Ping Zhang*, Yan-Bin Wang and Qiong Su

Crystal structure of bis{5-methoxy-2-(((2-oxo-2*H*-chromen-6-yl)imino)methyl)phenolato-κ²*N*,*O*} zinc(II), $C_{34}H_{24}N_2O_8Zn$

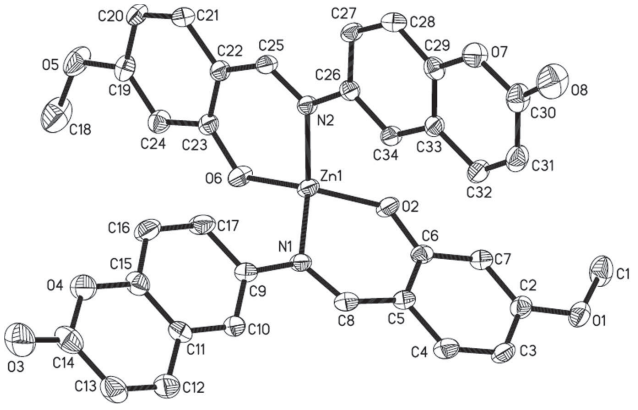

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.27 × 0.26 × 0.22 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.94 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω-scans
θ_{max}, completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9489, 4876, 0.020
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4335
$N(param)_{refined}$:	408
Programs:	Bruker programs [1], SHELX [2]

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Abstract

$C_{34}H_{24}N_2O_8Zn$, triclinic, $P\bar{1}$ (no. 2), $a = 9.1202(6)$ Å, $b = 12.2985(8)$ Å, $c = 12.9973(9)$ Å, $\alpha = 83.799(2)°$, $\beta = 76.063(2)°$, $\gamma = 81.385(2)°$, $Z = 2$, $V = 1395.02(16)$ Å^3, $R_{gt}(F) = 0.0292$, $wR_{ref}(F^2) = 0.0691$, $T = 296(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The ligand was synthesized according to a method reported previously [3, 4]. A solution of 2-hydroxy-5-methoxybenzaldehyde (168.2 mg, 1 mmol) in ethanol (5 ml) was added to a solution of 6-amino-chromen-2-one (161.2 mg, 1 mmol) in ethanol (10 ml). The mixture was stirred at 373 K for 6 h. After cooling to room temperature, the precipitates were collected. The product was dried *in vacuo* (yield 72.7%, m.p. 467–468 K). Anal. calcd. for $C_{17}H_{13}NO_4$ (%): C, 65.15; H, 4.44; N, 4.74. Found (%): C, 66.11; H, 4.33; N, 4.92.

A methanol solution (3 ml) of zinc(II) acetate dihydrate (2.2 mg, 0.01 mmol) was added dropwise to a ethyl acetate solution (4 ml) of 6-[(2-hydroxy-4-methoxy-benzylidene)-amino]-chromen-2-one (5.9 mg, 0.02 mmol) at room temperature. The color of the mixed solution turned to yellow immediately. After stirring for 10 min at room temperature, the mixture was filtered and the filtrate was allowed to stand at room temperature for a week. The solvent partially evaporated and yellow block crystals suitable for X-ray crystallographic analysis were obtained. Elemental analysis-Anal. calcd. for $C_{34}H_{24}N_2O_8Zn$ (%): C, 62.45; H, 3.70; N, 4.28. Found (%): C, 62.53; H, 3.58; N, 4.35.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Discussion

Metal complexes containing O, S, and N Schiff bases have been the subject of current interest because of their application in many fields, such as biological activity reagents [5–7], magnetic materials [8–11], luminescent materials [12–14], and supramolecular building [15–17].

X-ray crystallographic analysis of the Zn(II) complex reveals a mononuclear structure (*cf.* the figure). It crystallizes

***Corresponding author: Ping Zhang,** Northwest Minzu University, College of Chemical Engineering, Lanzhou 730030, P.R. China; and Key Laboratory for Utility of Environment-friendly Composite Materials and Biomass in Universities of Gansu Province, Lanzhou 730030, P.R. China, e-mail: gszhangping@126.com
Yan-Bin Wang and Qiong Su: Northwest Minzu University, College of Chemical Engineering, Lanzhou 730030, P.R. China

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

Atom	x	y	z	U_{iso}*/U_{eq}
C1	0.6028(3)	0.7541(2)	1.01772(19)	0.0364(6)
H1A	0.7035	0.7323	0.9766	0.055*
H1B	0.6065	0.7576	1.0905	0.055*
H1C	0.5640	0.8253	0.9901	0.055*
C2	0.4813(2)	0.66082(17)	0.91538(17)	0.0246(5)
C3	0.3867(3)	0.57961(17)	0.91688(17)	0.0273(5)
H3	0.3490	0.5390	0.9798	0.033*
C4	0.3517(3)	0.56173(17)	0.82474(17)	0.0273(5)
H4	0.2898	0.5078	0.8260	0.033*
C5	0.4057(2)	0.62196(16)	0.72643(16)	0.0220(4)
C6	0.5039(2)	0.70298(16)	0.72507(16)	0.0208(4)
C7	0.5407(2)	0.71963(16)	0.82147(16)	0.0222(4)
H7	0.6058	0.7709	0.8217	0.027*
C8	0.3577(2)	0.59388(16)	0.63712(17)	0.0236(5)
H8	0.2977	0.5369	0.6503	0.028*
C9	0.3271(2)	0.59785(16)	0.46024(17)	0.0221(4)
C10	0.2537(2)	0.50454(17)	0.47601(17)	0.0243(5)
H10	0.2422	0.4631	0.5410	0.029*
C11	0.1970(2)	0.47220(17)	0.39504(17)	0.0246(5)
C12	0.1176(3)	0.37721(19)	0.40816(19)	0.0337(5)
H12	0.1019	0.3351	0.4728	0.040*
C13	0.0662(3)	0.3492(2)	0.3279(2)	0.0362(6)
H13	0.0142	0.2879	0.3382	0.043*
C14	0.0890(3)	0.41137(19)	0.2254(2)	0.0359(6)
C15	0.2175(3)	0.53310(18)	0.29715(18)	0.0272(5)
C16	0.2930(3)	0.62487(19)	0.27887(19)	0.0349(6)
H16	0.3079	0.6645	0.2129	0.042*
C17	0.3462(3)	0.65701(18)	0.36056(18)	0.0307(5)
H17	0.3959	0.7195	0.3490	0.037*
C18	1.0854(3)	0.7387(2)	0.0437(2)	0.0518(8)
H18A	1.1355	0.7287	0.1017	0.078*
H18B	1.1604	0.7354	−0.0224	0.078*
H18C	1.0222	0.6814	0.0500	0.078*
C19	0.8720(2)	0.86096(18)	0.12963(17)	0.0262(5)
C20	0.7800(3)	0.96232(18)	0.11907(17)	0.0270(5)
H20	0.8049	1.0117	0.0601	0.032*
C21	0.6541(3)	0.98597(17)	0.19725(17)	0.0258(5)
H21	0.5922	1.0524	0.1900	0.031*
C22	0.6119(2)	0.91430(16)	0.28961(16)	0.0216(4)
C23	0.7082(2)	0.81277(16)	0.30090(16)	0.0208(4)
C24	0.8373(2)	0.78804(18)	0.21780(17)	0.0253(5)
H24	0.9000	0.7216	0.2226	0.030*
C25	0.4762(2)	0.95360(16)	0.36321(16)	0.0224(4)
H25	0.4272	1.0218	0.3436	0.027*
C26	0.2727(2)	0.95897(16)	0.51655(16)	0.0203(4)
C27	0.1978(2)	1.06238(16)	0.48689(17)	0.0228(4)
H27	0.2397	1.1012	0.4238	0.027*
C28	0.0630(2)	1.10620(17)	0.55088(17)	0.0252(5)
H28	0.0137	1.1739	0.5304	0.030*
C29	0.0009(2)	1.04997(17)	0.64517(17)	0.0231(5)
C30	−0.2049(3)	1.0495(2)	0.80146(18)	0.0322(5)
C31	−0.1330(3)	0.94277(19)	0.83469(18)	0.0316(5)
H31	−0.1799	0.9059	0.8975	0.038*
C32	−0.0010(3)	0.89561(18)	0.77756(17)	0.0283(5)
H32	0.0441	0.8282	0.8024	0.034*
C33	0.0719(2)	0.94833(17)	0.67799(16)	0.0221(4)
C34	0.2082(2)	0.90448(17)	0.61194(16)	0.0226(4)
H34	0.2570	0.8366	0.6327	0.027*
N1	0.38670(19)	0.63737(13)	0.53957(13)	0.0206(4)
N2	0.41149(19)	0.90674(13)	0.45446(13)	0.0194(4)
O1	0.50513(18)	0.67521(13)	1.01177(12)	0.0318(4)
O2	0.56026(16)	0.76425(11)	0.64012(11)	0.0240(3)
O3	0.0491(2)	0.39023(16)	0.14867(15)	0.0521(5)
O4	0.16316(19)	0.50358(13)	0.21484(13)	0.0354(4)
O5	0.99336(19)	0.84369(14)	0.04619(13)	0.0394(4)
O6	0.68377(16)	0.74078(11)	0.38353(11)	0.0256(3)
O7	−0.13397(17)	1.09851(12)	0.70506(12)	0.0297(4)
O8	−0.3203(2)	1.09966(16)	0.84904(15)	0.0510(5)
Zn1	0.51481(3)	0.76140(2)	0.50334(2)	0.02154(8)

in the triclinic system, space group $P\bar{1}$, and consists of one Zn(II) ion, and two bidentate deprotonated ligands. The coordination geometry of the Zn(II) center can be described as distorted tetrahedron. In addition, there are intermolecular non-classical hydrogen bond interactions which link the title complex to form a stable structure.

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