Crystal structure of bis(pyridine)chlorido(4-hydroxybenzoato-κ^1O) zinc(II), $C_{17}H_{15}ClN_2O_3Zn$

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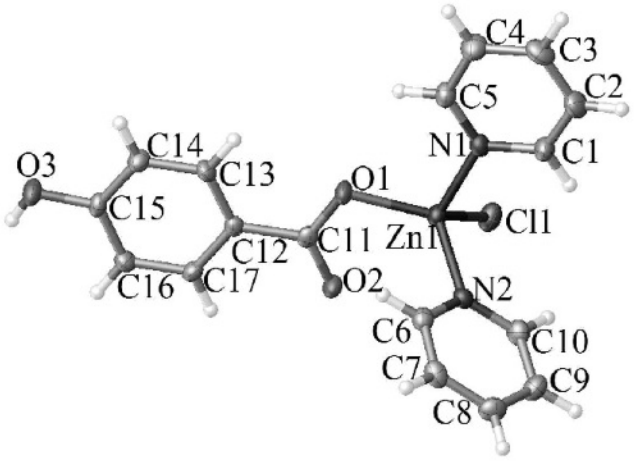
Received May 26, 2014, accepted September 22, 2014, available online October 10, 2014, CCDC no. 1267/4175



Abstract

$C_{17}H_{15}ClN_2O_3Zn$, monoclinic, $P2_1/n$ (no. 14), a = 10.0944(15) Å, b = 13.637(2) Å, c = 12.6014(19) Å, β = 105.745(3)°, V = 1669.6 Å^3, Z = 4, $R_{gt}(F)$ = 0.0379, $wR_{ref}(F^2)$ = 0.0858, T = 100 K.

Table 1. Data collection and handling.

Crystal:	colourless plates, size 0.03×0.17×0.26 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	16.48 cm^{-1}
Diffractometer, scan mode:	CCD area detector, ω
$2\theta_{max}$:	49.8°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	17342, 2888
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2258
$N(param)_{refined}$:	221
Programs:	SHELX [7], OLEX2 [8]

Source of material

The title compound ([Zn(py)$_2$(hbz)Cl]) was synthesized by adding 0.5 ml pyridine to the mixture of $ZnCl_2$ (0.136 g, 1.0 mmol) and 4-hydroxybenzoic acid (0.138 g, 1 mmol) in methanol. The solution was stirred for half an hour and then kept undisturbed at room temperature for slow evaporation. Colourless plate-shaped crystals of [Zn(py)$_2$(hbz)Cl] were yielded after around one week.

Experimental details

Hydrogen atoms expect for the hydroxyl H were treated as riding with C–H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C). The hydroxyl H was located in difference Fourier map, and distance constraints was applied with O–H = 0.84 Å.

Discussion

All the atoms are situated in general positions (Figure 1). A four coordinated Zn(II) center can be described as a distorted tetrahedron. The coordination sphere is consistuted by one chlorido ligand, two N atoms from two independent pyridine molecules, and one O from the carboxy group of 4-hydroxy-benzoato ligand. The two Zn–N bonds have very similar bond lengths, which are 2.046(3) and 2.042(3) Å for Zn1–N1 and Zn1–N2, respectively. The Zn–O bond is 1.957(2) Å in length, well in line with other reported Zn(II) complexes [1–5]. The distance between Cl1 and Zn1is 2.2189(10) Å, which is in the normal range of Zn–Cl bond as well. The hydroxyl group is not coordinating to Zn(II), but it forms a hydrogen bond with the adjacent complexes. The hydrogen bond is moderately strong [6] with the acceptor (A) and donor (D) distance of 2.694(3) Å. An equvalent O–H···O hydrogen bond is formed at the site of the uncoordinated carboxyl-O. In this way, the mononuclear molecules are extended to a one dimensional chain along crystallographic b direction. The geometry of the carboxyl group is also analyzed, and we found that the two C–O bonds are 1.283 and 1.243 Å, respectively.

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

Atom	Site	x	y	z	U_{iso}
H(3)	4e	–0.192(3)	1.294(3)	0.773(3)	0.04(1)
H(1)	4e	0.1852	0.5512	0.5440	0.035
H(2)	4e	0.3845	0.5230	0.4932	0.041
H(3A)	4e	0.5129	0.6562	0.4586	0.038
H(4)	4e	0.4380	0.8149	0.4814	0.040
H(5)	4e	0.2370	0.8366	0.5342	0.032
H(6)	4e	0.1558	0.7423	0.8280	0.029
H(7)	4e	0.2168	0.6575	0.9930	0.032
H(8)	4e	0.1612	0.4911	0.9956	0.035
H(9)	4e	0.0471	0.4140	0.8284	0.035
H(10)	4e	–0.0103	0.5055	0.6679	0.031
H(13)	4e	0.0857	1.0354	0.6436	0.028
H(14)	4e	0.0605	1.2006	0.6793	0.030
H(16)	4e	–0.2692	1.1358	0.7903	0.027
H(17)	4e	–0.2416	0.9709	0.7574	0.026

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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*	0.01738(4)	0.71484(3)	0.59322(3)	0.0240(2)	0.0179(2)	0.0254(2)	–0.0003(2)	0.0081(2)	–0.0009(2)
Cl(1)	4*e*	–0.15394(9)	0.64196(6)	0.47032(7)	0.0306(5)	0.0224(5)	0.0330(5)	–0.0014(4)	0.0014(4)	–0.0008(4)
O(1)	4*e*	0.0318(2)	0.8553(2)	0.6261(2)	0.029(1)	0.014(1)	0.035(2)	0.001(1)	0.015(1)	–0.003(1)
O(2)	4*e*	–0.1428(2)	0.8177(2)	0.6916(2)	0.029(1)	0.017(1)	0.034(2)	–0.004(1)	0.014(1)	–0.003(1)
O(3)	4*e*	–0.1231(3)	1.2817(2)	0.7515(2)	0.026(2)	0.017(1)	0.043(2)	–0.001(1)	0.013(1)	–0.004(1)
N(1)	4*e*	0.1936(3)	0.6962(2)	0.5450(2)	0.024(2)	0.021(2)	0.022(2)	0.002(1)	0.006(1)	–0.001(1)
N(2)	4*e*	0.0672(3)	0.6316(2)	0.7332(2)	0.022(2)	0.022(2)	0.020(2)	0.001(1)	0.008(1)	–0.001(1)
C(1)	4*e*	0.2378(4)	0.6056(3)	0.5316(3)	0.037(2)	0.020(2)	0.036(2)	–0.001(2)	0.017(2)	–0.003(2)
C(2)	4*e*	0.3555(4)	0.5882(3)	0.5008(3)	0.037(2)	0.030(2)	0.039(2)	0.009(2)	0.018(2)	0.001(2)
C(3)	4*e*	0.4313(4)	0.6665(3)	0.4809(3)	0.024(2)	0.045(3)	0.030(2)	0.004(2)	0.011(2)	–0.003(2)
C(4)	4*e*	0.3871(4)	0.7596(3)	0.4940(3)	0.028(2)	0.032(2)	0.042(2)	–0.004(2)	0.013(2)	–0.001(2)
C(5)	4*e*	0.2676(3)	0.7720(3)	0.5258(3)	0.026(2)	0.022(2)	0.031(2)	0.000(2)	0.007(2)	–0.003(2)
C(6)	4*e*	0.1333(3)	0.6747(3)	0.8285(3)	0.020(2)	0.023(2)	0.029(2)	–0.001(2)	0.008(2)	–0.002(2)
C(7)	4*e*	0.1699(3)	0.6248(3)	0.9269(3)	0.020(2)	0.032(2)	0.025(2)	0.002(2)	0.002(2)	–0.007(2)
C(8)	4*e*	0.1376(4)	0.5270(3)	0.9285(3)	0.027(2)	0.033(2)	0.025(2)	0.004(2)	0.005(2)	0.007(2)
C(9)	4*e*	0.0699(3)	0.4817(3)	0.8301(3)	0.029(2)	0.023(2)	0.034(2)	–0.003(2)	0.007(2)	0.003(2)
C(10)	4*e*	0.0365(3)	0.5366(3)	0.7350(3)	0.025(2)	0.026(2)	0.025(2)	–0.003(2)	0.004(2)	–0.004(2)
C(11)	4*e*	–0.0630(3)	0.8798(2)	0.6712(3)	0.023(2)	0.020(2)	0.016(2)	0.002(2)	0.001(2)	0.003(1)
C(12)	4*e*	–0.0754(3)	0.9860(2)	0.6962(3)	0.022(2)	0.018(2)	0.016(2)	0.002(2)	0.004(2)	0.000(1)
C(13)	4*e*	0.0133(3)	1.0556(2)	0.6735(3)	0.025(2)	0.022(2)	0.026(2)	0.003(2)	0.012(2)	–0.002(2)
C(14)	4*e*	–0.0022(3)	1.1539(3)	0.6939(3)	0.022(2)	0.021(2)	0.032(2)	–0.002(2)	0.010(2)	0.001(2)
C(15)	4*e*	–0.1092(3)	1.1844(2)	0.7357(3)	0.024(2)	0.015(2)	0.022(2)	0.001(2)	0.003(2)	–0.002(2)
C(16)	4*e*	–0.1971(3)	1.1155(2)	0.7600(3)	0.023(2)	0.023(2)	0.025(2)	0.002(2)	0.011(2)	–0.001(2)
C(17)	4*e*	–0.1806(3)	1.0176(2)	0.7405(3)	0.025(2)	0.019(2)	0.023(2)	–0.003(2)	0.008(2)	0.001(2)

Acknowledgments. The authors are grateful for support from Scientific and technological project of Henan Science and Technology Agency (142102210402).

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