The crystal structure of [(1,10-phenanthroline-κ²N,N)-bis(6-phenylpyridine-2-carboxylate-κ²N,O) nickel(II)] monohydrate, C₃₆H₂₆N₄O₅Ni

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Abstract
C₃₆H₂₆N₄O₅Ni, orthorhombic, P₂₁₂₁₂₁ (no. 19), a = 10.5860(9) Å, b = 10.6497(6) Å, c = 26.4492(15) Å, β = 90°, V = 2981.8(3) Å³, Z = 4, Rgt(F) = 0.0341, wRref(F²) = 0.0703, T = 200 K.
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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.

Source of material
The title compound has been synthesized as following: 1,10-phenanthroline (0.0405 g, 0.25 mmol), 6-phenylpyridine-2-carboxylic acid (0.0498 g, 0.25 mmol), Ni(O₂CMe)₂·4H₂O (0.0622 g, 0.25 mmol), and NaOH (0.010 g, 0.25 mmol) were dissolved into a solution of 22 mL 95% ethanol-water (v:v = 1:1) under constant heating and stirring. After the mixture was heated up to 70° C, the mixture continued to react for 5 h at this temperature. Then the reaction was then stopped and cooled down to room temperature and filtered. The needle-like crystals of [(1,10-phenanthroline-κ²N,N)-bis(6-phenylpyridine-2-carboxylate-κ²N,O) nickel(II)] monohydrate were received in 15 days.


IR: 1655 cm⁻¹ (C=O), 1386 cm⁻¹ (COO⁻).

Experimental details
The hydrogen atoms were positioned geometrically (C–H = 0.93 Å and O–H = 0.85 Å). Their Ueq values were set to 1.2Ueq or 1.5Ueq of the parent atoms.

Comment
In general, transition metal complexes may be self-assembled to create 1D, 2D, and 3D structures [5], and they have also exhibited potential applications in anti-tumor agents [6], antiviral agents [7], CO₂ photoreduction [8], effective adsorption of iodine [9], and so on. In our previous work, Co(II), Cu(II), Zn(II), and Pb(II) complexes...
of 6-phenylpyridine-2-carboxylates have been synthesized and structurally characterized [10–15].

The title compound was characterized through elemental analysis, infrared spectrum, and X-ray single-crystal diffraction. The molecular structure is composed of a Ni(II) ion, two 6-phenylpyridine-2-carboxylate ligands, one 1,10-phenanthroline ligand and one lattice water molecule. The Ni(II) ion coordinates with four N atoms (N1, N2, N3, N4). N1 and N2 atoms are from one 1,10-phenanthroline ligand, and N3, N4 atoms are from two different 6-phenylpyridine-2-carboxylate ligands, and two O atoms (O2, O3) from two different 6-phenylpyridine-2-carboxylate ligands, forming a distorted six-coordinated octahedral geometry. The Ni–O and Ni–N distances are 2.007(2) Å (Ni–O2), 2.008(3) Å (Ni1–O3), 2.087(3) Å (Ni1–N1), 2.115(3) Å (Ni1–N2), 2.211(3) Å (Ni1–N3), 2.167(3) Å (Ni1–N4), which is consistent with the literature. The sum of angles around Ni(II) ion is 362.59° (N3–Ni1–O2, 87.34(10)°; N3–Ni1–N2, 85.36(11)°; N2–Ni1–N4, 110.44(11)°; N4–Ni1–O2, 79.45(10)°), and the angle of O1–Ni1–N1 is 168.97(11)°, showing that O2, N3, N4 atoms are at the equatorial plane and O3, N1 atoms are at axial position. The dihedral angles between phenyl and pyridyl groups of the 6-phenylpyridine-2-carboxylate ligands are 66.0° (phenyl ring: C7–C8–C9–C10–C11–C12 and pyridyl ring: C1–C2–C3–C4–C5–C6) and 130.3° (phenyl ring: C19–C20–C21–C22–C23–C24 and pyridyl ring: C14–C15–C16–C17–C18–N3). The molecules form 1D chain structure by the O–H–O hydrogen bond between the lattice water molecule and a 6-phenylpyridine-2-carboxylate ligand.
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References