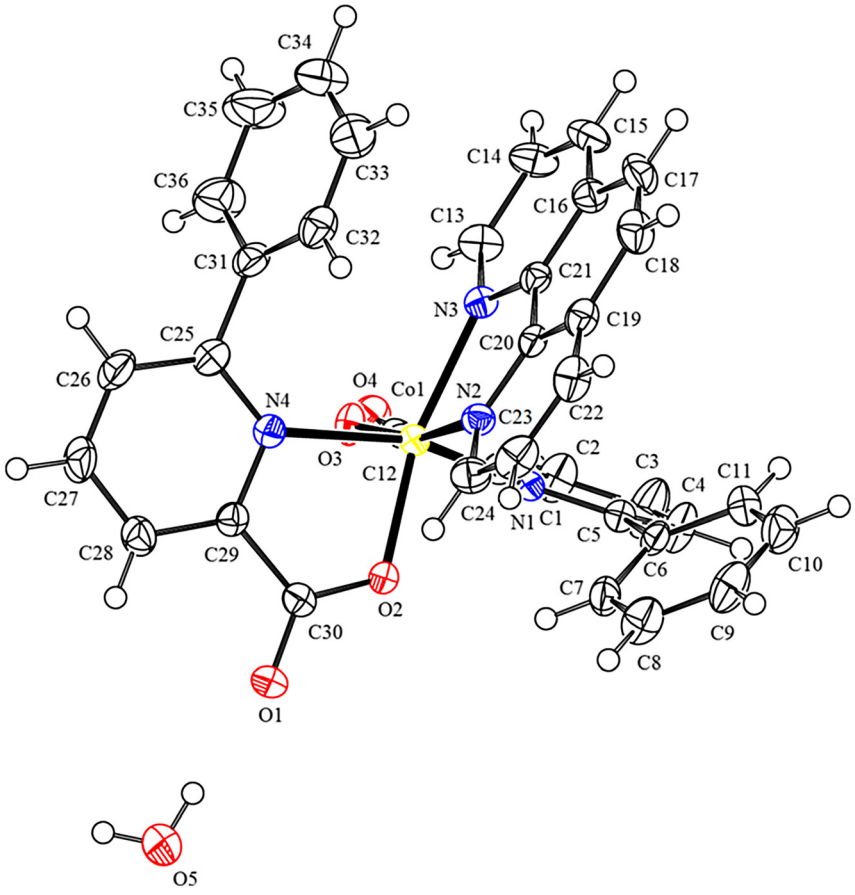
Xi-Shi Tai*, Zi-Jian Wang, Jian Ouyang, Yun-Fei Li, Wei Zhang, Wen-Lei Jia and Li-Hua Wang

The crystal structure of [(phenantroline-κ^2*N*, *N*′)-bis(6-phenylpyridine-2-carboxylate-κ^2*N*,*O*) cobalt(II)]monohydrate, $C_{36}H_{26}N_4O_5Co$



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Abstract

$C_{36}H_{26}N_4O_5Co$, triclinic, $P2_12_12_1$ (no. 19), a = 10.6380(5) Å, b = 10.6639(5) Å, c = 26.5443(15) Å, V = 3011.2(3) Å^3, Z = 4, $R_{gt}(F)$ = 0.0330, $wR_{ref}(F^2)$ = 0.0681, T = 200 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. https://orcid.org/0000-0002-0050-1900
Zi-Jian Wang, Kohodo (Weifang Free Trade Zone) Hydrogen Technology Co., Ltd, Weifang, Shandong 261031, P. R. China
Jian Ouyang, Yun-Fei Li, Wei Zhang and Wen-Lei Jia, Shenzhen Kohodo Hydrogen Energy Co., Ltd., Shenzhen, Guangdong 518109, P. R. China
Li-Hua Wang, College of Chemistry and Chemical Engineering, Weifang University, Weifang, Shandong 261061, P. R. China

Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was synthesized as follows: dissolving 0.0996 g (0.5 mmol) 6-phenylpyridine-2-carboxylic acid,

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.14 × 0.13 × 0.12 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.62 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	12,912, 5250, 0.031
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4822
$N(param)_{refined}$:	418
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}
Co1	0.57858 (4)	0.54695 (4)	0.59310 (2)	0.01996 (12)
O1	0.6157 (2)	0.4671 (2)	0.44444 (9)	0.0305 (6)
O2	0.5654 (2)	0.5574 (2)	0.51714 (8)	0.0266 (5)
O3	0.4737 (2)	0.3917 (2)	0.60417 (10)	0.0268 (6)
O4	0.2873 (2)	0.3191 (2)	0.62805 (9)	0.0313 (6)
N1	0.3837 (2)	0.6291 (2)	0.59868 (11)	0.0195 (6)
N2	0.7090 (2)	0.6989 (3)	0.59906 (11)	0.0222 (6)
N3	0.5865 (3)	0.5849 (2)	0.67342 (10)	0.0217 (6)
N4	0.7272 (3)	0.4141 (2)	0.56874 (11)	0.0217 (7)
C1	0.3044 (3)	0.5364 (3)	0.61220 (13)	0.0231 (8)
C2	0.1799 (3)	0.5557 (4)	0.62450 (15)	0.0365 (10)
H2	0.128633	0.489142	0.634021	0.044*
C3	0.1338 (4)	0.6760 (4)	0.62227 (18)	0.0475 (12)
H3	0.050281	0.692328	0.630306	0.057*
C4	0.2121 (4)	0.7714 (3)	0.60812 (16)	0.0373 (10)
H4	0.181603	0.852994	0.606290	0.045*
C5	0.3369 (3)	0.7470 (3)	0.59646 (14)	0.0229 (8)
C6	0.4202 (3)	0.8521 (3)	0.58087 (13)	0.0238 (8)
C7	0.4930 (3)	0.8449 (3)	0.53774 (14)	0.0282 (9)
H7	0.494578	0.771090	0.519114	0.034*
C8	0.5634 (4)	0.9471 (4)	0.52216 (16)	0.0393 (10)
H8	0.611724	0.941638	0.493057	0.047*
C9	0.5620 (4)	1.0565 (4)	0.54959 (16)	0.0396 (10)
H9	0.609684	1.124816	0.539119	0.048*
C10	0.4899 (4)	1.0648 (3)	0.59264 (17)	0.0401 (10)
H10	0.489645	1.138442	0.611372	0.048*
C11	0.4183 (4)	0.9642 (3)	0.60795 (13)	0.0316 (8)
H11	0.368236	0.971130	0.636544	0.038*
C12	0.3578 (3)	0.4041 (3)	0.61506 (13)	0.0231 (8)
C13	0.5277 (3)	0.5264 (4)	0.71042 (14)	0.0302 (9)
H13	0.482495	0.454368	0.702618	0.036*
C14	0.5294 (3)	0.5662 (4)	0.76058 (14)	0.0352 (10)
H14	0.484811	0.522567	0.785088	0.042*
C15	0.5976 (3)	0.6706 (4)	0.77306 (14)	0.0331 (9)
H15	0.599946	0.698801	0.806200	0.040*
C16	0.6641 (3)	0.7345 (3)	0.73525 (14)	0.0270 (9)
C17	0.7445 (4)	0.8397 (3)	0.74473 (15)	0.0338 (10)
H17	0.751067	0.870853	0.777343	0.041*
C18	0.8108 (3)	0.8945 (4)	0.70741 (15)	0.0320 (9)
H18	0.863461	0.961524	0.714888	0.038*
C19	0.8014 (3)	0.8510 (3)	0.65627 (15)	0.0265 (8)
C20	0.7220 (3)	0.7487 (3)	0.64583 (13)	0.0205 (8)
C21	0.6546 (3)	0.6887 (3)	0.68606 (13)	0.0214 (8)
C22	0.8702 (3)	0.9010 (4)	0.61628 (16)	0.0311 (9)
H22	0.923942	0.968518	0.621663	0.037*
C23	0.8586 (4)	0.8507 (4)	0.56934 (16)	0.0328 (10)
H23	0.904277	0.883152	0.542464	0.039*
C24	0.7763 (3)	0.7489 (3)	0.56216 (15)	0.0292 (9)
H24	0.768885	0.715072	0.530005	0.035*
C25	0.8039 (3)	0.3386 (3)	0.59500 (15)	0.0252 (8)
C26	0.8748 (4)	0.2457 (4)	0.57166 (16)	0.0349 (10)
H26	0.927776	0.194980	0.590652	0.042*
C27	0.8662 (4)	0.2290 (4)	0.52032 (16)	0.0372 (10)
H27	0.913620	0.167533	0.504311	0.045*
C28	0.7861 (3)	0.3048 (3)	0.49298 (15)	0.0300 (9)
H28	0.777494	0.294590	0.458360	0.036*
C29	0.7192 (3)	0.3961 (3)	0.51823 (13)	0.0214 (8)
C30	0.6278 (3)	0.4794 (3)	0.49053 (13)	0.0217 (8)
C31	0.8131 (3)	0.3566 (4)	0.65080 (15)	0.0296 (9)
C32	0.8626 (3)	0.4642 (4)	0.67090 (15)	0.0334 (9)
H32	0.888844	0.528165	0.649504	0.040*
C33	0.8742 (4)	0.4795 (4)	0.72253 (17)	0.0456 (12)
H33	0.909214	0.552488	0.735582	0.055*
C34	0.8340 (5)	0.3864 (5)	0.75426 (18)	0.0565 (13)
H34	0.840636	0.396828	0.788947	0.068*
C35	0.7834 (5)	0.2769 (5)	0.73479 (18)	0.0630 (15)
H35	0.756459	0.213521	0.756307	0.076*
C36	0.7733 (5)	0.2622 (4)	0.68298 (17)	0.0497 (12)
H36	0.739669	0.188744	0.669792	0.060*
O5	0.6169 (3)	0.3863 (3)	0.34543 (10)	0.0469 (8)
H5A	0.647835	0.313111	0.342863	0.070*
H5B	0.625375	0.412272	0.375535	0.070*

0.020 g (0.5 mmol) NaOH and 0.1245 g (0.5 mmol) $Co(CH_3COO)_2{\cdot}1H_2O$ mixture into 20 ml of water-95% ethanol (v:v = 1:2) at room temperature. A small amount of blue precipitation was immediately present in the solution. The mixture was stirred for 0.5 h at 75 °C, and 0.090 g (0.5 mmol) 1,10-phenanthroline was added to the reaction mixture. The reaction mixture was stirred for 5 h. The solution was cooled to room temperature and filtered. The yellow crystals of the title compound were received from the filtrate in four weeks.

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 1.2 or 1.5U_{eq} of the parent atoms.

Comment

Cobalt(II) complexes exhibit potential application properties in electrochemical property, catalytic activity, reversible magnetogenic property and antifungal activity [5–9]. 1,10-Phenanthroline was also an important nitrogen heterocycle ligand, and it also played an important role in enriching the structure and properties of the metal complexes [10]. Our research group has been on the synthesis and properties of metal complexes [11, 12]. In order to synthesize and characterize more metal complexes, a new Co(II) complex has been synthesized and structural characterized.

The asymmetric unit of the tile crystal structure consists of one Co(II) ion, two bidentate 6-phenylpyridine-2-carboxylate ligands, one 1,10-phenanthroline ligand, and one uncoordinated water molecule. The Co(II) ion is coordinated by two O atoms (O2 and O3), two N atoms (N1 and N4) from two 6-phenylpyridine-2-carboxylate ligands and two N atoms (N2 and N3) from one 1,10-phenanthroline ligand. The Co(II) atom forms a six-coordinated distorted octahedral coordination environment. The N1, N2, N4 and O3 atoms are at the equatorial plane and the N3 and O2 atoms are in the axial position (N3–Co1–O2, 166.01(9)°). The lengths of Co–N bonds and Co–O bonds are 2.256(3) Å (Co1–N1), 2.139(3) Å (Co1–N2), 2.172(3) Å (Co1–N3), 2.219(3) (Co1–N4), 2.024(2) (Co1–O2), 2.018(2) (Co1–O3), respectively. All geometric parameters are in the expected ranges [13].

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

References

1. Bruker. SAINT and SADABS; Bruker AXS Inc.: Madison, Wisconsin, USA, 2000.
2. Dolomanov O. V., Bourhis L. J., Gildea R. J., Howard J. A. K., Puschmann H. OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* 2009, *42*, 339–341.
3. Sheldrick G. M. Crystal structure refinement with SHELXL. *Acta Crystallogr.* 2015, *C71*, 3–8.
4. Brandenburg K. *Diamond*. Visual Crystal Structure Information System. (Ver. 3.2); Crystal Impact: Bonn, Germany, 2012.
5. Li T.-Y., Xu X.-D., Huang M.-F., Wang M., Wu Q. Crystal structure of tris(azido-k^1*N*)-(*N*-(2-aminoethyl)-*N*-methyl-1,3-propanediamine-k^3*N*,*N*′,*N*″)cobalt(III), $C_7H_{19}CoN_{12}$. *Z. Kristallogr. NCS* 2021, *236*, 357–358.
6. Balaraman L., Emhoff K.-A., Salem A.-M.-H., Hanna J., Alsabony M.-N., Bayachou M., Mundell J.-J., Boyd W.-C. Electrochemical studies of cobalt(II) diphenylazodioxide complexes. *Inorg. Chim. Acta*. 2020, *501*, 119277.
7. Gualandi A., Rodeghiero G., Perciaccante R., Jansen T.-P., Moreno-Cabrerizo C., Foucher C., Marchini M., Ceroni P., Cozzi P.-G. Catalytic photoredox allylation of aldehydes promoted by a cobalt complex. *Adv. Synth. Catal.* 2020, *363*, 1105–1111.
8. Bonnitcha P., Broadhouse K., Grieve S., Kolanowski J., New E., ONeill E., Renfrew A., Yin G. Reversible magnetogenic cobalt complexes. *RSC Adv.* 2016, *6*, 30021–30027.
9. Frei A., King A.-P., Lowe G.-J., Cain A.-K., Short F.-L., Dinh H., Elliott A.-G., Zuegg J., Wilson J.-J., Blaskovich M.-A.-T. Nontoxic cobalt(III) Schiff base complexes with broad-spectrum antifungal activity. *Chem. Eur J.* 2021, *27*, 2021–2029.
10. Wang L.-H., Liu L.-L., Cao S.-H., Tai X.-S. Crystal structure of poly[(m$_3$-3-carboxyadamantane-1-carboxylato-κ^3*O*:*O*′:*O*″)-(phenanthroline-κ^2 *N*,*N*′)sodium(II)], $C_{24}H_{23}N_2NaO_4$. *Z. Kristallogr. NCS* 2021, *236*, 745–747.
11. Du L.-C., Tai X.-S. The crystal structure of *catena*-poly[diaqua-bis(μ$_2$-2-((2-(2-phenylacetyl)hydrazineylidene) methyl)benzoato-κ^2*O*:*O*′)zinc(II)], $C_{32}H_{30}N_4O_8Zn$. *Z. Kristallogr. NCS* 2021, *236*, 843–844.
12. Wang L.-H., Kong F.-Y., Tai X.-S. Crystal structure and catalytic activity of poly[bis(3-bromo-2-hydroxybenzaldehyde)-2-aminopyrimidinemagnesium(II)] for hydrogenation of 1,3-butadiene. *Bull. Chem. React. Eng. Catal.* 2021, *16*, 260–266.
13. Smith P. W., Moore C. E., Rheingold A. L., Figueroa J. S. Coordination and structural properties of encumbering 6-mesityl-2-picolinate complexes. *Dalton Trans*. 2012, *41*, 8031–8038.