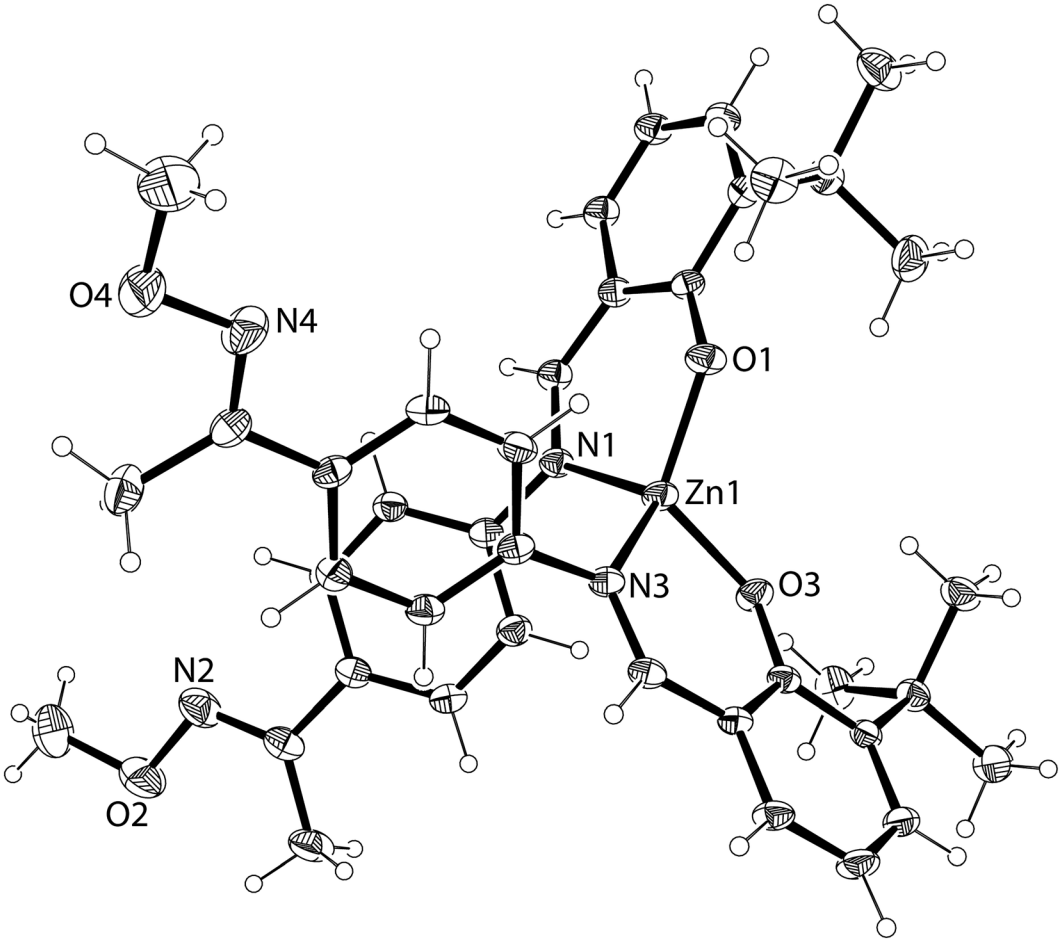
Ji-Xing Zhao*, Lei-Fang Wu and Da-Qun Chen

Crystal structure of bis{2-(*tert*-butyl)-6-((*E*)-((4-((*E*)-1-(methoxyimino)ethyl)phenyl)imino)methyl) phenolato-κ^2*N*,*O*}zinc(II), $C_{40}H_{46}N_4O_4Zn$



https://doi.org/10.1515/ncrs-2022-0135
Received March 20, 2022; accepted April 25, 2022;
published online May 17, 2022

Abstract

$C_{40}H_{46}N_4O_4Zn$, monoclinic, $P2_1/n$ (no. 14), a = 12.0198(4) Å, b = 28.0212(9) Å, c = 12.0655(4) Å, β = 110.727(2)°, V = 3800.8(2) Å^3, Z = 4, $R_{gt}(F)$ = 0.0442, $wR_{ref}(F^2)$ = 0.1076, T = 173(2) K.

***Corresponding author: Ji-Xing Zhao**, Analysis and Testing Center, Shihezi University, Xinjiang 832003, P. R. China,
E-mail: zhaojixing_2016@126.com. https://orcid.org/0000-0002-1322-1860
Lei-Fang Wu and Da-Qun Chen, Analysis and Testing Center, Shihezi University, Xinjiang 832003, P. R. China

CCDC no.: 2168527

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.24 × 0.19 × 0.18 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.69 mm^{-1}
Diffractometer, scan mode:	Bruker D8 Venture, φ and ω
θ_{max}, completeness:	26.7°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	42616, 8073, 0.050
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 6523
$N(param)_{refined}$:	452
Programs:	Bruker [1], SHELX [2, 3]

The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.28531 (2)	0.59356 (2)	0.71876 (2)	0.03305 (9)
C1	0.5173 (2)	0.60719 (8)	0.89700 (19)	0.0286 (5)
O1	0.45066 (15)	0.60809 (7)	0.78447 (14)	0.0381 (4)
N1	0.27742 (17)	0.55999 (7)	0.86204 (17)	0.0316 (4)
O2	−0.2156 (2)	0.39039 (10)	0.8898 (2)	0.0769 (7)
C2	0.4791 (2)	0.58542 (8)	0.9846 (2)	0.0308 (5)
N2	−0.1110 (2)	0.41379 (10)	0.8993 (2)	0.0579 (7)
N3	0.21874 (17)	0.55554 (7)	0.56924 (16)	0.0305 (4)
O3	0.17412 (16)	0.64464 (6)	0.66397 (14)	0.0371 (4)
C3	0.5550 (2)	0.58582 (9)	1.1052 (2)	0.0358 (6)
H3	0.528931	0.571428	1.163056	0.043*
N4	0.5128 (2)	0.36758 (9)	0.5701 (2)	0.0568 (7)
O4	0.5527 (2)	0.32112 (8)	0.5700 (2)	0.0719 (7)
C4	0.6639 (2)	0.60633 (9)	1.1395 (2)	0.0367 (6)
H4	0.713726	0.606700	1.220628	0.044*
C7	0.6801 (2)	0.65124 (9)	0.8440 (2)	0.0380 (6)
C6	0.6335 (2)	0.62825 (8)	0.9344 (2)	0.0294 (5)
C5	0.7017 (2)	0.62691 (9)	1.0537 (2)	0.0336 (5)
H5	0.778730	0.640799	1.078620	0.040*
C8	0.8056 (3)	0.67220 (12)	0.9037 (3)	0.0548 (8)
H8A	0.831102	0.687601	0.843741	0.082*
H8B	0.861244	0.646543	0.942182	0.082*
H8C	0.804269	0.695806	0.963139	0.082*
C9	0.5985 (3)	0.69204 (11)	0.7779 (3)	0.0541 (8)
H9A	0.628650	0.705628	0.719189	0.081*
H9B	0.596841	0.716829	0.834613	0.081*
H9C	0.517883	0.679733	0.737795	0.081*
C10	0.6889 (3)	0.61283 (12)	0.7565 (2)	0.0507 (7)
H10A	0.609285	0.600541	0.711721	0.076*
H10B	0.739526	0.586656	0.800382	0.076*
H10C	0.723535	0.626799	0.701584	0.076*
C11	0.3669 (2)	0.56243 (9)	0.9615 (2)	0.0333 (5)
H11	0.356441	0.546979	1.027232	0.040*
C12	0.1755 (2)	0.53315 (9)	0.8584 (2)	0.0313 (5)
C13	0.1858 (2)	0.49023 (9)	0.9189 (2)	0.0353 (5)
H13	0.262276	0.478283	0.964586	0.042*
C14	0.0859 (2)	0.46502 (9)	0.9131 (2)	0.0372 (6)
H14	0.094428	0.436041	0.956232	0.045*
C15	−0.0283 (2)	0.48112 (9)	0.8450 (2)	0.0338 (5)
C17	0.0632 (2)	0.54958 (10)	0.7893 (2)	0.0374 (6)
H17	0.055403	0.578402	0.745711	0.045*
C16	−0.0374 (2)	0.52405 (9)	0.7837 (2)	0.0367 (6)
H16	−0.113761	0.535959	0.737439	0.044*
C19	−0.2561 (3)	0.46941 (13)	0.7634 (3)	0.0561 (8)
H19A	−0.256719	0.479131	0.685205	0.084*
H19B	−0.278741	0.496590	0.802050	0.084*
H19C	−0.312928	0.443308	0.754426	0.084*
C18	−0.1348 (2)	0.45305 (11)	0.8372 (2)	0.0417 (6)
C20	−0.1791 (4)	0.34735 (16)	0.9604 (5)	0.122 (2)
H20A	−0.249432	0.330999	0.964903	0.183*
H20B	−0.125895	0.355817	1.040422	0.183*
H20C	−0.137277	0.326175	0.923532	0.183*
C21	0.0988 (2)	0.65239 (8)	0.55710 (19)	0.0286 (5)
C22	0.0767 (2)	0.61794 (8)	0.4645 (2)	0.0294 (5)
C23	−0.0024 (2)	0.62873 (10)	0.3488 (2)	0.0376 (6)
H23	−0.017488	0.605622	0.287580	0.045*
C24	−0.0570 (2)	0.67201 (10)	0.3248 (2)	0.0430 (6)
H24	−0.107651	0.679641	0.246451	0.052*
C25	−0.0382 (2)	0.70516 (9)	0.4161 (2)	0.0365 (6)
H25	−0.078138	0.734987	0.398007	0.044*
C26	0.0355 (2)	0.69664 (8)	0.5312 (2)	0.0298 (5)
C27	0.0529 (2)	0.73380 (9)	0.6291 (2)	0.0352 (5)
C28	0.0187 (3)	0.71220 (11)	0.7300 (2)	0.0502 (7)
H28A	−0.064310	0.701513	0.698486	0.075*
H28B	0.028018	0.736399	0.791270	0.075*
H28C	0.070500	0.684958	0.764379	0.075*
C29	0.1828 (2)	0.75064 (10)	0.6763 (2)	0.0456 (7)
H29A	0.204057	0.763347	0.610803	0.068*
H29B	0.234822	0.723657	0.712612	0.068*
H29C	0.192464	0.775654	0.735785	0.068*
C30	−0.0255 (3)	0.77773 (10)	0.5841 (3)	0.0497 (7)
H30A	−0.003624	0.793387	0.522108	0.075*
H30B	−0.013998	0.800012	0.649837	0.075*
H30C	−0.109143	0.767961	0.551537	0.075*
C31	0.1324 (2)	0.57196 (9)	0.4783 (2)	0.0317 (5)
H31	0.102438	0.550889	0.412699	0.038*
C32	0.2600 (2)	0.50837 (9)	0.56314 (19)	0.0303 (5)
C33	0.1848 (2)	0.46939 (9)	0.5347 (2)	0.0362 (6)
H33	0.101928	0.473760	0.517315	0.043*
C34	0.2289 (2)	0.42406 (9)	0.5312 (2)	0.0362 (5)
H34	0.175821	0.397685	0.511605	0.043*
C35	0.3499 (2)	0.41638 (9)	0.5559 (2)	0.0319 (5)
C36	0.4246 (2)	0.45621 (10)	0.5844 (2)	0.0401 (6)
H36	0.507273	0.452107	0.600330	0.048*
C37	0.3812 (2)	0.50118 (10)	0.5897 (2)	0.0387 (6)
H37	0.434312	0.527520	0.611742	0.046*
C38	0.3992 (2)	0.36799 (10)	0.5551 (2)	0.0385 (6)
C39	0.3211 (3)	0.32533 (10)	0.5376 (3)	0.0543 (8)
H39A	0.259822	0.326347	0.458279	0.081*
H39B	0.283125	0.325214	0.597317	0.081*
H39C	0.368948	0.296338	0.545716	0.081*
C40	0.6750 (3)	0.32505 (16)	0.5768 (5)	0.1062 (17)
H40A	0.711480	0.293293	0.588377	0.159*
H40B	0.719011	0.345653	0.643533	0.159*
H40C	0.677283	0.338863	0.502994	0.159*

of the atoms including atomic coordinates and displacement parameters.

Source of material

The title complex and its ligand were prepared by a similar method reported earlier [4–6]. The zinc(II) acetate dihydrate (109.76 mg, 0.5 mmol) dissolved in methanol solution (5 mL) was added to the organic ligand ((*E*)-1-(4-((*E*)-3-(*tert*-butyl)-2-hydroxybenzylidene)amino)phenyl)ethan-1-one O-methyl

oxime) (324.42 mg, 1 mmol) dissolved in dichloromethane(5 mL). The mixture was kept stirring at room temperature for 1 h. The filtrate was allowed to stand at room temperature 25 days in a quiet environment. Several clear yellow block crystals were obtained.

Experimental details

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

Comment

Transition metal complexes, especially Zn(II) complexes, have attracted much attention [7]. Zn(II) complexes with excellent fluorescence properties have received increasing attention [8–10]. What is more, Zn(II) complexes are widely applied in ion recognition [11] and supramolecular constructing [12, 13] fields and so on. Recently, we have also tried to investigate the title complex synthesis, structural characterization, and we predict that this complex also has excellent fluorescence properties [14].

In this paper, we report the crystal structure of the title complex characterised by X-ray crystallographic analysis (cf. the figure). All bond lengths and bond angles are within the normal ranges [6]. In the title complex, Zn1 is four-coordinated by two O atoms and two N atoms from two ligands. The Zn1—O1 bond length is 1.9050(17) Å and the Zn1—O3 is 1.9096(17) Å. The Zn1—N1 bond length is 2.000(2) Å and the Zn1—N3 is 2.0021(19) Å. The angle of O1—Zn1—N1 is 95.88(7)°, O3—Zn1—N1 is 114.23(8)°, O1—Zn1—N3 is 120.94(8)° and O1—Zn1—O3 is 118.89(8)°, respectively.

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.
Research funding: This project was supported by the Open Project Program of Shihezi University (KX000203).
Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

References

1. Bruker. *APEX2, SAINT and SADABS*; Bruker AXS Inc.: Madison, WI, USA, 2012.
2. Sheldrick G. M. *SHELXT* – integrated space-group and crystal-structure determination. *Acta Cryst.* 2015, *A71*, 3–8.
3. Sheldrick G. M. Crystal structure refinement with SHELXL. *Acta Cryst.* 2015, *C71*, 3–8.
4. Zhao J. X., Zhao L., Li P. P., Wang F., An Q. Q. Crystal structure of (*E*)-1-(4-(((*E*)-5-bromo-2-hydroxybenzylidene)amino)phenyl) ethan-1-one *O*-methyl oxime, $C_{16}H_{15}BrN_2O_2$. *Z. Kristallogr. N. Cryst. Struct.* 2017, *232*, 731–732.
5. Fu T., Ma J. X., Li Q. L., Wei P., Zhao J. X., Zhao L. Crystal structure of (*E*)-1-(4-(((*E*)-3,5-dichloro-2-hydroxybenzylidene)amino)phenyl) ethan-1-one O-methyl oxime, $C_{16}H_{14}Cl_2N_2O_2$. *Z. Kristallogr. N. Cryst. Struct.* 2018, *233*, 979–980.
6. Li Q. L., Li P. P., Ma J. X., Zhao J. X., Zhao L. Crystal structure of bis {2-((*E*)-((4-((*E*)-1-(methoxyimino)ethyl)phenyl)imino)methyl) phenolato-κ^2*N,O*}zinc(II), $C_{32}H_{30}N_4O_4Zn$. *Z. Kristallogr. N. Cryst. Struct.* 2018, *233*, 637–639.
7. Liu P. P., Wang C. Y., Zhang M., Song X. Q. Pentanuclear sandwich-type Zn^{II}–Ln^{III} clusters based on a new Salen-like salicylamide ligand: structure, near-infrared emission and magnetic properties. *Polyhedron* 2017, *129*, 133–140.
8. Dong Y. J., Li X. L., Zhang Y., Dong W. K. A highly selective visual and fluorescent sensor for Pb^{2+} and Zn^{2+} and crystal structure of Cu^{2+} complex based-on a novel single-armed Salamotype bisoxime. *Supramol. Chem.* 2017, *29*, 518–527.
9. Gao L., Wang F., Zhao Q., Zhang Y., Dong W. K. Mononuclear Zn(II) and trinuclear Ni(II) complexes derived from a coumarin-containing N_2O_2 ligand: syntheses, crystal structures and fluorescence properties. *Polyhedron* 2018, *139*, 7–16.
10. Xia X. Z., Xia L. X., Zhang G., Jiang Y. X., Sun F. G., Wu H. L. A 2–D Zn(II) coordination polymer based on 4,5- imidazoledicarboxylate and bis(benzimidazole) ligands: synthesis, crystal structure and fluorescence properties. *Z. Naturforsch. B* 2021, *76*, 313–318.
11. Dong W. K., Sunday F. A., Zhang Y., Sun Y. X., Dong X. Y. A reversible "turn-on" fluorescent sensor for selective detection of Zn^{2+}. *Sens. Actuators, B* 2017, *238*, 723–734.
12. Zheng S. S., Dong W. K., Zhang Y., Chen L., Ding Y. J. Four Salamo-type 3d–4f hetero-bimetallic [$Zn^{II}Ln^{III}$] complexes: syntheses, crystal structures, and luminescent and magnetic properties. *New J. Chem.* 2017, *41*, 4966–4973.
13. Chang J., Zhang H. J., Jia H. R., Sun Y. X. Binuclear nickel(II) and zinc(II) complexes based on 2-amino-3-hydroxy-pyridine Schiff base: syntheses, supramolecular structures and spectral properties. *Chin. J. Inorg. Chem.* 2018, *34*, 2097–2107.
14. Yu B., Sun Y. X., Yang C. J., Guo J. Q., Li J. Synthesis and crystal structures of an unexpected tetranuclear zinc(II) complex and a benzoquinone compound derived from Zn^{II-} and Cd^{II-} promoted reactivity of Schiff base ligands. *Z. Anorg. Allg. Chem.* 2017, *643*, 689–698.