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# A novel cyano-bridged heteronuclear complex exhibiting C–H…Ni close interaction: $[Cd(C_4H_7N)_2Ni(\mu-CN)_4]_n$

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# 1. Introduction

The field of transition metal cyanide chemistry has a remarkable history that spans almost three centuries, dating back to the earlier 18th century. The wide availability of cyano complexes together with their diverse bonding and structural chemistry has led to their widespread applications in the field of material chemistry [1]. Functional polymeric cyano complexes can be prepared with two or more dentate ligands. These types of materials are packed to form crystal structures due to bridging groups and intermolecular interactions [2]. Tetracyanonickelate complexes [3,4] have nitrogens in the square  $[Ni(CN)_4]^{2-}$  anion to form additional coordination bonds enhancing dimensionality of the structure [4,5]. The ability of the tetracyanonickelate anion to form oligo- and polynuclear compounds was mainly exploited in connection with their ability to form Hofmann-type and analogous clathrates [6]. Tetracvanonickelates exhibiting especially low-dimensional structures for magnetic applications attract the interest of chemists and physicists [7-9].

The Hofmann-type compounds  $[ML_2M'(CN)_4]_n$ , which were first prepared by Hofmann in 1897 [10] and extensively studied by Iwamoto and others, show 2D structures with variety of small molecules intercalated between the layers [11,12]. Based on this structure, metal(II) tetracyanonickelate complexes have been developed

# ABSTRACT

The cyano-bridged heteronuclear polymeric complex,  $[Cd(pyr)_2Ni(\mu-CN)_4]_n$ , **1** (pyr = 3-pyrroline or 2,5dihydropyrrole), has been synthesized and characterized by FT-IR, Raman spectroscopy, thermal and elemental analyses. The crystal structure of **1** has been determined by X-ray single crystal diffraction. The complex crystallizes in orthorhombic system and space group *Pmna*. In **1**, Ni(II) ion is coordinated by four cyano ligands, and the Cd(II) ion is coordinated by four bridging cyanide ligands and two *trans* pyr ligands. The coordination environment of the Cd(II) ion described as distorted octahedral geometry, whereas around the Ni(II) centre has square planar geometry. The crystallographic analysis reveals that the weak intermolecular C–H…Ni interaction was found to be hydrogen bonding interaction, resulting in a 3D framework. Vibration assignments were given for all the observed bands and the spectral feature also supported to the structure of polymeric complex. The decomposition reaction take places in the temperature range 30–700 °C in the static air atmosphere.

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using N-donor ligands 2-methylpyrazine [13], triethylenetetramine [14,15], 2-aminomethylpyridine [16]. The Hofmann-type host framework is formed from infinite  $\{M-Ni(CN)_4\}_n$  layers with four planar coordination around Ni atom [17].

Non-covalent interactions are very important in biological structure, supramolecular chemistry and molecular recognition. When a C–H bond of transition metal ligands is oriented towards the metal ion, indicating some weak interaction between the metal and the H atom, this has been considered as an intramolecular hydrogen bonding. The most interesting feature of this structure is the C–H…Ni hydrogen bonding interaction. These weak interactions have facilitated the formation of the coordination bond between Cd(II) and the N donor of the pyr ligands. These intermolecular interactions give three-dimensional framework.

As far as we know, no vibrational and structural studies have been reported for the transition metal(II)-cyano complexes with pyr ligand. Here we report the results of our study on synthesis, chemical, spectral and structural characterization of one novel cyano-bridged heteronuclear polymeric complex,  $[Cd(pyr)_2Ni(\mu-CN)_4]_n(1)$ .

# 2. Experimental

# 2.1. Materials and instrumentation

Cd(II) chloride (CdCl<sub>2</sub>), potassium cyanide (KCN) and 3-pyrroline were purchased from commercial sources and used without further purification. The carbon, hydrogen and nitrogen content were

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analysed with a LECO CHNS-932 analyzer. The FT-IR spectrum was recorded in the range 4000–400 cm<sup>-1</sup> on a Perkin–Elmer 100 FT-IR spectrometer, using the KBr pellet technique. The Raman spectrum was recorded in the range of 4000–250 cm<sup>-1</sup> on a Bruker Senterra Dispersive Raman instrument using laser excitation of 785 nm. Per-kin–Elmer Diamond TG/DTA thermal analyzer was used to record simultaneous TG, DTG and DTA curves in the static air atmosphere at a heating rate of 10 K min<sup>-1</sup> in the temperature range 30–700 °C using platinum crucibles.

#### 2.2. Synthesis

# 2.2.1. Cd[Ni(CN)<sub>4</sub>]

A mixture of a solution of NiCl<sub>2</sub>·6H<sub>2</sub>O (1.18 g, 5 mmol) in water (20 mL) and a solution of KCN (1.30 g, 20 mmol) in water (20 mL) was added dropwise with stirring at 50 °C to a solution of CdCl<sub>2</sub> (0.92 g, 5 mmol) in water (20 mL). The mixture was refluxed with stirring for 2 h at 50 °C in a temperature-controlled bath and then the solution was cooled to room temperature.

# 2.2.2. $[Cd(pyr)_2Ni(\mu-CN)_4]_n$

A solution of 3-pyrroline (0.346 g, 5 mmol) in ethanol (10 mL) was added dropwise upon stirring to a solution of  $Cd[Ni(CN)_4]$  (1.371 g, 5 mmol) in water (30 mL). The solutions were refluxed

with stirring for 12 h at 60 °C. The reaction mixture was cooled to room temperature. The colorless crystals formed were filtered and washed with 10 mL of water and acetone and dried in air. The product obtained was left overnight in the open air. The yellow color plates like crystals formed on the top of solution were filtered. The C, H, N analysis for the sample was carried out and the results were found to fit well with the proposed formulae. The result is as follows (% found, % calculated):  $Cd(C_4H_7N)_2Ni(CN)_4$ : C(34.54/34.87), N(20.14/20.33), H(3.43/3.41).

#### 2.3. X-ray crystallography

Diffraction experiments were carried out at 296 K on a Stoe IPDS diffractometer. The structures were solved by direct methods and refined using the programs SHELXS97 and SHELXL97 [18]. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares methods [18]. The hydrogen atoms were placed in geometrically idealized positions and refined as riding atoms. The following procedures were implemented in our analysis: data collection: X-Area, cell refinement: X-Area, data reduction: X-RED [19]; program(s) used for molecular graphics were as follows: OR-TEP-3 for Windows [20]; software used to prepare material for publication: WinGX [21].



Fig. 1. The FT-IR (a) and Raman (b) spectra of 1.

#### 3. Results and discussion

#### 3.1. Vibrational spectra

The FT-IR and Raman spectra of **1** are given in Fig. 1a and b, respectively. Up to now, there has been no extensive vibrational study of pyr, although the microwave and infrared spectra on pyr and its N-deuterated species have been reported [22]. Therefore the spectral features due to the pyr in **1** were evaluated through the measured infrared frequencies of the free molecule. Additionally, normal mode frequencies and assignments of pyr (in gas phase) have been calculated at the B3LYP/6-311G(d, p) level by using the package Gaussian 03 [23]. The tentative assignments and the wavenumbers of the vibrational bands of the 3-pyrroline observed in the FT-IR and Raman spectra of 1 are presented in Table 1, together with the wavenumbers for the calculated data of the pyr. In the FT-IR and Raman spectra of 1, the absorption band at 3291 cm<sup>-1</sup> is assigned to the NH stretching frequency which is lower than the corresponding value for the pyr molecule (3440 cm<sup>-1</sup>) and characteristic of bonded Cd–NH group. This downward frequency shift can be explained as being due to weakening of the N-H bonds for electron draining from the N atom on account of its coordination to the Cd atom. A metal-dependent frequency shift is also observed for the NH wagging mode: e.g., the band at about 878 cm<sup>-1</sup> can be assigned to the NH bending vibration derived from the similar degenerate mode in **1**. The NH wagging mode shifts to higher frequency in complex form (892 cm<sup>-1</sup>). These shifts can be explained as the coupling of the internal mode of the pyr with M–N vibrations.

In the spectra of **1** the dominant feature is represented by strong and sharp well identifiable bands due to the v(CN) stretching vibrations. The  $v(C \equiv N)$  vibrations are the most important absorption bands for the complexes since the  $v(C \equiv N)$  vibrational peaks in the FT-IR and Raman spectra are used to elucidate the bridging formation in the polymeric complexes [2]. The vibrational wavenumbers of the  $[Ni(CN)_4]^{2-}$  group for **1** are given in Table 2. In order to assign the bands attributable to the  $[Ni(CN)_4]^{2-}$  ion in the

#### Table 1

The vibrational wavenumbers (cm<sup>-1</sup>) and assignments of pyr in **1**.

Assignment [2	2] pyr	pyr		1	
	Calculated	Experimental	FT-IR	Raman	
v(NH)	3447	3440 m	3291 w	3289 m	
v(CH)	3098	-	3049 vw	3049 w	
v(CH)	3075	3070 m	2957 vw	2959 m	
v(CH)	2931	2947 m	2931 vw	2931 m	
v(CH)	2879	2836 s	2878 vw	2878 s	
v(C=C)	1616	1615 m	1633 w	1604 w	
$\delta(CH_2)$	1461	1473 m	1478 wv	1475 w	
$\delta(CH_2)$	1454	1456 vw	1462 w	-	
$\delta(CH_2)$	1407	1412 m	1413 w	1414 w	
$\delta(CH_2)$	1320	1327 m	1331 w	-	
$\delta(CH)$	1306	1311 vw	-	-	
$\delta(CH_2)$	1273	1283 vw	-	1292 w	
$\delta(CH_2)$	1198	1180 m	1191 w	-	
v(CN)	1154	1153 vw	1166 w	-	
$\delta(CH)$	1081	1084 s	1079 m	1100 w	
v(CC)	1065	1064 vw	1056 m	-	
$\delta(CH_2)$	1021	1031 s	1028 vw	-	
$\delta(CH_2)$	981	965 m	968 s	971 w	
$\delta(CH_2)$	931	928 w	956 m	962 w	
γ(CH)	921	906 s	918 w	-	
$\delta(NH)$	878	866 vw	892 s	890 vw	
γring	779	789 vw	790 vw	780 vw	
$\gamma_{ring}(CH)$	736	725 vw	734 m	-	
$\gamma(NH)$	692	663 vs	674 s	675 w	
τ(CH)	652	662 vs	649 w	650 vw	

\* Abbreviations used: v, stretching;  $\delta$ , deformation; w, wagging; t, twisting; r, rocking; s, strong; m, medium; w, weak; sh, shoulder; v, very.

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The vibrational wavenumbers  $(cm^{-1})$  of the  $[Ni(CN)_4]^{2-}$  unit in **1**.

Assignment <sup>b</sup>	Na <sub>2</sub> [Ni(CN) <sub>4</sub> ] [24]	Cd-Ni-Py <sup>a</sup> [25]	1
$A_{1g}$ , $v(CN)$	(2149) vs	(2172) vs	(2164) vs
$B_{1g}$ , $v(CN)$	(2141) vs	(2160) s	-
$E_u, v(CN)$	2132 vs	2154 s	2146 vs
$v(^{13}CN)$	2087 sh	2111 w	2109 vw
$E_u$ , $v(NiC)$	543 w	543 w	545 w
$A_{2u}$ , $\pi$ (NiCN)	448 w	-	-
$E_u, \delta(NiCN)$	421 s	425 s	423 vs

The bands observed in the Raman spectra are given in parentheses.

<sup>a</sup> Cd-Ni-Py: [Cd(py)<sub>2</sub>Ni(CN)<sub>4</sub>].

<sup>b</sup> Abbreviations used: s, strong; m, medium; w, weak; sh, shoulder; v, very. The symbols  $\nu$ ,  $\delta$  and  $\pi$  refer to valence, in-plane and out-of-plane vibrations, respectively.

Table 3

Crystal data and structure refinement parameters for complex 1.

	1
Empirical formula	C <sub>12</sub> H <sub>14</sub> CdN <sub>6</sub> Ni
Formula weight	413.40
Temperature (K)	293 (2)
Wavelength (Å)	0.71073 ΜοΚα
Crystal system	Orthorhombic
Space group	Pmna
a (Å)	7.824 (2)
b (Å)	6.922 (1)
c (Å)	14.407 (2)
V (Å <sup>3</sup> )	780.2 (2)
Z	
Absorption coefficient (mm <sup>1</sup> )	2.57
$D_{\text{calc}}$ (Mg m <sup>3</sup> )	1.760
Theta range for data collection (°)	2.83-27.50
Measured reflections	2907
Independent reflections	947
Absorption correction	Integration Stoe X-RED
	Stoe and Cie [19]
Refinement method	Full-matrix least-squares on $F^2$
Final <i>R</i> indices $[I > 2\sigma(I)]$	$R_{\rm int} = 0.047$
Final R indices (all data)	R1 = 0.034
	$wR^2 = 0.089$
Goodness-of-fit on $F^2$	1.16
$\Delta  ho_{ m max}  ({ m e} { m \AA}^{-3})$	0.56
$\Delta  ho_{ m min}  ({ m e} {\rm \AA}^{-3})$	-0.65

spectra, we refer to the work of McCullough et al. who presented vibrational data for the salt Na2[Ni(CN)4] in the solid state [24] and [Cd(py)<sub>2</sub>Ni(CN)<sub>4</sub>] [25] for comparison. The assigned wavenumbers of the  $[Ni(CN)_4]^{2-}$  units of **1** appear to be much higher than those for isolated  $[Ni(CN)_4]^{2-}$  ion. The CN stretching mode, v(CN), is observed at 2146  $\text{cm}^{-1}$  in the FT-IR spectrum of **1** whereas the IR active v(CN) mode  $(E_u)$  of free  $[Ni(CN)_4]^{2-}$  group is observed at 2132 cm<sup>-1</sup> in the FT-IR spectrum of solid Na<sub>2</sub>[Ni(CN)<sub>4</sub>]. The upward shift of 14 cm<sup>-1</sup> on going from  $CN^-$  to  $Ni(CN)_4^{2-}$  was explained as the mechanical coupling of the Ni–C(CN) stretching mode with the v(CN) [25]. Such frequency shifts have been observed for the other cyano-bridged complexes [2,13-17,26,27] and are attributed to the mechanical coupling of the internal modes of  $[Ni(CN)_4]^{2-1}$ with the M-NC vibrations. It follows that the N-termini of the  $[Ni(CN)_4]^{2-}$  group are bound to a Cd atom in the complex investigated.

# 3.2. Crystal structure

The molecular structure of **1** with the atom labelling is shown in Fig. 2. Experimental data are listed in Table 3. The selected bond



**Fig. 2.** Molecular structure of **1** with atom-labelling scheme [symmetry codes: (i) -1 + x, *y*, *z*; (ii) -1 + x, 1 + y, *z*; (iii) *x*, 1 - y, 1 - z; (iv) 1 - x, *y*, *z*; (v) 1 - x, 1 - y, 1 - z; (vi) *x*, 2 - y, 1 - z].

lengths and angles are given in Table 4. Single X-ray crystal analysis reveals that the complex **1** crystallizes in the orthorhombic space group *Pmna*, which is a two-dimensional coordination polymer. Each nickel(II) ion is coordinated by four cyano ligands, forming a square planar geometry. The Ni1–C5 bond distance of 1.869 (3) Å is also similar to those found in reported tetracyanonickelate(II) complexes [13–18]. In **1**, the Cd(II) ion is also coordinated by four bridging cyanide ligands and two trans pyr ligands, forming distorted octahedral geometry (Fig. 2). The structure consists of corrugated and cyano-bridged heteropolynuclear two-dimensional

 Table 4

 Selected geometric parameters (Å, °) for complex 1.

Bond distances	Bond angle	es			
C5-Ni1	1.869 (3)	C5 <sup>ii</sup> -Ni1- C5	91.6 (2)	N1–Cd1– N2 <sup>vi</sup>	98.0 (1)
N1-Cd1	2.300 (5)	C5 <sup>iii</sup> –Ni1– C5	88.4 (2)	N1–Cd1– N2 <sup>v</sup>	83.3 (1)
N2-Cd1	2.374 (3)	N1-Cd1- N2	82.0 (1)	N1 <sup>v</sup> –Cd1– N1	159.7 (2)
		N1–Cd1– N2 <sup>i</sup>	96.8 (1)	N2 <sup>i</sup> –Cd1– N2	93.6 (1)
				N2 <sup>v</sup> –Cd1– N2	86.4 (1)

Symmetry codes: (i) -x + 1, y, z; (ii) -x, y, z; (iii) x, -y + 2, -z + 1; (iv) -x, -y + 2, -z + 1; (v) x, -y + 1, -z + 1; (vi) -x + 1, -y + 1, -z + 1.

networks. The intralayer  $Cd \cdots Cd^i$  (i: -1 + x, y, z) and  $Cd \cdots Cd^{ii}$  (ii: -1 + x, 1 + y, z) distances are 7.824 and 10.446 Å, whereas the shortest interlayer  $Cd \cdots Cd^{iii}$  (iii: 1/2 - x, 1 - y, -1/2 + z) distance is 8.197 Å. The Cd1-N2 = C5 bond angle (153.75°) is found to be slightly bent.

The most interesting structural features of complex is the presence of obvious C–H···M interaction between the Ni(II) center and H3 atom of pyr ligand. The crystal packing of complex is stabilized through interlayer weak C–H···Ni hydrogen bonding interaction, resulting in a 3D framework (Fig. 3). The Ni···H distance of 2.760 Å, Ni···C distance of 3.505 Å and C–H···Ni angle of 137.79° are similar to those values for reported Ni(II) complexes [28–30]. This interactions should be well described as being of a weak intermolecular C–H···Ni hydrogen bonding. To the best of our knowledge, this manner has not been reported so far although there are many complexes of tetracyanonickelate(II) [13–17]. This interlayer interaction gives three-dimensional framework.



Fig. 3. Unit cell structure in 1.

#### 3.3. Thermal analysis

A thermal decomposition behavior of the complex was performed in static atmosphere of air in the temperature range 30–700 °C. Thermal decomposition of the complex proceeds in the two stages. The complex is thermally stable up to about 105 °C. In the first stage range of 105–198 °C, the endothermic peak is related to the release of the one pyr ligand (found 16.67, calcd. 16.72%). In the second stage between 307 and 384 °C, the strong exothermic mass loss processes corresponds to the decomposition of other 3-pyr and cyanide ligands (DTA<sub>max</sub> = 377 °C). The final solid product is CdO + NiO.

# 4. Conclusions

The cyano-bridged heteronuclear polymeric complex **1** was synthesized and characterized by FT-IR spectroscopy, Raman spectroscopy, elemental analysis, thermal analysis and single crystal X-ray diffraction techniques. The complex **1** has shown that it has similar structure with linkage between the square planar  $[Ni(CN)_4]^{2-}$  and the octahedral Cd(II) through cyano bridges. The six coordination of Cd(II) is satisfied by four terminal N of the cyano groups and two pyr molecules. Additionally, CH...Ni(II) interaction is discussed in terms of X-ray crystal structural study.

# Supplementary data

CCDC 718826 contains the supplementary crystallographic data for **1**. This data can be obtained free of charge via http:// www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 (0)1223-336033; or e-mail: deposit@ccdc.cam.ac.uk.

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