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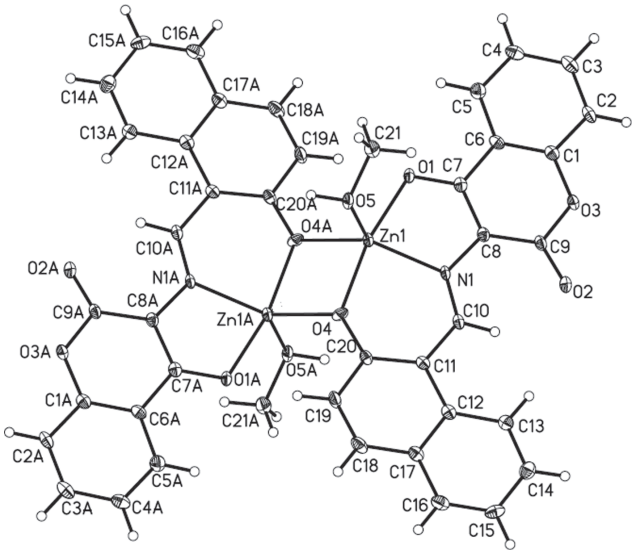
Crystal structure of dimethanol-bis{3-(((2-oxidonaphthalen-1-yl) methylene)amino)-2-oxo-2*H*-chromen-4-olato-κ³*O*,*N*:*O*′}dizinc(II), $C_{42}H_{30}Zn_2N_2O_{10}$



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Abstract

$C_{42}H_{30}Zn_2N_2O_{10}$, monoclinic, $P2_1/c$ (no. 14), $a = 8.5451(9)$ Å, $b = 11.6897(12)$ Å, $c = 18.4893(19)$ Å, $\beta = 100.733(3)°$, $Z = 2$, $V = 1814.6(3)$ Å^3, $R_{gt}(F) = 0.0404$, $wR_{ref}(F^2) = 0.1029$, $T = 296(2)$ 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 materials

Synthesis of the ligand HL: The ligand was synthesized according to an analogous method reported previously in the literature [3, 4]. To an ethanol solution (5 mL) of 2-hydroxy-1-naphthaldehyde (172.2 mg, 1 mmol) was added an ethanol solution (5 mL) of 3-amino-4-hydroxy-2*H*-chromen-2-one (177.2 mg, 1 mmol). The solution was stirred under reflux at 434 K for 6 h. Cooling to room temperature gave a precipitate, which was filtered and washed with ethanol and hexane. The product was dried under vacuum and a yellow solid was obtained (yield 65.5%, m.p. 554-556 K). Elemental analysis-anal. calcd. for $C_{20}H_{13}NO_4$ (%): C, 72.50; H, 3.96; N, 4.23. Found (%): C, 73.47; H, 3.13; N, 4.65.

Synthesis of the zinc(II) complex: To a stirred solution of the ligand (3.31 mg, 0.01 mmol) in methanol (6 mL) was added zinc(II) acetate dihydrate (3.00 mg, 0.014 mmol) in methanol (1 mL) at room temperature. The resultant yellow solution was allowed to evaporate at room temperature in the dark for about two weeks. Colourless block crystals were obtained. Elemental analysis-anal. calcd. for $C_{42}H_{30}Zn_2N_2O_{10}$ (%): C, 59.11; H, 3.54; N, 3.28. Found (%): C, 59.92; H, 3.35; N, 3.36.

Table 1: Data collection and handling.

Crystal:	Block, colourless
Size:	0.27 × 0.25 × 0.21 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	1.39 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω-scans
$2\theta_{max}$, completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	11436, 3191, 0.043
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2629
$N(param)_{refined}$:	248
Programs:	Bruker programs [1], SHELX [2]

Experimental details

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

Discussion

Schiff base compounds and their derivatives can coordinate metal ions as chelating ligand [5–7]. These Schiff base ligands and their metal complexes could be utilized in obtaining luminescence materials [8–11], biological systems [12], magnetic materials [13–15], and supramolecular constructing [16, 17].

The binuclear Zn(II) complex of the title structure consists of two Zn(II) atoms, two tridentate ligand units L^{2-}, two coordinated methanol molecules. As shown in the figure, the Zn(II) center (Zn1 or Zn1A) is coordinated by one N1 and two O atoms (O1, O4) from a tridentate ligand unit, and one O

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.10396(4)	0.61094(3)	0.51075(2)	0.02014(14)
N1	0.3475(3)	0.5981(2)	0.54322(14)	0.0163(6)
O1	0.1682(3)	0.74634(19)	0.45394(13)	0.0246(6)
O2	0.6928(3)	0.6533(2)	0.57022(14)	0.0266(6)
O3	0.6491(3)	0.80050(19)	0.49485(13)	0.0227(5)
O4	0.0873(3)	0.45830(19)	0.55981(12)	0.0218(5)
O5	−0.0045(3)	0.7068(2)	0.57928(14)	0.0258(6)
H5A	−0.1129	0.6951	0.5723	0.031*
C1	0.5501(4)	0.8736(3)	0.44904(18)	0.0203(7)
C2	0.6235(4)	0.9639(3)	0.41851(19)	0.0249(8)
H2	0.7335	0.9728	0.4292	0.030*
C3	0.5291(4)	1.0393(3)	0.37228(19)	0.0286(8)
H3	0.5761	1.0996	0.3513	0.034*
C4	0.3656(5)	1.0264(3)	0.3567(2)	0.0290(8)
H4	0.3035	1.0786	0.3259	0.035*
C5	0.2932(4)	0.9368(3)	0.38644(19)	0.0267(8)
H5	0.1831	0.9283	0.3754	0.032*
C6	0.3870(4)	0.8585(3)	0.43351(18)	0.0197(7)
C7	0.3191(4)	0.7618(3)	0.46688(17)	0.0186(7)
C8	0.4233(4)	0.6886(3)	0.51282(18)	0.0179(7)
C9	0.5901(4)	0.7095(3)	0.52825(18)	0.0193(7)
C10	0.4243(4)	0.5198(3)	0.58451(17)	0.0176(7)
H10	0.5349	0.5222	0.5909	0.021*
C11	0.3566(4)	0.4280(3)	0.62214(17)	0.0174(7)
C12	0.4672(4)	0.3598(3)	0.67370(17)	0.0189(7)
C13	0.6358(4)	0.3761(3)	0.68869(18)	0.0219(7)
H13	0.6793	0.4360	0.6659	0.026*
C14	0.7344(4)	0.3064(3)	0.73540(19)	0.0287(8)
H14	0.8437	0.3191	0.7432	0.034*
C15	0.6750(4)	0.2157(3)	0.77219(19)	0.0282(8)
H15	0.7436	0.1684	0.8039	0.034*
C16	0.5143(5)	0.1988(3)	0.7604(2)	0.0287(8)
H16	0.4737	0.1395	0.7849	0.034*
C17	0.4081(4)	0.2685(3)	0.71198(18)	0.0217(7)
C18	0.2418(4)	0.2496(3)	0.69943(19)	0.0278(8)
H18	0.2022	0.1919	0.7256	0.033*
C19	0.1381(4)	0.3120(3)	0.65096(19)	0.0251(8)
H19	0.0296	0.2964	0.6445	0.030*
C20	0.1932(4)	0.4019(3)	0.60938(17)	0.019
C21	0.0126(5)	0.8301(3)	0.5826(2)	0.0354(9)
H21A	0.1234	0.8496	0.5952	0.053*
H21B	−0.0425	0.8600	0.6193	0.053*
H21C	−0.0320	0.8624	0.5356	0.053*

atom (O5) from a methanol. These two [ZnL(MeOH)] moieties are bridged via two μ_2-O4 atoms (phenolato oxygen) to form a penta-coordination. The coordination geometry of the Zn(II) centers can be described as slightly distorted tetragonal-pyramidal with $\tau = 0.17$.

Meanwhile, a 3D network was formed by intermolecular hydrogen bonds (O5—H5A···O2, O5—H5A···O3) and π···π interactions with the centroid-centroid distances of 3.43–3.81 Å.

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