used as received. A mixture of $ZnCl_2$ (0.0204 g, 0.15 mmol), and the Schiff-base ligand ((1*E*,1′*E*)-*N*,*N*′-((1,4-phenylenebis(propane-2,2-diyl))bis(4,1-phenylene))bis(1-(pyridin-2-yl)methanimine) (L)) (0.0796 g, 0.10 mmol) was dissolved in water (10 mL) under stirring. The resulting mixture was left standing for several days to give a colorless crystalline product (Yield: 63% based on the added amounts of $ZnCl_2$).

Table 1: Data collection and handling.

Crystal:	Colourless, block, size 0.49×0.50×0.53 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	16.92 cm^{-1}
Diffractometer, scan mode:	Bruker SMART APEX CCD, ω scan
$2\theta_{max}$:	54.96°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4042, 4042
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3058
$N(param)_{refined}$:	208
Programs:	Bruker programs [3], SHELX [4]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1)	4*e*	1.1580	0.0667	0.5314	0.076
H(2)	4*e*	1.3478	0.0889	0.4136	0.083
H(3)	4*e*	1.3227	0.1952	0.3225	0.085
H(4)	4*e*	1.1051	0.2805	0.3514	0.073
H(6)	4*e*	0.8478	0.3132	0.4469	0.061
H(8)	4*e*	0.7436	0.3950	0.5456	0.064
H(9)	4*e*	0.5323	0.4658	0.6072	0.065
H(11)	4*e*	0.2690	0.2891	0.6750	0.059
H(12)	4*e*	0.4899	0.2180	0.6240	0.060
H(14A)	4*e*	0.3993	0.4717	0.8155	0.109
H(14B)	4*e*	0.2376	0.5246	0.7777	0.109
H(14C)	4*e*	0.4036	0.5224	0.7189	0.109
H(15A)	4*e*	0.1771	0.3705	0.8031	0.103
H(15B)	4*e*	0.0457	0.3556	0.6975	0.103
H(15C)	4*e*	0.0197	0.4249	0.7633	0.103
H(17)	4*e*	0.1968	0.4089	0.4742	0.055
H(18)	4*e*	−0.0070	0.5421	0.6663	0.055

Experimental details

All H atoms were refined using a riding model, with C—H distances of 0.93 Å and U_{iso}(H) values of $1.2U_{eq}$(C) for aromatic

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Table 3: Atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	4*e*	1.1478(4)	0.1104(2)	0.4951(2)	0.075(2)	0.058(2)	0.058(2)	0.023(2)	0.017(2)	0.003(1)
C(2)	4*e*	1.2618(5)	0.1232(2)	0.4242(3)	0.071(2)	0.074(2)	0.067(2)	0.020(2)	0.023(2)	−0.005(2)
C(3)	4*e*	1.2469(5)	0.1858(2)	0.3707(3)	0.073(2)	0.083(2)	0.062(2)	0.006(2)	0.030(2)	−0.005(2)
C(4)	4*e*	1.1173(4)	0.2368(2)	0.3876(2)	0.070(2)	0.060(2)	0.054(2)	0.003(1)	0.018(1)	0.003(1)
C(5)	4*e*	1.0086(4)	0.2202(2)	0.4594(2)	0.054(1)	0.052(1)	0.042(1)	0.005(1)	0.006(1)	−0.002(1)
C(6)	4*e*	0.8681(4)	0.2694(1)	0.4825(2)	0.054(1)	0.048(1)	0.049(1)	0.009(1)	0.006(1)	0.004(1)
C(7)	4*e*	0.6386(3)	0.2987(1)	0.5806(2)	0.040(1)	0.041(1)	0.050(1)	0.007(1)	0.001(1)	0.002(1)
C(8)	4*e*	0.6503(4)	0.3736(2)	0.5737(2)	0.041(1)	0.045(1)	0.076(2)	0.003(1)	0.013(1)	0.008(1)
C(9)	4*e*	0.5215(4)	0.4156(1)	0.6092(2)	0.043(1)	0.038(1)	0.081(2)	0.004(1)	0.012(1)	0.006(1)
C(10)	4*e*	0.3761(3)	0.3859(1)	0.6480(2)	0.037(1)	0.043(1)	0.050(1)	0.0061(9)	−0.000(1)	0.002(1)
C(11)	4*e*	0.3660(3)	0.3109(1)	0.6510(2)	0.041(1)	0.046(1)	0.059(2)	−0.002(1)	0.006(1)	0.004(1)
C(12)	4*e*	0.4974(4)	0.2682(1)	0.6192(2)	0.050(1)	0.037(1)	0.062(2)	0.001(1)	0.006(1)	0.005(1)
C(13)	4*e*	0.2336(3)	0.4352(1)	0.6827(2)	0.043(1)	0.048(1)	0.048(1)	0.009(1)	0.005(1)	0.001(1)
C(14)	4*e*	0.3272(5)	0.4939(2)	0.7555(3)	0.065(2)	0.074(2)	0.071(2)	0.020(2)	−0.010(2)	−0.021(2)
C(15)	4*e*	0.1072(4)	0.3925(2)	0.7422(2)	0.072(2)	0.074(2)	0.069(2)	0.028(2)	0.034(2)	0.025(2)
C(16)	4*e*	0.1162(3)	0.4693(1)	0.5864(2)	0.034(1)	0.037(1)	0.051(1)	0.0013(9)	0.009(1)	0.0011(9)
C(17)	4*e*	0.1175(3)	0.4456(1)	0.4855(2)	0.041(1)	0.042(1)	0.055(1)	0.011(1)	0.011(1)	−0.003(1)
C(18)	4*e*	−0.0034(3)	0.5246(1)	0.5994(2)	0.046(1)	0.046(1)	0.047(1)	0.010(1)	0.011(1)	−0.003(1)
N(1)	4*e*	1.0252(3)	0.1574(1)	0.5137(2)	0.054(1)	0.054(1)	0.050(1)	0.010(1)	0.011(1)	0.002(1)
N(2)	4*e*	0.7729(3)	0.2521(1)	0.5518(2)	0.044(1)	0.045(1)	0.054(1)	0.0073(9)	0.0061(9)	0.0019(9)
Cl(1)	4*e*	0.6601(1)	0.06869(5)	0.6156(1)	0.0810(6)	0.0612(5)	0.164(1)	−0.0088(5)	0.0119(7)	0.0222(6)
Cl(2)	4*e*	1.0246(2)	0.18354(6)	0.77780(7)	0.1196(8)	0.0787(6)	0.0638(5)	0.0226(6)	−0.0097(5)	−0.0091(4)
Zn(1)	4*e*	0.85997(4)	0.15503(2)	0.62656(2)	0.0567(2)	0.0446(2)	0.0546(2)	0.0100(1)	0.0154(1)	0.0059(1)

and Schiff-base groups, and 0.96 Å and U_{iso}(H) values of $1.5U_{eq}$(C) for methyl groups.

Discussion

There is one Zn(II), two chlorido ligands and one half of the organic ligand L in the asymmetric unit. There is an inversion center that occurs at the centroid of the central benzene ring in the molecule. Therefore, the ligand L uses a *meso*-configuration to render the structure achiral [1]. The total molecule exhibits a symmetrical Z-shaped structure. For crystallographically unique part of L, two phenyl rings and one pyridyl ring are not coplanar with each other. The metal center (Zn1 atom) is tetrahedrally coordinated by two N atoms from L and two chlorido ligands. The bond angles Zn1 are in the range of 80.25(9)–120.62(5)°, defining a significantly distorted tetrahedron. The Zn–N distances (2.073(2) Å for Zn1–N1 and 2.088(2) Å for Zn1–N2) and the Zn–Cl bond lengths (2.175(1) Å for Zn1–Cl1 and 2.195(1) Å for Zn1–Cl2) are in normal ranges [2]. The most interesting structural feature for title compound is the hydrogen-bonding role in stabilizing open three-dimensional framework. Each chlorido ligand takes part in the formation of weak C—H···Cl H-bonding interactions with the C atoms of pyridine rings. The two H-bonding performances result in a complicated supramolecular three-dimensional framework.

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