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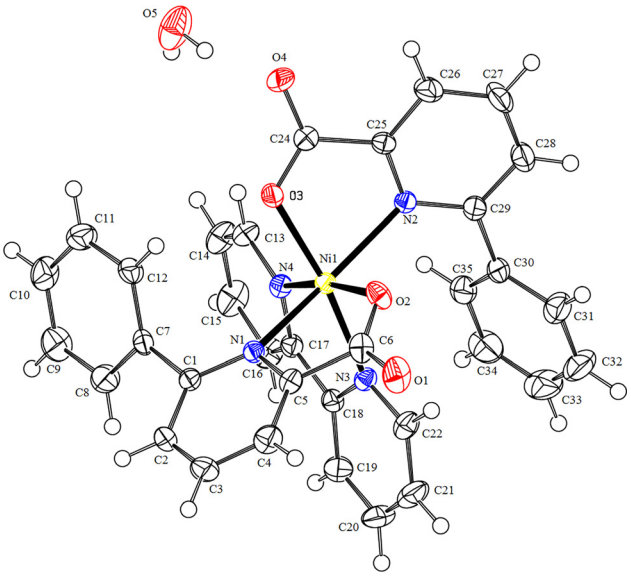
The crystal structure of [(2,2′-bipyridine-κ²*N*,*N*)-bis(6-phenylpyridine-2-carboxylato- κ²*N*,*O*) nickel(II)] monohydrate, $C_{34}H_{26}N_4O_5Ni$



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Abstract

$C_{34}H_{26}N_4O_5Ni$, monoclinic, *C*2/*c* (no. 15), a = 29.3459(13) Å, b = 10.2867(4) Å, c = 19.8780(9) Å, β = 107.243(5)°, V = 5730.9(4) Å^3, Z = 8, $R_{gt}(F)$ = 0.0326, w$R_{ref}(F^2)$ = 0.0817, T = 200K.

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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:	Colourless block
Size:	0.14 × 0.11 × 0.10 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.73 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	13553, 5050, 0.029
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4373
$N(param)_{refined}$:	400
Programs:	Bruker [1], Olex2 [2], SHELX [3], Diamond [4]

Source of material

To 0.2488 g (1.0 mmol) $Ni(CH_3COO)_2{\cdot}4H_2O$ was added a solution of 0.1992 g (1.0 mmol) 6-phenylpyridine-2-carboxylic acid and 0.040 g (1.0 mmol) NaOH in 20 mL ethanol-distilled water (v:v = 1:1) with stirring. After 30 min, 0.1562 g (1.0 mmol) 2,2′-bipyridine was added. Then the solution was heated at 75 °C for 6 h. After cooled to room temperature, the solution was filtered and volatiled slowly at room temperature. The block crystals of the title compound were obtained after 30 days. **Elemental analysis** (%) calcd. for $C_{34}H_{26}N_4O_5Ni$: C, 64.83; H, 4.13; N, 8.90. Found (%): C, 64.99; H, 4.36; N, 8.69.

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

The studies on the properties and structures of metal complexes have been one of the priorities of coordination chemists. Because they showed wide potential application for example [5–8]. Tai's research team reported the

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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}
Ni1	0.37812 (2)	0.42744 (2)	0.31050 (2)	0.01678 (9)
O1	0.36054 (5)	0.49693 (16)	0.49901 (8)	0.0351 (4)
O2	0.38738 (5)	0.51119 (14)	0.40550 (7)	0.0251 (3)
O3	0.36154 (5)	0.59180 (13)	0.25273 (8)	0.0240 (3)
O4	0.39089 (5)	0.77336 (13)	0.22049 (8)	0.0282 (3)
N1	0.30634 (5)	0.40977 (14)	0.32063 (8)	0.0171 (4)
N2	0.44915 (5)	0.50927 (15)	0.32391 (8)	0.0179 (4)
N3	0.38758 (5)	0.23826 (15)	0.35524 (9)	0.0192 (4)
N4	0.37223 (5)	0.31111 (16)	0.22302 (8)	0.0195 (4)
C1	0.26496 (7)	0.36150 (18)	0.27780 (10)	0.0200 (4)
C2	0.22850 (7)	0.3218 (2)	0.30462 (12)	0.0269 (5)
H2	0.200866	0.285318	0.274779	0.032*
C3	0.23317 (7)	0.3362 (2)	0.37491 (12)	0.0317 (5)
H3	0.208928	0.309696	0.393148	0.038*
C4	0.27436 (7)	0.3906 (2)	0.41802 (12)	0.0292 (5)
H4	0.278101	0.403825	0.465635	0.035*
C5	0.31003 (7)	0.42513 (18)	0.38916 (10)	0.0201 (4)
C6	0.35639 (7)	0.4827 (2)	0.43571 (11)	0.0238 (5)
C7	0.25687 (7)	0.36060 (19)	0.20070 (11)	0.0217 (4)
C8	0.23635 (8)	0.2545 (2)	0.15954 (12)	0.0337 (5)
H8	0.230389	0.178792	0.181035	0.040*
C9	0.22473 (9)	0.2605 (2)	0.08695 (13)	0.0391 (6)
H9	0.211395	0.188565	0.059926	0.047*
C10	0.23281 (8)	0.3724 (2)	0.05465 (12)	0.0355 (6)
H10	0.224872	0.376449	0.005796	0.043*
C11	0.25276 (8)	0.4790 (2)	0.09484 (12)	0.0340 (5)
H11	0.258002	0.555131	0.072986	0.041*
C12	0.26491 (7)	0.4729 (2)	0.16724 (11)	0.0258 (5)
H12	0.278644	0.544817	0.193978	0.031*
C13	0.37075 (7)	0.3531 (2)	0.15890 (10)	0.0252 (5)
H13	0.370348	0.442177	0.150840	0.030*
C14	0.36981 (8)	0.2699 (2)	0.10407 (12)	0.0341 (6)
H14	0.368987	0.302254	0.060035	0.041*
C15	0.37011 (8)	0.1381 (2)	0.11597 (12)	0.0360 (6)
H15	0.369466	0.080002	0.079854	0.043*
C16	0.37137 (8)	0.0927 (2)	0.18162 (12)	0.0300 (5)
H16	0.371559	0.003919	0.190436	0.036*
C17	0.37235 (7)	0.18171 (19)	0.23436 (10)	0.0201 (4)
C18	0.37564 (6)	0.1422 (2)	0.30681 (10)	0.0204 (4)
C19	0.36774 (8)	0.0157 (2)	0.32513 (12)	0.0310 (5)
H19	0.359627	−0.049051	0.290996	0.037*
C20	0.37205 (8)	−0.0125 (2)	0.39419 (13)	0.0381 (6)
H20	0.366040	−0.096108	0.407257	0.046*
C21	0.38532 (8)	0.0840 (2)	0.44368 (13)	0.0355 (6)
H21	0.388757	0.066594	0.490839	0.043*
C22	0.39350 (7)	0.2072 (2)	0.42252 (11)	0.0266 (5)
H22	0.403594	0.271438	0.456605	0.032*
C24	0.39499 (7)	0.67046 (19)	0.25470 (10)	0.0202 (4)
C25	0.44351 (6)	0.63412 (19)	0.30278 (10)	0.0194 (4)
C26	0.47900 (7)	0.7262 (2)	0.32388 (12)	0.0299 (5)
H26	0.473912	0.811046	0.307144	0.036*
C27	0.52231 (8)	0.6901 (2)	0.37041 (13)	0.0351 (6)
H27	0.546590	0.750798	0.386568	0.042*
C28	0.52884 (7)	0.5631 (2)	0.39232 (12)	0.0300 (5)
H28	0.557696	0.536946	0.423668	0.036*
C29	0.49216 (7)	0.4735 (2)	0.36752 (10)	0.0212 (4)
C30	0.50000 (7)	0.3348 (2)	0.38690 (11)	0.0238 (5)
C31	0.52156 (8)	0.2984 (2)	0.45652 (13)	0.0358 (6)
H31	0.530867	0.361368	0.491477	0.043*
C32	0.52911 (9)	0.1682 (3)	0.47355 (15)	0.0489 (7)
H32	0.542910	0.143620	0.520184	0.059*
C33	0.51618 (9)	0.0743 (3)	0.42137 (18)	0.0525 (8)
H33	0.521383	−0.013085	0.433109	0.063*
C34	0.49568 (8)	0.1099 (2)	0.35224 (15)	0.0429 (6)
H34	0.487361	0.046892	0.317151	0.051*
C35	0.48754 (7)	0.2399 (2)	0.33535 (13)	0.0294 (5)
H35	0.473498	0.263874	0.288680	0.035*
O5	0.36041 (7)	0.7513 (2)	0.07137 (10)	0.0522 (5)
H5A	0.367315	0.744953	0.115915	0.078*
H5B	0.360572	0.673382	0.057214	0.078*

structures of Mn(II), Co(II), Cu(II), Zn(II) and Pb(II) complexes using 6-phenylpyridine-2-carboxylate ligand [9–15]. In view of the above studies, in this work, we reported a Ni(II) complex, using 6-phenylpyridine-2-carboxylic acid, $Ni(CH_3COO)_2{\cdot}4H_2O$.

The molecular structure of the title complex is shown in the figure. The Ni(II) complex is made up of a Ni(II) ion, two 6-phenylpyridine-2-carboxylate ligands, one 2,2′-bipyridine ligand and one lattice water molecule. The title complex is for example isomorphous to the related manganese(II) complex [9]. The 6-phenylpyridine-2-carboxylate ligands adopt a bidentate coordination mode. The Ni(II) ion is six-coordinated with two N atoms (N1, N2) and two O atoms (O2, O3) from two different 6-phenylpyridine-2-carboxylate ligands, two N atoms (N3, N4) from one 2,2′-bipyridine ligand, respectively. Which forms a distorted octahedral coordination polyhedron. The sum of bond angles of O2–Ni1–N1 (79.35(6)°), N2–Ni1–O2 (82.11(6)°), N2–Ni1–N4 (99.42(6)°) and N4–Ni1–N1 (100.74(6)°) is 361.62°, and N3–Ni1–O3 is 169.88(6)°), indicating that the center Ni(II) ion is in the same plane with N1,O2,N2,O4 atoms and N3, O3 atoms are at the axial position. The bond lengths of Ni1–N1, Ni1–O2, Ni1–N2, Ni1–N4, Ni1–O3 and Ni1–N3 are 2.1822(15), 2.0193(13), 2.1896(15), 2.0755(16), 2.0206(13) and 2.1233(16) Å, respectively, which are consistent with those reported in the literature [5]. The complexes are interconnected by intermolecular O–H···O hydrogen bonds including oxygen atoms of lattice water molecules and the carboxyl oxygen atoms of 6-phenylpyridine-2-carboxylate ligand to form chain architecture.

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

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