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Crystal structure of poly[($\mu_2$-5-hydroxyisophthalato-$\kappa^4O,O':O'',O'''$)-($\mu_2$-1,4-bis(2-methylimidazolyl)-1-butene-$N':N'$)nickel(II)], C$_{20}$H$_{20}$NiN$_{4}$O$_{5}$

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Abstract
C$_{20}$H$_{20}$NiN$_{4}$O$_{5}$, monoclinic, $P2_1/n$ (no. 14), $a = 8.8571(7)$ Å, $b = 20.4827(14)$ Å, $c = 10.9374(8)$ Å, $\beta = 101.235(3)^\circ$, $V = 1946.2(2)$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.0697$, $wR_{ref}(F^2) = 0.1486$, $T = 193(2)$ K.

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The molecular structure is shown in the Figure 1. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of materials

All chemicals were purchased from commercial sources and used as received. A mixture of nickel nitrate hexahydrate (29.8 mg, 0.1 mmol), 5-hydroxyisophthalic acid (Hip) (17.0 mg,
2 Experimental details

The structure was solved by Direct Methods with the SHELXS-2018 program. All H-atoms from C-atoms were positioned with idealized geometry and refined isotropically \(U_{eq}(H) = 1.2\) or 1.5 \(U_{eq}(C)\) using a riding model with C–H = 0.950, 0.980, and 0.990 Å.

3 Comment

In the past two decades, metal-organic frameworks (MOFs) have attracted intense interest of chemists because of novel and diverse topological architectures.\(^5\)\(^7\) As we know, some isophthalic acids have been used in preparation of MOFs.\(^8\)\(^10\) And, some nickel complexes have been reported with 1,4-bis-(imidazolyl)butane.\(^11\)\(^13\) However, there is no report about the study of nickel MOFs based on 1,4-bis-(2-methylimidazolyl)-1-butene to date. In this paper, we have prepared a new coordination polymer using 5-hydroxysophthalic acid and 1,4-bis(2-methylimidazolyl)-1-butene constructing \([\text{Ni(ip)(bimb)}]_n\). Single-crystal structure analysis revealed that the title compound crystalized in the monoclinic space group \(P2_1/n\) with two-dimensional layer framework. The ORTEP diagram is presented in Figure 1. The asymmetric unit consists of one Ni(II), one ip anion, and one bimb co-ligand. Each Ni(II) atom is coordinated with four oxygen atoms from two Hip\(^2\)-ligands, two nitrogen atoms from two bimb ligands, which forms a slightly distorted octahedral coordination geometry with NiO\(_6\)N\(_2\). The Ni–O and Ni–N lengths are 2.059(3)–2.203(3) Å and 2.048(4)–2.054(4) Å, respectively. In the title compound, the ip\(^2\)-ligand serves as a \(\mu_2\)-bridge linking two adjacent Ni\(^{II}\) ions in the bis-chelating mode to give rise to a one-dimensional chain, while such one-dimensional chains are further double-bridged by bimb ligands into a two-dimensional layer structure.

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References