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A LADDER-LIKE COBALT(II) COORDINATION POLYMER INCORPARATING PIVALATE AND 4,4′-BIPYRIDINE LIGANDS

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Abstract

A new one-dimensional (1D) coordination polymer $[Co(piv)_2(4,4'\text{-bpy})]_n$ (**1**) (where Hpiv = pivalic acid, 4,4′-bpy = 4,4′-bipyridine) has been synthesized via the solvothermal reaction of a dinuclear $[Co_2(H_2O)(piv)_4(Hpiv)_4]$ complex with 4,4′-bipyridine. Single-crystal X-ray diffraction analysis reveals that the structure of **1** adopts a distinctive ladder-like chain architecture. In this structural motif, dinuclear $[Co_2(piv)_4]$ subunits function as the rigid rungs, while the elongated 4,4′-bpy ligands act as the rails, which together define the ladder-like topology of the coordination polymer. Within the chains, the 4,4′-bpy exo-ligand bridge the Co(II) centers with a Co···Co separation of 11.407 Å, while the pivalate ligands facilitate inter-chain connectivity through double-bridging modes, resulting in a significantly shorter Co···Co separation of 4.155 Å. The influence of the various types of intermolecular interactions on the crystal packing was evaluated using Hirshfeld surface analysis and 2D fingerprint plots.

Keywords: ladder-like, coordination polymer, cobalt, pivalic acid, 4,4′-bipyridine, X-ray structure, Hirshfeld surface analysis.

UN POLIMER COORDINATIV DE COBALT(II) DE TIP SCARĂ CARE ÎNCORPOREAZĂ LIGANZI DE PIVALAT ȘI 4,4′-BIPIRIDINĂ

Resumat

Un nou polimer de coordinativ unidimensional (1D), $[Co(piv)_2(4,4'\text{-bpy})]_n$ (**1**) (unde Hpiv = acid pivalic, 4,4′-bpy = 4,4′-bipiridină), a fost sintetizat prin reacția solvotermală a unui complex dinuclear $[Co_2(H_2O)(piv)_4(Hpiv)_4]$ cu 4,4′-bipiridină. Analiza prin difracție de raze X pe monocristal relevă faptul că structura compusului **1** constă din lanțuri de tip scară. În acest motiv structural, subunitățile dinucleare $[Co_2(piv)_4]$ funcționează ca trepte rigide, în timp ce liganzii alungiți de 4,4′-bpy servesc drept trepte, care împreună definesc topologia de tip scară a polimerului coordinativ. În cadrul lanțurilor, exo-ligandul 4,4′-bpy leagă centrele Co(II) cu o separare Co···Co de 11,407 Å, în timp ce liganzii pivalați facilitează conectivitatea inter-lanț prin moduri de dublă punte, rezultând o separare Co···Co semnificativ mai scurtă de 4,155 Å. Influența diverselor tipuri de interacțiuni intermoleculare asupra împachetării cristaline a fost evaluată ulterior prin analiza suprafeței Hirshfeld și prin diagrame de amprentă 2D.

Cuvinte-cheie: tip scară, polimer coordnativ, cobalt, 4,4′-bipiridină, acid trimetilacetic, structură cu raze X, analiza suprafaței Hirshfeld.

Introduction

The design and synthesis of coordination polymers (CPs) based on transition metal ions and organic bridging ligands have become a focal point in materials science [1-4]. Among the transition metals, cobalt occupies a prominent position due to its versatile coordination geometries, multiple oxidation states, and potential for exhibiting interesting magnetic and catalytic properties [5-8]. The structural diversity of cobalt-based CPs, in conjunction with their tunable architectures, offers significant potential for the development of functional porous materials that exhibit desirable physical and chemical characteristics [9-11].

A fundamental strategy employed in the field of crystal engineering of cobalt-based systems involves the utilization of carboxylate groups as preferred spacer ligands, often in conjunction

with select auxiliary co-ligands [8, 11-14]. Specifically, pivalate ligands have proven highly effective in stabilizing both discrete clusters and extended frameworks [8,15-17]. The pivalate moiety is particularly advantageous as it combines the robust coordination ability of the carboxylate group with the significant steric bulk and hydrophobic nature of the *tert*-butyl group. These features enable the regulated assembly of metal clusters, where pivalate ligands frequently function as terminal or bridging units, thereby determining the ultimate dimensionality of the framework [18-20]. On the other hand, the 4,4′-bipyridine (4,4′-bpy) ligand facilitates the formation of various topologies, including 1D chains, 2D layers, and 3D frameworks [21]. Despite the established utility of both pivalates and 4,4′-bpy in coordination chemistry, the library of cobalt-based coordination polymers featuring this specific combination remains remarkably sparse. A survey of the Cambridge Structural Database (CSD) [22] reveals only two reported cobalt-pivalate polymers bridged by 4,4′-bpy (refcodes: ILUXOD [19] and YEHGAV [20]). The aforementioned examples are both constituted by two-dimensional (2D) polymeric layers that are characterized by the presence of honeycomb-like cavities.

As cobalt-based coordination polymers with these ligands have not been extensively explored, the present study seeks to expand the structural landscape of this family. We report the synthesis and structural characterization of a new one-dimensional (1D) ladder-like coordination polymer, $[Co(piv)_2(4,4'\text{-bpy})]_n$ (**1**) (where Hpiv = pivalic acid, 4,4′-bpy = 4,4′-bipyridine). The structure of **1** was elucidated using single-crystal X-ray diffraction, complemented by IR and TG analyses to establish structure-property relationships. Additionally, Hirshfeld surface analysis was conducted to provide a quantitative and qualitative assessment of the intermolecular interactions governing the crystalline packing of this new cobalt architecture.

Experimental section

Method and materials. Commercially available chemicals were used without further purification. All reactions were carried out under aerobic conditions using commercial grade solvents. Cobalt(II) pivalate was prepared by the method described in literature [23]. Thermogravimetric analysis measurements were performed on METTLER TOLEDO thermogravimetric analyzer TGA/DSC3 in nitrogen atmosphere with heating rate of 5 K/min from 25 to 600 °C. The hydro(solvo)thermal synthesis was carried out in cylindrical PTFE-lined stainless-steel autoclave, which were heated in a Memmert UFP 400 programmable oven. The FT-IR spectrum were recorded using a Perkin Elmer FT-IR Spectrum spectrophotometer within the 650-4000 cm^{-1} range. HS analysis and two-dimensional (2D) fingerprint plots diagrams generated by CrystalExplorer [24-25] were performed to investigate the nature and quantitative contributions of intermolecular interactions in crystal assembly. The 2D fingerprint plots were displayed using the 0.6–2.8 Å expanded view, with the scale for the d_i (inside) and d_e (outside) distances displayed on the plot axes.

Synthesis of $[Co(piv)_2(4,4'\text{-bpy})]_n$ (1). A mixture containing $[Co_2(H_2O)(piv)_4(Hpiv)_4]$ (0.28 g, 0.295 mmol), NaN_3 (0.01 g, 0.15 mmol), and 4,4′-bpy (0.023 g, 0.15 mmol) in 6 mL of ethanol was stirred to homogenize and then transferred to a cylindrical PTFE-lined stainless-steel autoclave and slowly heated in an oven for 2 h to reach 120°C The temperature was held constant for an additional 48 h, followed by cooling for 48 h to room temperature. Dark-orange, needle-shaped crystals suitable for single-crystal X-ray diffraction were filtered off, washed with a small amount of water and then cold ethanol, and dried in air. Yield: 0.033 g, 13% (based on Co). Notably, while sodium azide does not coordinate to metal center, it acts as a necessary template for the formation of the crystals; blank experiments preformed without sodium azide failed to yield any crystalline product. FT-IR (cm^{-1}) 2951 (m), 2927 (m), 2864 (sh), 1585 (vs), 1544 (sh), 1481 (s), 1459 (sh), 1418 (vs), 1375 (sh), 1355 (s), 1291 (sh), 1221 (vs), 1208 (sh), 1103 (w), 1071 (m), 954 (m), 934 (w), 895 (s), 811 (vs), 732 (m), 630 (vs), 600 (s).

Crystallography. Single-crystal X-ray diffraction experiments for **1** were performed at 293 K on a Xcalibur E CCD diffractometer equipped with graphite-monochromatized Mo Kα radiation. The positions of the metal atoms were determined using direct methods. The other atoms were subsequently identified through alternating cycles of least-squares refinement and difference Fourier map analysis. All non-hydrogen atoms were refined anisotropically using a full-matrix least-squares approach implemented in the SHELX software package [26]. The experimental data are presented in Table 1 and selected bond distances and angles in Table 3. Crystallographic data for the structure have been deposited with the Cambridge Crystallographic Data Centre (CCDC) under the accession number: 2538525.

Results and disscusion

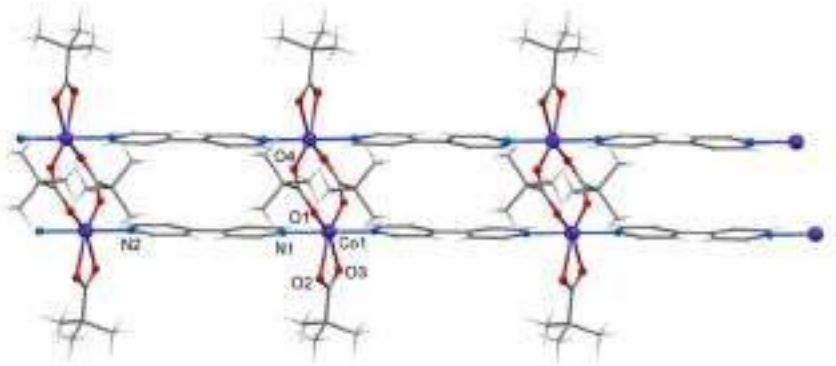
Structural Characterization

Single crystal X-ray analysis reveals that 1 crystallizes in the monoclinic $P2_1/c$ space group, with unit cell parameters a = 11.3930(8), b = 11.4065(7), c = 16.4614(9) Å, β = 101.144(6)°, V = 2098.9(2) Å^3 (Table 1). The X-ray analysis shows that 1 represent the ladder type 1D coordination polymer, in which dimeric [$Co_2(piv)_4$] units serve as ladder rungs, while the 4,4′-bpy ligands serve as the rails (Fig. 1a). In this arrangement, the 4,4′-bpy molecules function as linear spacers, effectively separating the metal nodes along the chain. The pivalate groups play a dual role: they satisfy the coordination requirements of the Co(II) ions and facilitate inter-chain connectivity. Their bulky *tert*-butyl groups govern the supramolecular assembly, providing steric hindrance that prevent the formation of higher-dimensional frameworks. Survey of CSD reveals only two examples of similar ladder-like cobalt polymer with phenyl [27], and trifluoroacetic acid [28] carboxylate ligands.

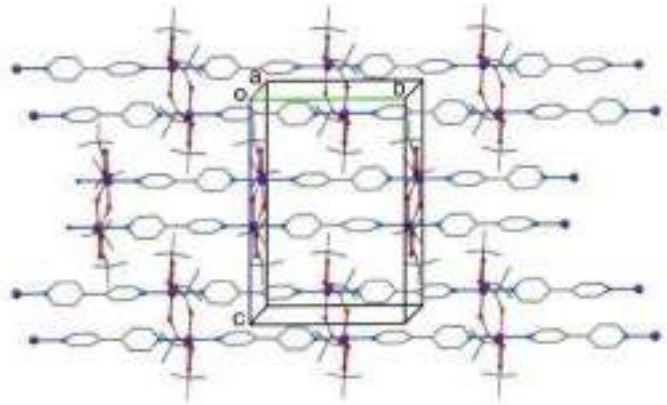
The coordination environment around the cobalt center is best described as a distorted N_2O_4 octahedron. This geometry is further confirmed by Continuous Shape Measure (CShM) analysis [29-30], which yields a value of 2.738, indicating a clear deviation from the ideal octahedral (*O*$_h$, *OC*-6) symmetry (Table 2). The coordination sphere is composed of four oxygen atoms from three pivalate ligands (comprising two bridging and one chelating group) and two nitrogen atoms from 4,4′-bpy ligands occupying *trans*-positions. The Co–O bond distances range from 2.024(2) to 2.241(2) Å, while the Co–N bond distances are similar and equal 2.151(2) and 2.155(2) Å (Table 3). Two pivalate ligands adopt a μ_2-bridging mode, linking adjacent cobalt centers into dinuclear [Co_2] units with a Co···Co separation of 4.1553(5) Å. These units are further extended into a 1D polymeric ladder-like structure by the 4,4′-bpy spacers, which bridge the metal nodes along the chain with a Co···Co separation of 11.4065(9) Å. In the crystal lattice, these chains are parallel and running along the *b* crystallographic axis (Fig. 1b).

IR Spectroscopy and Thermal Analysis

The IR spectrum of 1 exhibits characteristic asymmetric and symmetric absorption bands corresponding to the coordinated pivalate ligands and the 4,4′-bpy linkers. Aliphatic C–H asymmetric and symmetric stretching vibrations of the *tert*-butyl fragments of the pivalates, along with the aromatic C–H stretching vibrations of 4,4′-bpy ligands, appear in the 2951-2864 cm^{-1} range. Bands at 1481 cm^{-1} and in the 1418-1355 cm^{-1} region are attributed to asymmetric and symmetric C–H bending vibrations, respectively. Strong characteristic bands in the region of 1585-1544 cm^{-1} are assigned to the asymmetric stretching vibrations of the coordinated carboxylate groups, ν_{as}(COO), overlapping with the ν(C=N) stretching of the 4,4′-bpy ligands. The band at 1418 cm^{-1} corresponds to symmetric ν_s(COO) stretching modes of the carboxylate groups. Further, the absorption at 1221 cm^{-1} is associated with C–N stretching and in-plane aromatic ring vibrations of the 4,4′-bpy ligand, while the peak at 1072 cm^{-1} is attributed to pyridyl rings deformations. In the lower-frequency region, peaks at 895, 811, and 732 cm^{-1} correspond to the out-of-plane C–H bending vibrations of the 4,4′-bpy pyridine rings.



(a)



(b)

Figure 1. (a) View of the ladder-like 1D polymer in the structure; (b) View of the crystal packing of 1, showing the parallel arrangement of the chains along the *b* axis.

Table 1. Crystal data and details of structural determinations for 1

Formula	$C_{20}H_{26}CoN_2O_4$
*M*r / g·mol^{-1}	417.36
Crystal system	Monoclinic
Space group	$P2_1/c$
a/Å	11.3930(8)
b/Å	11.4065(7)
c/Å	16.4614(9)
α/°	90
β/°	101.144(6)
γ/°	90
V/Å^3	2098.9(2)
Z	4
Final R_1, wR_2 (%)	0.0473, 0.1057
R indices R_1, wR_2 (all data) (%)	0.0804, 0.1196

Table 2. Continuous shape measures (CShM) for the coordination geometry of the Co center in 1

	JPPY-6	*TPR*-6	*OC*-6	*PPY*-6	*HP*-6
ML6	Johnson pentagonal pyramid J2 (C_{5v})	Trigonal prism (D_{3h})	Octahedron (O_h)	Pentagonal pyramid (C_{5v})	Hexagon (D_{6h})
Co1	27.166	11.223	**2.738**	23.156	33.019

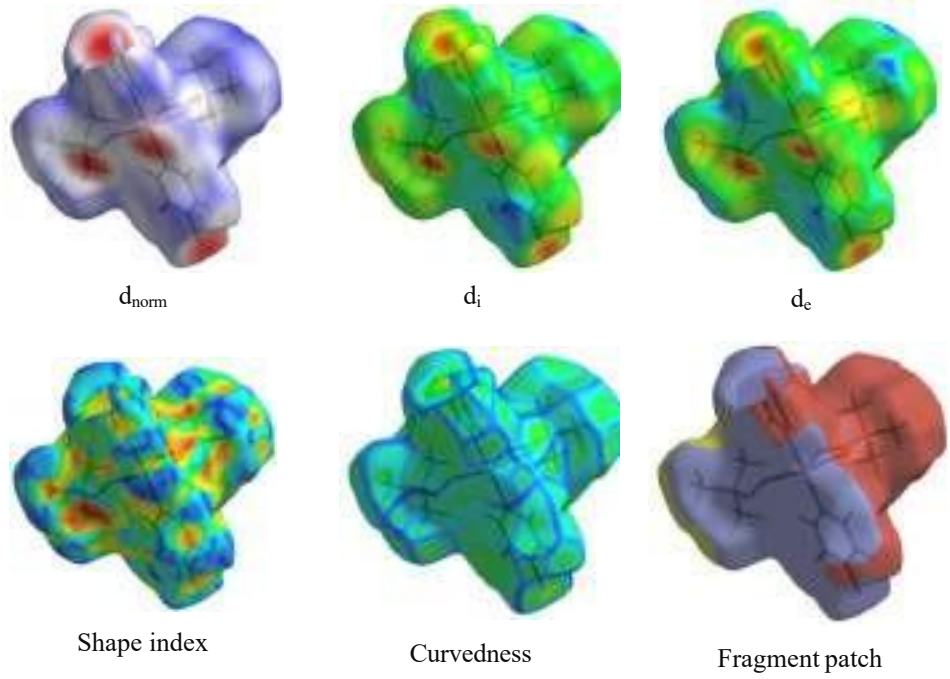
Table 3. Selected bond distances (Å) and angles (°) in 1

Co(1)–O(1)	2.025(2)	O(4)–Co(1)–N(2)	86.77(9)
Co(1)–O(4)	2.026(2)	O(3)–Co(1)–N(2)	91.55(9)
Co(1)–O(3)	2.144(2)	O(1)–Co(1)–N(1)	90.67(8)
Co(1)–N(2)	2.151(2)	O(4)–Co(1)–N(1)	93.54(8)
Co(1)–N(1)	2.156(2)	O(3)–Co(1)–N(1)	88.49(8)
Co(1)–O(2)	2.241(2)	N(2)–Co(1)–N(1)	179.68(9)
O(1)–Co(1)–O(4)	115.57(9)	O(1)–Co(1)–O(2)	92.97(8)
O(1)–Co(1)–O(3)	152.52(9)	O(4)–Co(1)–O(2)	151.43(9)
O(4)–Co(1)–O(3)	91.89(9)	O(3)–Co(1)–O(2)	59.55(8)
O(1)–Co(1)–N(2)	89.15(9)	N(2)–Co(1)–O(2)	92.60(8)
		N(1)–Co(1)–O(2)	87.15(8)

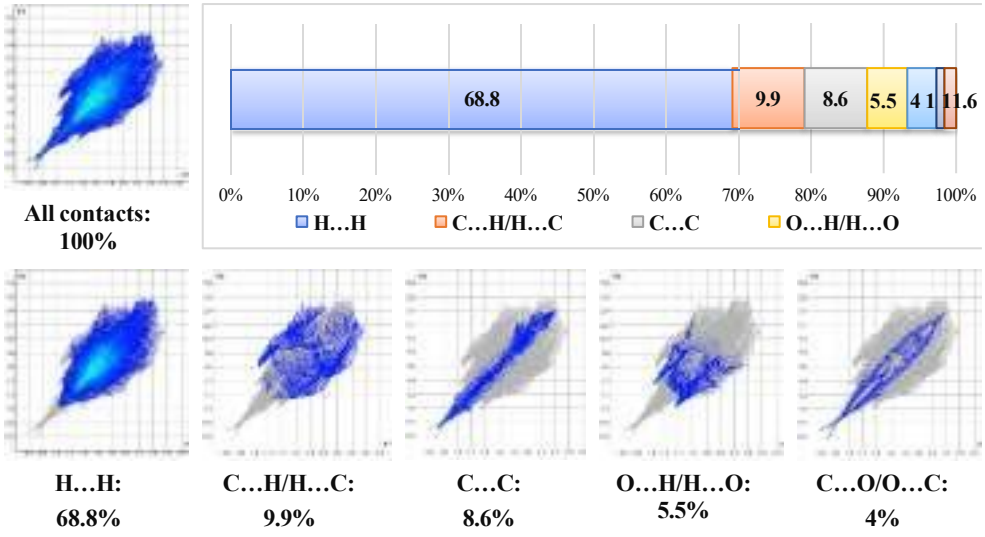
The thermal analysis of coordination polymer 1 reveals that the material is stable up to 180 °C. Above this temperature, a significant mass loss of 85.8% (calc. 85.8%) occurs in the temperature range up to 290 °C, corresponding to simultaneous decomposition of both pivalate and 4,4′-bpy ligands. The next stage, between 313 °C and 330 °C, involves the complete decomposition of the framework, resulting in a solid residue of CoO. The DTA curve exhibits a thermal effect associated with the degradation of the organic ligands with a minor endothermic peak at 310 °C.

Hirshfeld Surface Calculation

The Hirshfeld molecular surfaces for a fragment of the one-dimensional polymeric compound $[Co(piv)_2(4,4'\text{-bpy})]_n$ (1) was generated at high resolution, with the three-dimensional surfaces mapped over d_{norm} using a fixed color scale ranging from -1.2138 to +1.7015 (Fig. 2a). The two-dimensional (2D) fingerprint plots were employed to quantify the contributions of all intermolecular contacts (Fig. 2b). The analysis reveals that H···H interactions dominate, comprising 68.8% of the Hirshfeld surface and reflecting their prevalence in the crystal packing. The C···H/H···C contacts represent the second most significant contribution (9.9%), suggesting the presence of weak C–H···π interactions within the lattice. In addition, C···C interactions account for 8.6%, which can be attributed to π-π stacking between the aromatic rings of the 4,4′-bpy ligands. Hydrogen bond O···H/H···O contacts contribute 5.5%, indicating weak hydrogen bonding involving carboxylate oxygen atoms. Furthermore, C···O/O···C interactions contribute 4.0%, while other minor contacts collectively represent 3.2% of the Hirshfeld surface.



(a)



(b)

Figure 2. (a) View of the Hirshfeld surface for the $[Co(piv)_2(4,4'\text{-bpy})]_n$ (1) decorated with different properties. (b) 2D fingerprint plot with the relative contributions of all contacts mapped over d_{norm} in 1

Conclusions

In conclusion, a new 1D coordination polymer, $[Co(piv)_2(4,4'\text{-bpy})]_n$ (**1**), has been synthesized and structurally characterized. The polymer structure exhibits a distinct ladder-like topology based on $[Co_2(piv)_4]$ building units, which function as the structural "rungs" of the ladder. These dimeric nodes are interconnected by rigid 4,4'-bpy ligands acting as "rails" that extend the coordination network along the *b* axis in **1**. This specific 1D architecture is further stabilized by the peripheral *tert*-butyl groups of the pivalate ligands, which effectively shield the polymeric chains and prevent inter-chain cross-linking into higher-dimensional networks. The results demonstrate that the synergy between rigid aromatic spacers and sterically demanding carboxylates is an effective strategy for engineering stable, low-dimensional molecular architectures.

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