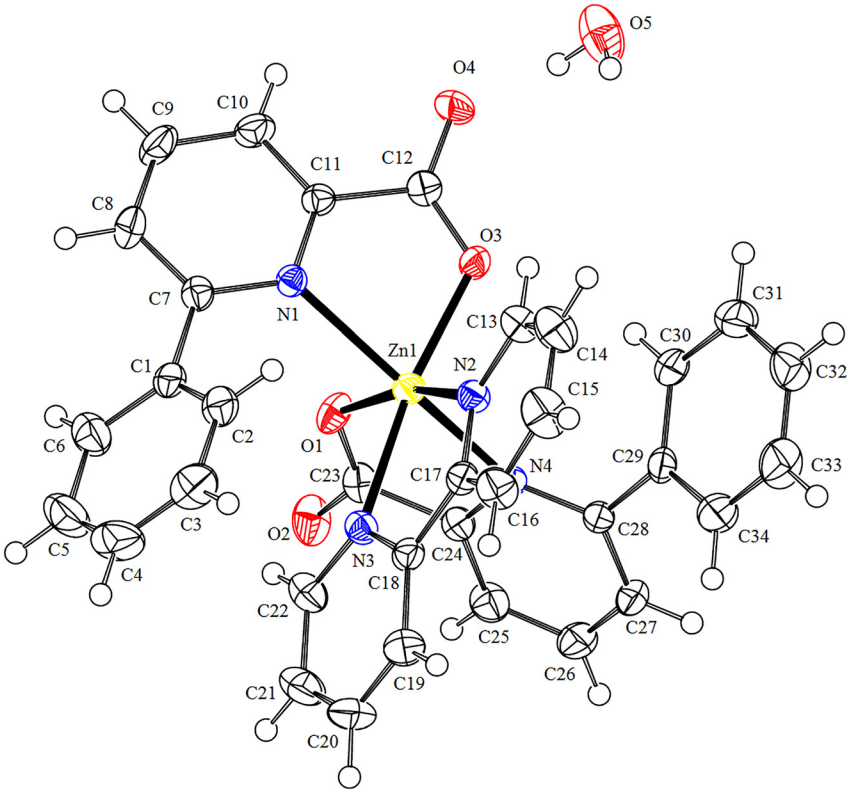
Li-Hua Wang, Zi-Jian Wang, Jian Ouyang and Xi-Shi Tai*

The crystal structure of bis(6-phenylpyridine-2-carboxylate-κ²*N*,*O*)-(2,2′-bipyridine-κ²*N*,*N*′) zinc(II) monohydrate, $C_{34}H_{26}N_4O_5Zn$



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Abstract

$C_{34}H_{26}N_4O_5Zn$, monoclinic, *C*2/*c* (no. 15), a = 29.3891(18) Å, b = 10.3260(5) Å, c = 19.9101(11) Å, V = 5783.1(6) Å^3, Z = 8, $R_{gt}(F)$ = 0.0334, $wR_{ref}(F^2)$ = 0.0759, T = 199.99(10) K.

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***Corresponding author: Xi-Shi Tai,** College of Chemistry and Chemical Engineering, Weifang University, Weifang, Shandong 261061, P. R. China, E-mail: taixs@wfu.edu.cn
Li-Hua Wang, College of Chemistry and Chemical Engineering, Weifang University, Weifang, Shandong 261061, P. R. China
Zi-Jian Wang, Kohodo (Weifang Free Trade Zone) Hydrogen Technology Co., Ltd, Weifang, Shandong 261031, P. R. China
Jian Ouyang, Shenzhen Kohodo Hydrogen Energy Co., Ltd., Shenzhen, Guangdong 518109, P. R. China

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.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.14 × 0.12 × 0.11 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.90 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	13,471, 5096, 0.029
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 4316
$N(param)_{refined}$:	400
Programs:	Bruker [1], Olex2 [2], SHELX [3], Diamond [4]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.62131 (2)	0.43010 (2)	0.69251 (2)	0.02110 (9)
O1	0.61301 (5)	0.50693 (15)	0.59526 (7)	0.0284 (4)
O2	0.63959 (6)	0.49391 (18)	0.50125 (8)	0.0379 (4)
O3	0.63571 (5)	0.59258 (14)	0.75338 (8)	0.0269 (4)
O4	0.60628 (6)	0.77589 (15)	0.78246 (8)	0.0314 (4)
N1	0.54826 (6)	0.51672 (17)	0.67644 (9)	0.0200 (4)
N2	0.62764 (6)	0.30605 (17)	0.78023 (9)	0.0222 (4)
N3	0.61256 (6)	0.23249 (18)	0.64736 (9)	0.0229 (4)
N4	0.69599 (6)	0.41319 (16)	0.67950 (9)	0.0194 (4)
C1	0.49824 (7)	0.3454 (2)	0.61133 (11)	0.0255 (5)
C2	0.51094 (8)	0.2502 (2)	0.66254 (13)	0.0315 (6)
H2	0.524628	0.273600	0.709147	0.038*
C3	0.50341 (9)	0.1208 (3)	0.64482 (15)	0.0429 (7)
H3	0.511809	0.057497	0.679425	0.051*
C4	0.48346 (10)	0.0862 (3)	0.57588 (17)	0.0520 (8)
H4	0.478621	−0.000802	0.563893	0.062*
C5	0.47058 (10)	0.1798 (3)	0.52431 (15)	0.0500 (8)
H5	0.457420	0.155557	0.477721	0.060*
C6	0.47717 (9)	0.3097 (3)	0.54173 (13)	0.0370 (6)
H6	0.467599	0.372814	0.507161	0.044*
C7	0.50583 (7)	0.4835 (2)	0.63127 (11)	0.0228 (5)
C8	0.47035 (8)	0.5748 (2)	0.60564 (12)	0.0309 (6)
H8	0.441740	0.550460	0.573676	0.037*
C9	0.47769 (8)	0.7011 (2)	0.62771 (13)	0.0350 (6)
H9	0.454351	0.763325	0.610490	0.042*
C10	0.52019 (8)	0.7341 (2)	0.67578 (12)	0.0307 (6)
H10	0.525476	0.818331	0.692874	0.037*
C11	0.55468 (7)	0.6407 (2)	0.69812 (10)	0.0214 (5)
C12	0.60258 (8)	0.6734 (2)	0.74878 (11)	0.0231 (5)
C13	0.62941 (8)	0.3478 (2)	0.84450 (11)	0.0289 (5)
H13	0.629834	0.436527	0.852614	0.035*
C14	0.63062 (9)	0.2648 (3)	0.89928 (12)	0.0373 (6)
H14	0.631501	0.296769	0.943310	0.045*
C15	0.63048 (9)	0.1341 (3)	0.88725 (13)	0.0408 (7)
H15	0.631529	0.076126	0.923389	0.049*
C16	0.62880 (9)	0.0890 (2)	0.82153 (12)	0.0332 (6)
H16	0.628625	0.000476	0.812770	0.040*
C17	0.62736 (7)	0.1774 (2)	0.76868 (11)	0.0221 (5)
C18	0.62397 (7)	0.1376 (2)	0.69596 (11)	0.0232 (5)
C19	0.63141 (9)	0.0113 (2)	0.67787 (13)	0.0349 (6)
H19	0.639180	−0.052976	0.712011	0.042*
C20	0.62719 (9)	−0.0178 (3)	0.60898 (14)	0.0436 (7)
H20	0.632753	−0.101656	0.596159	0.052*
C21	0.61467 (9)	0.0782 (3)	0.55926 (13)	0.0394 (6)
H21	0.611406	0.060489	0.512292	0.047*
C22	0.60707 (8)	0.2010 (2)	0.58044 (11)	0.0307 (6)
H22	0.597655	0.265193	0.546507	0.037*
C23	0.64424 (8)	0.4806 (2)	0.56483 (11)	0.0256 (5)
C24	0.69087 (7)	0.4252 (2)	0.61022 (11)	0.0223 (5)
C25	0.72567 (8)	0.3885 (2)	0.58015 (12)	0.0312 (6)
H25	0.721263	0.400063	0.532367	0.037*
C26	0.76693 (8)	0.3344 (3)	0.62185 (13)	0.0356 (6)
H26	0.790594	0.307004	0.602605	0.043*
C27	0.77262 (8)	0.3217 (2)	0.69272 (12)	0.0304 (6)
H27	0.800237	0.284952	0.721751	0.036*
C28	0.73697 (7)	0.3638 (2)	0.72081 (11)	0.0219 (5)
C29	0.74529 (7)	0.3629 (2)	0.79792 (11)	0.0237 (5)
C30	0.73529 (8)	0.4723 (2)	0.83122 (11)	0.0291 (5)
H30	0.720988	0.543326	0.804671	0.035*
C31	0.74636 (9)	0.4771 (3)	0.90346 (12)	0.0381 (6)
H31	0.740133	0.551937	0.925236	0.046*
C32	0.76653 (9)	0.3718 (3)	0.94349 (12)	0.0404 (7)
H32	0.773620	0.375257	0.992109	0.048*
C33	0.77612 (10)	0.2620 (3)	0.91141 (13)	0.0431 (7)
H33	0.789444	0.190381	0.938273	0.052*
C34	0.76599 (9)	0.2575 (2)	0.83893 (12)	0.0370 (6)
H34	0.773122	0.183233	0.817547	0.044*
O5	0.63939 (7)	0.7549 (2)	0.93091 (9)	0.0536 (5)
H5A	0.630054	0.748931	0.886422	0.080*
H5B	0.639956	0.677169	0.945226	0.080*

Source of material

Dissolving 0.0549 g zinc(II) acetate dihydrate (0.25 mmol), 0.020 g of NaOH (0.5 mmol) and 0.0996 g of 6-phenyl-pyridine-2-carboxylic acid (0.5 mmol) in 25 ml of water-95% ethanol (v:v = 1:1) at room temperature yielded a colorless solution. The mixture solution was heated to 80 °C and stirred for 1 h. Then 0.078 g 2,2′-bipyridine (0.5 mmol) was added to the solution, and the reaction mixture was continuously stirred for 3.5 h at 80 °C. After the reaction was cooled to room temperature, it was filtered. After 17 days, colorless crystals of the title compound were obtained from the filtrate.

Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.93 Å and O–H = 0.85 Å). Their U_{iso} values were set to $1.2U_{eq}$ or $1.5U_{eq}$ of the parent atoms.

Comment

Over the past decades, studies on the triternary zinc complexes have received extensive researches because of their fascinating structure [5, 6] and appealing properties [7–9], especially in photocytotoxic activity, antimalarial activity, photoluminescent property and phosphatase-like activity. So the studies on the structure and property of triternary complexes based on Zn(II) center has been one of the hot spots of coordination chemistry. In previous research in

our research group, the structure and properties of some triternary zinc complexes have been studied [10, 11].

The title structure is made up of one Zn(II) ion, two 6-phenylpyridine-2-carboxylate ligands, one 2,2′-bipyridine ligand and one lattice water molecule. In the crystal structure, both 6-phenylpyridine-2-carboxylate and 2,2′-bipyridine act as bidentate ligands. The Zn(II) ion is six-coordinated with two O atoms (O1 and O3) and two N atoms (N1 and N4) from two different 6-phenylpyridine-2-carboxylate ligands, two N atoms (N2 and N3) from one 2,2′-bipyridine ligand. The Zn(II) atom form a distorted octahedral coordination geometry with N1, N2, N4 and O1 defining the equatorial plane. The lengths of Zn–N bonds and Zn–O bonds are 2.1301(17)–2.2900(16) and 2.0407(14)–2.0411(15) Å, respectively. The bond angles and bond lengths agree with those reported in the literature [12].

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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