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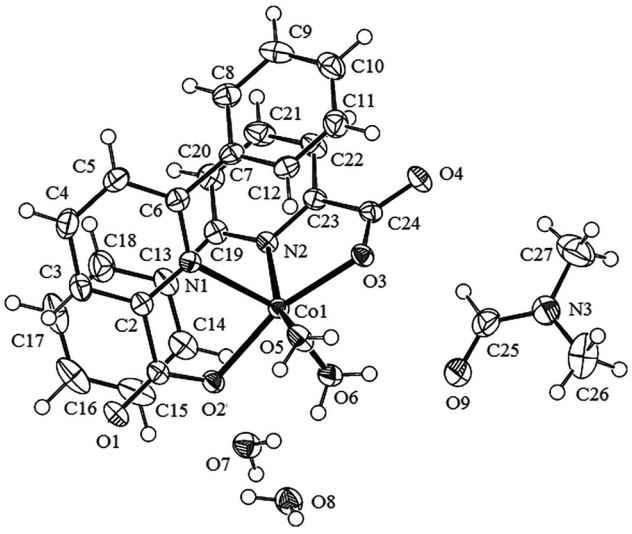
The crystal structure of diaqua-bis(6-phenylpyridine-2-carboxylato-κ²*N*,*O*)cobalt(II)–water–*N*,*N*-dimethylformamide(1/2/1), $C_{27}H_{31}N_3O_9Co$



https://doi.org/10.1515/ncrs-2022-0067
Received February 7, 2022; accepted March 7, 2022;
published online March 16, 2022

Abstract

$C_{27}H_{31}N_3O_9Co$, monoclinic, $P2_1/n$ (no. 14), a = 10.9230(6) Å, b = 11.1166(8) Å, c = 22.8312(15) Å, β = 93.404(6)°, V = 2767.4(3) Å^3, Z = 4, $R_{gt}(F)$ = 0.0349, $wR_{ref}(F^2)$ = 0.0893, T = 200 K.

CCDC no.: 2156796

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:	Pink block
Size:	0.14 × 0.12 × 0.10 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.68 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	13,563, 4867, 0.031
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 4159
$N(param)_{refined}$:	383
Programs:	Bruker [1], Olex2 [2], SHELX [3], Diamond [4]

Source of material

The synthesis of the title compound was performed as following: 0.0498 g 6-phenylpyridine-2-carboxylic acid (0.25 mmol) and 0.010 g NaOH (0.25 mmol) were completely dissolved in 15 mL water-ethanol (v:v = 1:2) in 100 mL round bottom flask with stirring. A 5 mL solution of 0.0623 g $Co(CH_3COO)_2{\cdot}4H_2O$ (0.25 mmol) in water was added to the above mixture and the pink precipitation appeared. Then 5 mL *N*,*N*-dimethylformamide was added and the pink precipitation disappeared, the reaction was continued for 3 h at 80 °C. The solution was filtered and put in a static place. The pink crystals of the title compound appeared in the filtrate after three weeks.

Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.93–0.96 Å and O–H = 0.78–0.85 Å). Their U_{iso} values were set to 1.2U_{eq} or 1.5U_{eq} of the parent atoms.

Comment

The metal-aza ligand complexes have rich and diverse structures and promising properties in many areas such as antibacterial activity, photocatalytic activity and fluorescence

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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}
Co1	0.31460 (2)	0.55978 (2)	0.40778 (2)	0.01919 (11)
O1	−0.03005 (11)	0.67410 (13)	0.44519 (6)	0.0293 (4)
O2	0.13146 (12)	0.56288 (12)	0.42410 (6)	0.0234 (3)
O3	0.49810 (11)	0.51207 (13)	0.40438 (6)	0.0226 (3)
O4	0.65499 (12)	0.49012 (14)	0.34602 (6)	0.0297 (4)
O5	0.34231 (16)	0.56230 (15)	0.49954 (7)	0.0302 (4)
O6	0.27611 (12)	0.37761 (13)	0.39266 (6)	0.0279 (3)
H6A	0.335379	0.334911	0.407114	0.042*
H6B	0.215026	0.356674	0.411942	0.042*
N1	0.26976 (14)	0.75535 (15)	0.40911 (7)	0.0198 (4)
N2	0.35292 (13)	0.59450 (15)	0.31530 (7)	0.0195 (4)
C1	0.07741 (17)	0.66118 (19)	0.43095 (9)	0.0217 (5)
C2	0.15119 (17)	0.77319 (19)	0.41943 (9)	0.0217 (5)
C3	0.09712 (19)	0.8852 (2)	0.41919 (10)	0.0303 (5)
H3	0.015445	0.894062	0.427789	0.036*
C4	0.1670 (2)	0.9842 (2)	0.40589 (11)	0.0362 (6)
H4	0.133058	1.060920	0.404768	0.043*
C5	0.2880 (2)	0.9667 (2)	0.39435 (11)	0.0332 (6)
H5	0.335960	1.031877	0.384473	0.040*
C6	0.33882 (18)	0.85232 (19)	0.39737 (9)	0.0239 (5)
C7	0.47216 (18)	0.83473 (18)	0.39098 (9)	0.0238 (5)
C8	0.52929 (19)	0.8866 (2)	0.34463 (10)	0.0301 (5)
H8	0.483416	0.930985	0.316648	0.036*
C9	0.6543 (2)	0.8727 (2)	0.33971 (11)	0.0363 (6)
H9	0.691685	0.906280	0.308010	0.044*
C10	0.7235 (2)	0.8091 (2)	0.38183 (11)	0.0365 (6)
H10	0.807541	0.800330	0.378771	0.044*
C11	0.66716 (19)	0.7588 (2)	0.42841 (11)	0.0335 (6)
H11	0.713683	0.716417	0.456914	0.040*
C12	0.54221 (18)	0.77083 (19)	0.43316 (10)	0.0269 (5)
H12	0.504993	0.736111	0.464627	0.032*
C13	0.14809 (18)	0.6530 (2)	0.27841 (9)	0.0265 (5)
C14	0.08517 (19)	0.5503 (2)	0.29358 (9)	0.0315 (5)
H14	0.127844	0.479227	0.301692	0.038*
C15	−0.0413 (2)	0.5532 (3)	0.29669 (10)	0.0400 (6)
H15	−0.083369	0.484029	0.306460	0.048*
C16	−0.1043 (2)	0.6584 (3)	0.28533 (11)	0.0480 (7)
H16	−0.189032	0.660228	0.287468	0.058*
C17	−0.0427 (2)	0.7609 (3)	0.27082 (12)	0.0510 (8)
H17	−0.085710	0.832180	0.263810	0.061*
C18	0.0830 (2)	0.7584 (2)	0.26661 (11)	0.0387 (6)
H18	0.124114	0.827484	0.255837	0.046*
C19	0.28224 (17)	0.64727 (19)	0.27171 (9)	0.0237 (5)
C20	0.33157 (19)	0.6906 (2)	0.22150 (9)	0.0311 (5)
H20	0.281640	0.729971	0.193178	0.037*
C21	0.45419 (19)	0.6757 (2)	0.21335 (10)	0.0347 (6)
H21	0.488283	0.705016	0.179816	0.042*
C22	0.52583 (18)	0.6163 (2)	0.25603 (9)	0.0288 (5)
H22	0.608253	0.601249	0.250857	0.035*
C23	0.47324 (17)	0.57966 (18)	0.30627 (9)	0.0216 (5)
C24	0.54948 (17)	0.52228 (18)	0.35633 (9)	0.0218 (5)
O7	0.15093 (16)	0.54436 (16)	0.57116 (8)	0.0322 (4)
O8	0.05795 (14)	0.29062 (15)	0.43328 (7)	0.0349 (4)
H8A	0.059393	0.286367	0.470503	0.052*
H8B	0.008693	0.347930	0.424532	0.052*
O9	0.45195 (15)	0.21200 (15)	0.41020 (9)	0.0507 (5)
N3	0.65200 (16)	0.16699 (17)	0.40300 (9)	0.0358 (5)
C25	0.5496 (2)	0.2223 (2)	0.38623 (12)	0.0407 (6)
H25	0.550841	0.272906	0.353853	0.049*
C26	0.6579 (3)	0.0915 (3)	0.45460 (12)	0.0556 (8)
H26A	0.718570	0.122505	0.482777	0.083*
H26B	0.679560	0.011091	0.443922	0.083*
H26C	0.579350	0.090762	0.471399	0.083*
C27	0.7632 (2)	0.1845 (3)	0.37237 (15)	0.0641 (9)
H27A	0.748002	0.241612	0.341223	0.096*
H27B	0.788269	0.109288	0.356289	0.096*
H27C	0.826891	0.214348	0.399312	0.096*
H7A	0.204 (2)	0.535 (2)	0.5980 (11)	0.029 (7)*
H7B	0.117 (3)	0.484 (3)	0.5631 (14)	0.063 (11)*
H5A	0.278 (2)	0.560 (2)	0.5158 (11)	0.034 (7)*
H5B	0.393 (2)	0.537 (2)	0.5215 (12)	0.048 (9)*

properties, and so forth [5–9]. 6-Phenylpyridine-2-carboxylate ligands can provide both nitrogen atom and oxygen atoms coordination with metal atoms. We have reported some metal complexes using 6-phenylpyridine-2-carboxylate as the major ligand [10–13].

The structural analysis shows that the title Co(II) complex forms a one-dimensional chain structure by O–H···O hydrogen bonds. The asymmetric unit contains one Co(II) ion, two bidentate 6-phenylpyridine-2-carboxylate ligands, two coordinated water molecules, one uncoordinated *N*,*N*-dimethylformamide molecule and two lattice water molecules. The Co(II) ion is six-coordinated with two carboxylate O atoms (Co1–O2 = 2.0568(13) Å, Co1–O3 = 2.0793(13) Å), two pyridine N atoms (Co1–N1 = 2.2291(17) Å, Co1–N2 = 2.2108(16) Å) from two different 6-phenylpyridine-2-carboxylate ligands, and two O atoms (Co1–O5 = 2.0991(16) Å, Co1–O6 = 2.0928(14) Å) from two coordinated water molecules, forming a distorted octahedral geometry. The rich hydrogen bond interactions (O5–H5A···O7, 2.7367(2) Å; O5–H5B···O3, 2.8426(3) Å; O6–H6A···O9, 2.6735(2) Å; O6–H6B···O8, 2.7815(2) Å; O7–H7A···O4, 2.7822(2) Å; O7–H7B···O1, 2.7789(2) Å; O8–H8A···O1, 2.8365(2) Å; O8–H8B···O7, 2.9247(2) Å) formed by water molecules, 6-phenylpyridine-2-carboxylate ligands and *N*,*N*-dimethylformamide molecules help to construct the crystal packing. The O–Co1–O, O–Co1–N and N–Co1–N bond angles are 81.84(5)–163.97(6)°, 76.37(6)–154.67(6)° and 84.09(6)°, 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 National Natural Science Foundation of China (No. 21171132), the Natural Science Foundation of Shandong (ZR2014BL003), the Project of Shandong Province Higher Educational Science and Technology Program (J14LC01) and Science Foundation of Weifang (2020ZJ1054).

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

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