Wang Li-Hua, Liang Lei and Tai Xi-Shi*

The crystal structure 2,2'-bipyridine- κ^2N,N' -(2-(3-amino-4-chlorobenzoyl)benzoato- κ^1O)-(2-(3-amino-4-chlorobenzoyl)benzoato- κ^2O,O')zinc(II) – ethanol (1/1), $C_{40}H_{32}Cl_2N_4O_7Zn$

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.13 × 0.11 × 0.09 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.88 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	25.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	16321, 6406, 0.043
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 5112
$N(\text{param})_{\text{refined}}$:	502
Programs:	Bruker [1], Olex2 [2], SHELX [3], Diamond [4]

<https://doi.org/10.1515/ncrs-2020-0261>

Received May 27, 2020; accepted August 13, 2020; available online August 25, 2020

Abstract

$C_{40}H_{32}Cl_2N_4O_7Zn$, monoclinic, $P2_1/c$ (no. 14), $a = 13.5114(8)$ Å, $b = 16.5735(7)$ Å, $c = 17.0403(9)$ Å, $\beta = 107.528(6)^\circ$, $V = 3638.7(3)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0398$, $wR_{\text{ref}}(F^2) = 0.0831$, $T = 100$ K.

CCDC no.: 2023128

The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

0.1378 g 2-(3-Amino-4-chloro-benzoyl)benzoic acid (0.5 mmol), 0.020 g NaOH (0.5 mmol) and 0.0780 g

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.34474(2)	0.35986(2)	0.58398(2)	0.01581(10)
Cl1	0.23354(6)	0.47766(5)	0.21345(4)	0.02819(19)
Cl2	0.20843(5)	0.74272(4)	0.76205(4)	0.02696(18)
O1	−0.02269(15)	0.29723(12)	0.44381(12)	0.0271(5)
O2	0.34630(15)	0.19617(12)	0.57818(11)	0.0255(5)
O3	0.22322(14)	0.28999(11)	0.54183(10)	0.0199(4)
O4	0.37922(16)	0.36922(11)	0.70717(11)	0.0264(5)
O5	0.52489(17)	0.36857(11)	0.67401(11)	0.0295(5)
O6	0.31600(16)	0.35665(12)	0.86597(13)	0.0309(5)
O7	−0.09230(15)	0.21257(13)	0.56274(12)	0.0280(5)
H7	−0.082068	0.230596	0.521040	0.042*
N1	0.2695(2)	0.30022(19)	0.24191(16)	0.0273(6)
H1A	0.286(2)	0.2533(18)	0.2525(17)	0.018(9)*
H1B	0.294(2)	0.3321(19)	0.2091(18)	0.031(9)*
N2	0.40791(17)	0.36563(13)	0.48843(12)	0.0164(5)
N3	0.30515(16)	0.47661(13)	0.54452(12)	0.0164(5)
N4	0.4340(2)	0.69564(14)	0.81109(15)	0.0199(6)
H4A	0.403006	0.741060	0.810727	0.024*
H4B	0.494(3)	0.689(2)	0.8383(19)	0.040(11)*
C1	0.1770(2)	0.15828(16)	0.49308(15)	0.0147(6)
C2	0.1971(2)	0.07587(17)	0.50263(16)	0.0195(6)
H2	0.260572	0.058240	0.537290	0.023*
C3	0.1239(2)	0.01976(17)	0.46123(16)	0.0213(7)
H3	0.138101	−0.035132	0.468175	0.026*
C4	0.0298(2)	0.04586(17)	0.40963(16)	0.0219(7)
H4	−0.019778	0.008391	0.382069	0.026*
C5	0.0087(2)	0.12757(17)	0.39867(16)	0.0202(6)
H5	−0.054857	0.144612	0.363621	0.024*
C6	0.0821(2)	0.18453(16)	0.43978(15)	0.0153(6)

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C7	0.0512(2)	0.27186(17)	0.42353(16)	0.0190(6)
C8	0.1006(2)	0.32339(16)	0.37458(15)	0.0172(6)
C9	0.1660(2)	0.28938(16)	0.33473(15)	0.0168(6)
H9	0.182269	0.234826	0.342166	0.020*
C10	0.2083(2)	0.33516(17)	0.28353(15)	0.0170(6)
C11	0.1828(2)	0.41745(17)	0.27580(15)	0.0201(6)
C12	0.1183(2)	0.45184(17)	0.31616(16)	0.0224(7)
H12	0.103177	0.506643	0.309986	0.027*
C13	0.0767(2)	0.40576(16)	0.36521(16)	0.0198(6)
H13	0.033000	0.428941	0.391937	0.024*
C14	0.2559(2)	0.21720(17)	0.54166(16)	0.0186(6)
C15	0.4599(2)	0.30682(16)	0.46380(16)	0.0199(6)
H15	0.467141	0.257146	0.490322	0.024*
C16	0.5031(2)	0.31691(17)	0.40094(16)	0.0224(7)
H16	0.539060	0.275063	0.385386	0.027*
C17	0.4918(2)	0.39041(17)	0.36158(16)	0.0217(7)
H17	0.520230	0.398758	0.318839	0.026*
C18	0.4381(2)	0.45179(16)	0.38583(15)	0.0166(6)
H18	0.430367	0.501771	0.359882	0.020*
C19	0.39603(19)	0.43771(15)	0.44943(15)	0.0137(6)
C20	0.33572(19)	0.49916(16)	0.47936(15)	0.0148(6)
C21	0.3125(2)	0.57513(16)	0.44437(16)	0.0200(6)
H21	0.334457	0.590034	0.399709	0.024*
C22	0.2561(2)	0.62842(17)	0.47669(18)	0.0261(7)
H22	0.239428	0.679411	0.453741	0.031*
C23	0.2250(2)	0.60494(17)	0.54361(18)	0.0270(7)
H23	0.186979	0.639735	0.566305	0.032*
C24	0.2514(2)	0.52901(17)	0.57578(17)	0.0240(7)
H24	0.231175	0.513392	0.621085	0.029*
C25	0.4774(3)	0.37229(15)	0.72666(16)	0.0229(7)
C26	0.5377(2)	0.37897(15)	0.81644(15)	0.0139(6)
C27	0.6437(2)	0.36437(15)	0.84157(16)	0.0195(6)
H27	0.677330	0.354774	0.802213	0.023*
C28	0.7004(2)	0.36382(16)	0.92418(17)	0.0215(6)
H28	0.771318	0.353244	0.940309	0.026*
C29	0.6502(2)	0.37920(16)	0.98231(17)	0.0225(7)
H29	0.687742	0.379086	1.037898	0.027*
C30	0.5450(2)	0.39471(16)	0.95868(16)	0.0193(6)
H30	0.512297	0.405419	0.998390	0.023*
C31	0.4872(2)	0.39443(15)	0.87534(15)	0.0152(6)
C32	0.3722(2)	0.40937(16)	0.85364(16)	0.0182(6)
C33	0.3325(2)	0.49129(16)	0.82517(15)	0.0154(6)
C34	0.4004(2)	0.55475(15)	0.82762(14)	0.0146(6)
H34	0.471324	0.544410	0.842815	0.018*
C35	0.3654(2)	0.63382(15)	0.80793(15)	0.0139(6)
C36	0.2576(2)	0.64503(16)	0.78386(15)	0.0173(6)
C37	0.1890(2)	0.58174(17)	0.77938(16)	0.0204(6)
H37	0.117828	0.591240	0.762214	0.024*
C38	0.2259(2)	0.50529(17)	0.80023(15)	0.0197(6)
H38	0.180056	0.462859	0.797751	0.024*
C39	−0.0033(2)	0.22575(19)	0.63107(18)	0.0299(7)
H39A	0.056804	0.203085	0.619176	0.036*
H39B	−0.011905	0.197551	0.678476	0.036*
C40	0.0165(3)	0.3140(2)	0.6522(2)	0.0420(9)
H40A	0.026484	0.342135	0.605880	0.063*
H40B	0.077493	0.319446	0.698617	0.063*
H40C	−0.042015	0.336547	0.665362	0.063*

2,2'-bipyridine (0.5 mmol) were dissolved in 15 mL of a water-95% ethanol (*v:v* = 1:2) solution with stirring at R.T. After the solid was dissolved, 0.1097 g zinc acetate dihydrate (0.5 mmol) was added. The mixture was heated to 75 °C and stirred for 5 h. Filter after reaction, colorless crystals of the title compound were received from the filtrate in three weeks.

Experimental details

Hydrogen atoms were positioned geometrically (C—H = 0.93–0.97 Å, O—H = 0.82 Å and N—H = 0.81–0.90 Å). The *U*_{iso} values were set to 1.2*U*_{eq} or 1.5*U*_{eq} of the parent atoms.

Comment

Zn(II) complexes display excellent properties and potential applications in many ways such as luminescent sensor, explosives detection, antitumor activity, and catalytic degradation [5–8]. As part of our study, some metal complexes have been synthesized and characterized [9–12].

The asymmetric unit of the title structure contains one Zn(II) ion, one 2,2'-bipyridine ligand, two 2-(3-amino-4-chloro-benzoyl)benzoate ligands and one uncoordinated ethanol molecule. In the title complex, two carboxylate groups of two 2-(3-amino-4-chloro-benzoyl)benzoate ligands adopt two coordination modes (monodentate and bidentate). The Zn(II) ion is five-coordinated with three carboxylic O atoms from two benzoate ligands (O3, O4 and O5), and two N atoms from one 2,2'-bipyridine ligand (N2 and N3), and forms a distorted square pyramidal coordination geometry. The Zn—O distances are 1.9602(18) Å (Zn1—O3), 2.0146(18) Å (Zn1—O4), 2.460(2) Å (Zn1—O5), respectively. The Zn—N distances are 2.056(2) Å (Zn1—N2) and 2.065(2) Å (Zn1—N3).

Acknowledgements: This project was supported by the National Natural Science Foundation of China (no. 21171132), the Natural Science Foundation of Shandong (ZR2014BL003), the project of Shandong Province Higher Educational Science and Technology Program (J14LC01) and Science Foundation of Weifang.

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