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Vibrational Spectroscopic Study of 6-Aminouracil Tetracyanonickelate Complexes

6-Aminouracil Tetracyanonickelate Komplekslerinin Titreşim Spektroskopisi ile İncelenmesi

Research Article

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ABSTRACT

The FT-IR, FT-Raman and far-IR spectra of two dimensional coordination polymer compounds, $M(6AU)_2Ni(CN)_4$ (where M = Mn, Co, Ni and Cd; 6AU = 6-aminouracil = 4-amino-2,6-dihydroxypyrimidine) were reported for the first time. 6-aminouracil molecules are found to involve coordination through one of the pyrimidine ring nitrogen atoms. The spectral features suggest that the compounds are similar in structure to the Hofmann type two dimensional coordination polymer compounds, formed with $Ni(CN)_4^{2-}$ ions bridged by $M(6AU)_2^{2+}$ cations. Vibrational bands originated from both 6AU and $Ni(CN)_4$ group were assigned.

Key Words
6-aminouracil, far-IR, FT-IR, FT-Raman spectra, Hofmann type complexes

ÖZET

İki boyutlu kordinasyon polimer kompleksleri $M(6AU)_2Ni(CN)_4$ (burada M = Mn, Co, Ni ve Cd; 6AU = 6-aminouracil = 4-amino-2,6-dihydroxypyrimidine) ilk kez elde edilmiş ve FT-IR, FT-Raman ve far-IR ile incelenmiştir. 6-aminouracil molekülleri pirimidin halkasının azot atomlarının biri ile kordinasyon yaptığı bulunmuştur. $Ni(CN)_4^{2-}$ iyonları ile $M(6AU)_2^{2+}$ katyonlarının kordinasyonu sonucu, Hofmann tipi iki boyutlu kordinasyon polimer bileşikleri oluşturduğu spektral özellikler ile desteklenmiştir. 6AU ve $Ni(CN)_4$ grubunun her ikisinden kaynaklanan titreşim bandları tanımlanmıştır.

Anahtar Kelimeler
6-aminouracil, far-IR, FT-IR, FT-Raman spektrum, Hofmann tipi kompleksler

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INTRODUCTION

The derivatives of uracil deserve particular attention among all series of derivatives of nucleic pyrimidine bases. Some of the derivatives of uracil exhibit significant pharmacological activity and have been used as as antitumor, antibacterial, and antiviral drugs. The 6-aminouracil and 6-amino substituted derivatives of thymine have been found to be the competitive inhibitors of human thymidine phosphorylase [1,2]. The derivatives of uracils have very important applications in organic synthesis [3]. The 6-aminouracils find wide application as starting materials for the synthesis of many fused uracils of biological significance, for example, phenylazo-[3], pyrano-, pyrido-, pyrazolo-, pyrimido- and pyridazino-pyrimidines [4]. Some derivatives of 6-aminouracil were synthesized and their possible diuretic, smooth muscle relaxant, and cardiovascular effects were studied [5]. The 6-aminouracil is used extensively as an intermediate in the synthesis of a number of compounds containing the pyrimidine ring, including the manufacture of the important sulphanilamide drug sulfadimethoxin [6]. It has been found to inhibit the uracil-DNA glycosylase [7] and the dihydropyrimidine dehydrogenase enzymes [8].

The well known Hofmann-type two dimensional complexes, $\{M(L)_2Ni(CN)_4\}$, are built by stacking the twodimensional nickel cyanide sheets in layers [9,10]. The two-dimensional sheet is constructed by the alternate linkage between square-planar Ni(II) and octahedral M(II) (M = Mn, Fe, Co, Ni, Cu, Zn or Cd) through the cyanide bridges. The octahedral coordination of M(II) is satisfied by four N-terminals of the cyano groups and two nitrogen atoms of the two N-donor ligands (L) in a trans configuration, protruding above and below the sheet [9,10]. In this study, 6-aminouracil tetracyanonickelate, $M(6AU)_2Ni(CN)_4$ {where M = Mn, Co, Ni or Cd; 6AU = 6-aminouracil, abbreviated hereafter as M–Ni–6AU}, coordination polymer compounds have been prepared for the first time, and their FT-IR (400–4000 cm^{-1}), FT-Raman (50–4000 cm^{-1}) and Far-IR (20–400 cm^{-1}) spectra are reported. These complexes are an example of two dimensional coordination polymers in tetracyanometallate-bridged systems. The aims of this study are to examine the coordination sensitive ligand modes and to determine vibrational wavenumbers of modes arising from metal–ligand bonds {$\nu(M–N)_{6AU}$, $\delta(N–M–N)_{6AU}$} by studying isostructural complexes $\{M(6AU)_2Ni(CN)_4\}$.

EXPERIMENTAL

All chemicals used were reagent grade (Aldrich) and they were used without further purification. The complexes M-Ni-6AU (M= Mn, Co, Ni or Cd) were prepared as following: at first 1 mmol of MCl_2 was dissolved in the distilled water, then to this solution 1 mmol of $K_2Ni(CN)_4$ dissolved in distilled water was added under stirring. After a short time slightly more than 2 mmol of the 6-aminouracil solution in alcohol were added to the mixture prepared drop wise, again under stirring. The final mixture was left for stirring around a week at room temperature. The obtained product was filtered and washed with water, ethanol and ether successively and dried in a desiccator which included P_2O_5.

The freshly prepared compounds were analyzed for C, H and N by a LECO CHNS-932 analyzer with the following results (found % / calculated %). The analytical results were agreement with the proposed formula.

$Mn(C_4H_5N_2O_2)_2Ni(CN)_4$: C= 30.28/30.54, H= 2.35/2.13, N= 29.06/29.68
$Co(C_4H_5N_2O_2)_2Ni(CN)_4$: C= 31.02/30.28, H= 2.33/2.11, N= 29.12/29.43
$Ni(C_4H_5N_2O_2)_2Ni(CN)_4$: C= 30.15/30.30, H= 2.09/2.11, N= 29.21/29.44
$Cd(C_4H_5N_2O_2)_2Ni(CN)_4$: C= 27.09/27.22, H= 1.44/1.90, N= 26.23/26.45

The FT-IR (4000-400 cm^{-1}) spectra between KBr windows as Nujol or hexachloro-1,3-butadiene mulls and far-infrared (400-20 cm^{-1}) spectra between polyethylene plates as Nujol mulls of the compounds were recorded via a Bruker Optics IFS66v/s FT-IR spectrometer with 2 cm^{-1} resolution in vacuum. FT-Raman spectra (4000-70 cm^{-1}) of the compounds were recorded using a Bruker Senterra Dispersive Raman microscope spectrometer with 532 or 633 nm excitations from a 3B diode laser having 3 cm^{-1}

resolution in the region of 3700 and 60 cm^{-1}. Far-IR spectra of the nujol mulls between polyethylene windows of the samples were recorded on a Perkin-Elmer System 2000 FT-IR Interferometer resolutions (4 cm^{-1} resolution).

RESULTS AND DISCUSSION

The structural formula of 6AU is given Figure 1. The FT-IR, FT-Raman and far-IR spectra of $M(6AU)_2Ni(CN)_4$ (where M= Mn, Co, Ni and Cd) are found to be very similar, suggesting that they have isomorphous crystal structures. The FT-IR, FT-Raman and far-IR spectra of the $M(6AU)_2Ni(CN)_4$ (where M= Mn, Co, Ni and Cd) complexes are given in Figure 2, 3 and 4, respectively. The assignments were divided into two groups arising from the 6-aminouracil and the $Ni(CN)_4$ ions.

6-aminouracil vibrations

The first detailed vibrational assignments for 6-aminouracil was made by S. Aruna and G. Shanmugam [11], where they reported the calculated and experimental frequencies of 6-aminouracil. The 36 fundamental modes of 6AU may be classified according to the molecular point group C_s into 25 A′ symmetry species (in-plane) and 11 A″ species (out-of-plane). Since all the vibrations are IR and Raman active, the absence of Raman spectra present no serious difficulty.

6-aminouracil has different sites, therefore, has different binding modes. It can coordinate through one of the pyrimidine ring nitrogen, the C=O and / or-NH_2 groups. Therefore, vibrational wavenumbers of 6AU in M-Ni-6AU complexes studied are carefully investigated.

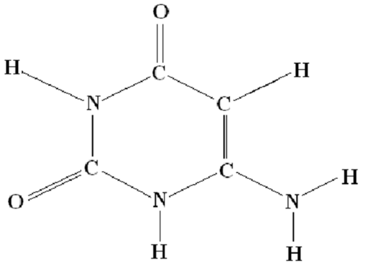

Figure 1. Structural formula of 6-aminouracil

If the coordination occurs through the amino nitrogen atom, it is expected that a great reduction would take place in the NH_2 stretching NH_2 bending and C-NH_2 stretching wavenumbers (e.g., [12]), and when coordination occurs through the oxgen of carbonly group, negative shift at υ(C=O) mode of coordinated molecule with respect to the free ligand is expected [13]. On the other hand when the aromatic ring nitrogen involves in complex formation, certain ring modes are affected [13]. In order to determine the coordination site of 6-aminouracil in $M(6AU)_2Ni(CN)_4$ (M= Mn, Co, Ni and Cd) complexes, the wavenumbers of 6-aminouracil in complexes are compared with those of free 6-aminouracil. Some selected fundamental modes of complexes are reported in Table 1. The spectroscopic results indicated that tha amino group hydrogen bonding interaction in comparison with those of other M-Ni-6AU complexes.

We observed four broad bands corresponding to stretching vibrations $\nu(NH_2)$ and their wave numbers are found to be higher in value than those of free 6-aminouracil. A positive shift of these absorptions is usually regarded as signifying that the ligand is not NH_2-bonded. This band indicates the presence of 6-aminouracil in $M(6AU)_2Ni(CN)_4$ (M= Mn, Co, Ni and Cd) complexes in its amine form and the rather broad character of the NH_2 vibration bands is suggestive of H bond participation [14]. In addition, NH_2 scissoring mode of 6-aminouracil is observed at 1659 cm^{-1} for 6-aminouracil and around 1657 cm^{-1} for complexes. These results suggested that the NH_2 groups of 6-aminouracil are not involved in the coordination with the metal ions and are in good agreement with those reported in the literature [3,15].

The υ(C=O) mode is observed at 1735 cm^{-1} for solid 6AU and around 1741 cm^{-1} in the FT-IR spectra of complexes, indicating that the ligand not coordinate to the metal ions through (C=O) group. The bands at 1596, 1388, 1289, 1048 and 979 cm^{-1} in the FT-IR spectra (at 1606, 1404, 1304, 1074 and 990 cm^{-1} in the FT-Raman spectra) with ring contribution exhibit intensity changes and shift to higher wavenumbers in complexes. All of these data suggest binding between the metal (II) and the ring N atom of the 6-aminouracil. Analogous shifts on coordination were observed in creatinine [16], pyrazinamide [17],

Table 1. The vibrational vawenumbers (cm^{-1}) of 6-aminouracil in the M-Ni-6AU complexes.

Sym.	6-aminouracil				Mn-6AU-Ni		Co-6AU-Ni		Ni-6AU-Ni		Cd-6AU-Ni		PED(%)[a]
	υ_{exp}			υ_{cal}[a]									
	IR[a]	IR[b]	Raman[b]		IR	Raman	IR	Raman	IR	Raman	IR	Raman	
A′	3400	3415s		3363	3416m		3415m		3419m		3417m		υNH (99)
A′	3340	3392m		3310	3392m,sh		3390m		3288m,sh		3392m,sh		$\upsilon_{as}NH_2$ (100)
A′	3240			3257									υNH (99)
A′	3170	3173vs		3145	3173s		3182s		3196s		3178m		$\upsilon_{s}NH_2$ (99)
A′	2905	2905w		2902	2908w		2908w		2908w		2908w		υCH (99)
A′	1865			1860									υC=O(60), υC=C(24), υCC(14)
A′	1735	1747m,sh		1744	1739m,sh		1741m,sh		1739m,sh		1743w,sh		υC=O(52), υC=C(20), υCN(12)
A′	1721	1716m,sh		1721	1702m		1707m		1699m		1711m		υCN(48), υCN(21), υC=C(20)
A′	1649	1659vs		1650	1658s		1657s	1631m	1658s		1659m,sh		δNH_2 (56), υCN(14)
		1624vs	1604m		1623vs		1624vs		1626vs		1627vs		
A′	1590	1596vs		1570	1595vs	1606m	1597vs		1592s,sh	1606m	1599s,sh	1606w	υCN(26), βNH (24), υCN (16)
A′	1525	1523s	1552m	1512	1527m	1526w	1526m	1524vw	1526m,sh	1526w	1530m	1526w	βNH (48), υCN (17), βCH (14)
A′	1460	1456s		1475	1456m		1456m		1468m		1455m		βCH (52)
A′	1395	1388s	1402vs	1397	1391s	1404w	1389s	1413w	1379s	1402vw	1391s	1402vw	υCN (23), βCH (22), δNCN (17)
A′	1310	1289m	1324vs	1308	1290m	1304vw	1289m		1292m	1294vw	1290m	1294vw	υCN (20), δCCN (18), υCN (17)
A′	1235	1234m		1256	1237m	1253vw	1237m	1246vw	1234m	1251w	1236m	11251	ρNH_2 (70)
A′	1120	1124w		1115	1124w	1169vw	1124w		1122w	1182vw	1125w		υCN (20), υC=C (16), δCCC (13)
		1104w			1105vw		1104w			1083w	1104w		
A′	1065	1048		1092	1047w		1049w	1074vw	1049w		1049w	1083w	υCN (20), βCH (20), υC=C (14), δCNC (12)
A′	1020	1024		1017	1025vw		1024vw		1019vw		1025vw		υCN (21), υCC (20), ρNH_2 (15), δCCN (11)
A′	990	979w		1001	982w	990w	980w	995m	980w	985w	982w	985w	υCN (21), υCC (20), δNCC (17), δCNC (15)
A″	885	878m		878	878w	946w	875w		859m		878w		πNH (57), πC=C (12)
A″	815	803m,sh		827	807m	816vw	805m	828vw	817w		805m		πNH (46), τCN (26)
A″	775	781vs		782	783m		782m	789vw	784m	772vw	783m	772vw	τCN (27), τCC (21), πCH (18)
A″	745	729w		732	734w		731w		733w		731w		πCN (42), πNH (12), τCN (10)
A′	675	683m		651	683w	692vs	681w	693vs	682w	692vs	683w	692vs	δNCC (21), δCCN (17), υC=O (11)
A′	630	644m		625	647w		647w	632vw	646w		649w		βC=O (37), βC=O (24)
A″	560	625m		564	628w	553m	627w	565w	624w		628w		ωNH_2 (51), τCN(10)
A′	525	546s		518	545m		545m		554m	554m	545m	554w	δNCN (30), δCCN (21), δCNC (19), δCCC (16)
A″	500	515m		508	517w,sh	491vw	515w,sh		521w	531w	520w	531vw	τNH_2 (39), τCN(14), πNH (11)
A′	508			505									βC=O (48), βC=O (29)
A′	495	441w		485	437s		443s		445s		430s		δNCC (31), δCNC (23), δCCN (13), δNCN (11)
A″	430	416w		435				419vw					πC=O (63), πC=C (12)
A″	385	386w		385	386w	392vw	388w	393vw	390w	419vw		397vw	τCN (26), τCC (24),), τC=O (16), πCH (11)
A′	385	372w		370	373w		372w		371w	378vw	373w		βCN (58), βC=O (18)
A″	285	285w		279	285w		278w	296vw	285w	277vw	286w		τC=C (28),), τCC (17), τCN (16)
A″	260	267w		243	261w		262vw		267vs		267vw	241vw	τCN (27),), τC=C (21), τCN (19), τNH_2 (11)

[a] Taken from Ref. [11]. [b] This study,

Abb: ν, stretching; ω, wagging; δ, bending; π, out-of-plane bending; ρ, rocking; τ, torsion; vs: very strong, s: strong, m: medium, w: weak, vw: very weak, sh: shoulder.

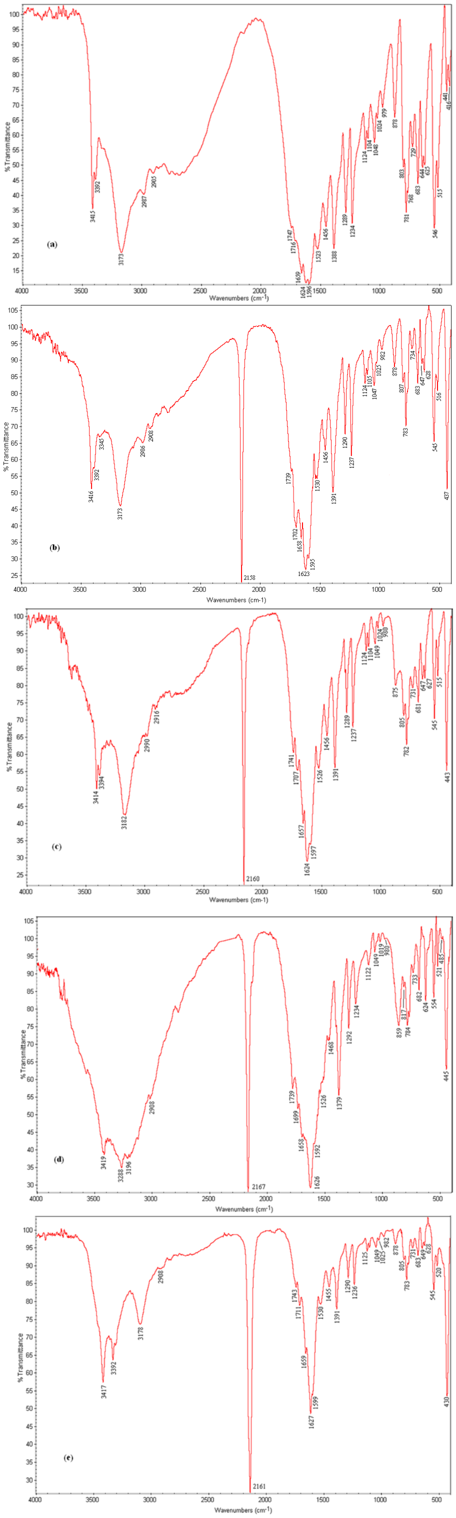

Figure 2. The FT-IR spectra of Hofmann-6AU compounds in KBr: (a) 6AU (ligand), (b) Mn-6AU-Ni, (c) Co-6AU-Ni, (d) Ni-6AU-Ni and (e) Cd-6AU-Ni.

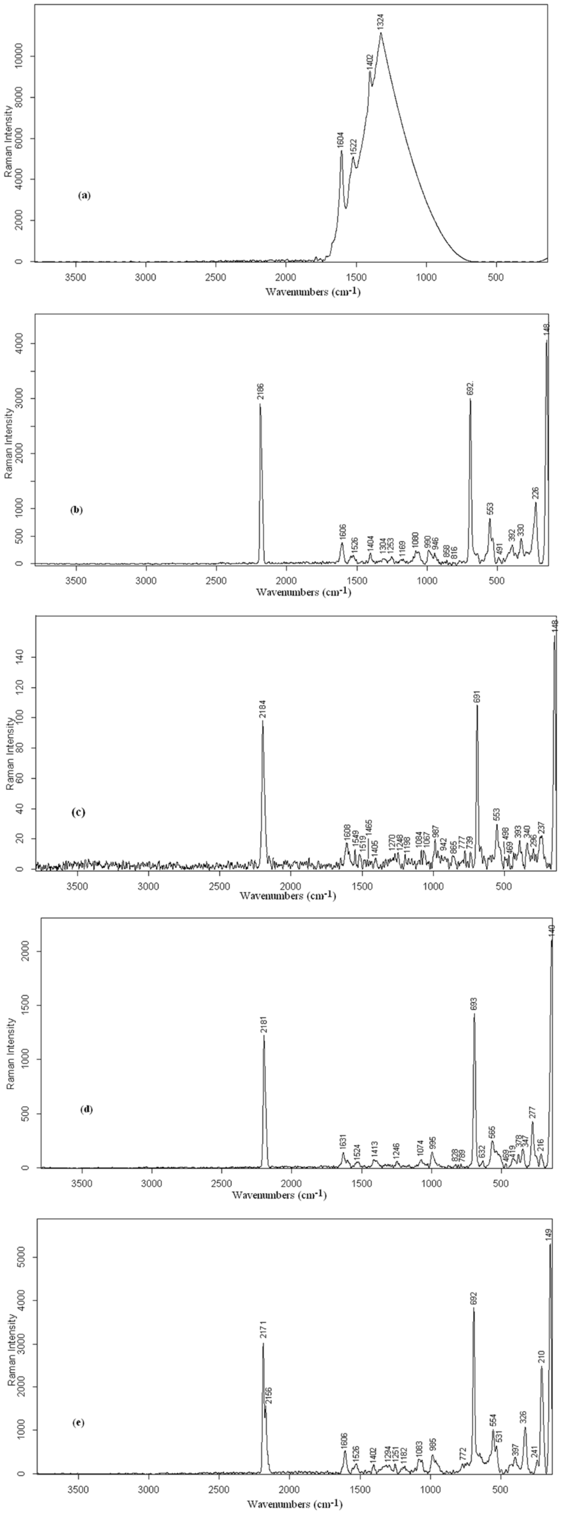

Figure 3. The FT-Raman spectra of Hofmann-6AU compounds in KBr: (a) 6AU (ligand), (b) Mn-6AU-Ni, (c) Co-6AU-Ni, (d) Ni-6AU-Ni and (e) Cd-6AU-Ni.

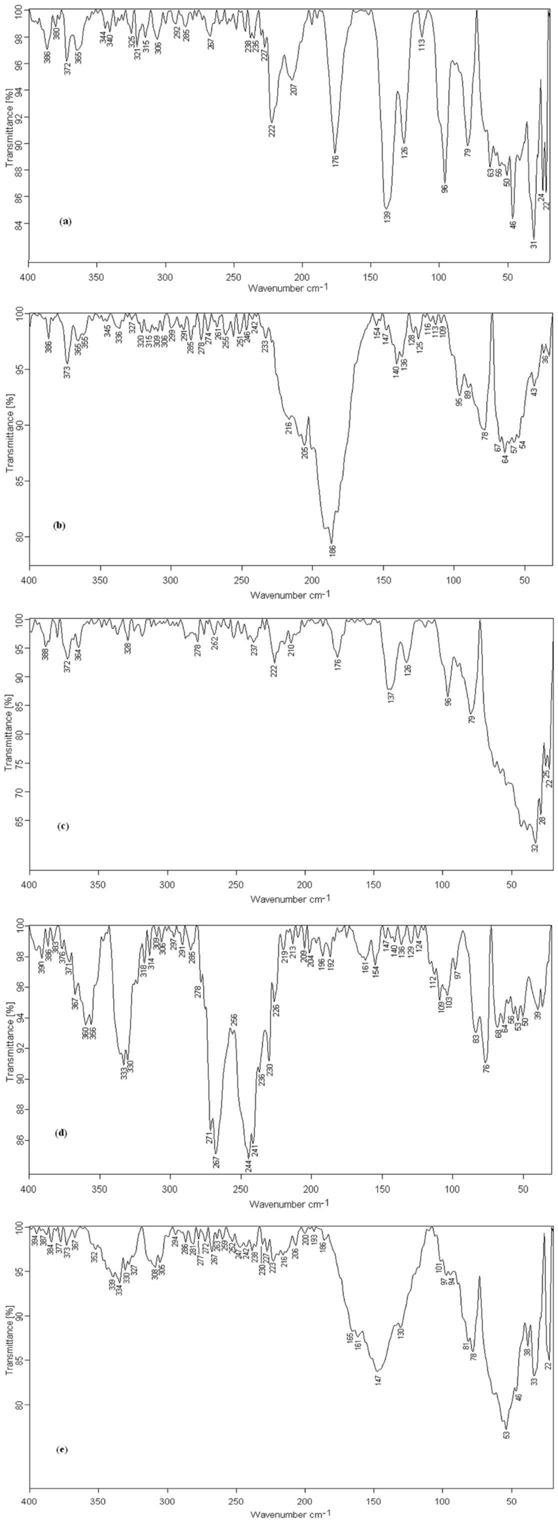

Figure 4. The far-IR spectra of Hofmann–6AU compounds (a) 6AU (ligand), (b) Mn-6AU-Ni, (c) Co-6AU-Ni, (d) Ni-6AU-Ni and (e) Cd-6AU-Ni.

2-aminopyrimidine [18], 4-aminopyrimidine [19,20] complexes and are explained as the coupling of the internal modes of the aromatic molecule with the M-N vibrations [16-20].

$Ni(CN)_4$ group vibrations

The vibrational wavenumbers of the $Ni(CN)_4$ group for the complexes studied are given in Table 2 together with those Hofmann type clathrates [21-23] and $K_2Ni(CN)_4$ [13, 22] for comparison. As seen in Table 2, the vibrational wavenumbers of $Ni(CN)_4$ groups are found to be much higher than those of $Ni(CN)_4$ in $K_2Ni(CN)_4$ salt. The higher wavenumbers in M-Ni-6AU, compared to the free $Ni(CN)_4$, are caused by coordination of tetracyanonickelate ion, through the nitrogen atoms to metal (M). Such upward wavenumber shift have been observed for Hofmannn type clathrates [23] and pyrazinamide complexes $M(PZA)_2Ni(CN)_4$ (M= Mn, Ni, Zn or Cd; PZA= pyrazinamide) [17], in which both ends of the CN group are coordinated, and explained as the mechanical coupling of the internal modes of $Ni(CN)_4$ with the M-NC vibrations [17]. The presence of just two υ(CN) Raman active bands and one IR active bands confirms that nickel atoms have a square planer environment. Far-IR and Raman bands below 300 cm^{-1} region is assigned based on the comparison with the Raman spectra of Hofmann type clathrates and tetracyanonickelate complexes [21,22] where available. Far-IR and Raman spectral investigation of M-Ni-6AU complexes enable us the determine coordination mode of 6AU. As seen in Table 2, the vibrational modes of $\upsilon(M\text{-}L)_{6AU}$ and $\delta(NMN)_{6AU}$ are found to close where expected for υ(M-L) and $\delta(NMN)_L$ (L= NH_3) for Hofmann type clathrates, which confirms coordination of 6AU through ring nitrogen.

CONCLUSIONS

FT-IR and far-IR and FT-Raman spectroscopy provides a powerful means to assess the coordination mode on 6-aminouracil. From these spectroscopic studies it is concluded that 6-aminouracil complexes have similar structures constructed by linkage between the square planer $Ni(CN)_4^{2-}$ and the octahedral M(II) through

Table 2. Vibrational wavenumbers of tetracyanonickelate group and metal-6AU vibrations.

Assignment	$K_2Ni(CN)_4$ [a]	$M(NH_3)_2Ni(CN)_4.2Bz$ [b]		M-Ni-PZA [c]		M-Ni-6AU			
		M= Mn	M= Cd	Mn	Cd	Mn	Co	Ni	Cd
υ(CN) E_u	2124[d]	2152[e]	2156[e]	2149vs	2150vs	2158s	2160vs	2164vs	2161vs
					548vw				
υ(Ni-CN) E_u	538	544	554	547w		545m	545m	554m	545m
π(NiCN), A_u	444	448	446	460vw	456sh				
δ(NiCN) E_u	419	428	425	434vs	429vs	437s	443s	445s	430s
υ(M-L)$_L$		204	179			205s	210w	244vs	242w
δ(NiCN)E_g		204	148			186vs	137s	154w	147s
υ(CN) A_g			2175	2171vs	2164vs	2186 vs	2184vs	2181vs	2171vs
υ(CN) B_g			2164	2158s	2177s				2156sh
υ(Ni-CN)A_g	405	462-477	445-450	439w	441w		469vw	469vw	-
δ(NiCN)E_g	302	312-322	305-307	316m	312m	330vw	340vw	347vw	326w
υ(M-L)$_L$		200-206	190-192	197s	182s	226w	237vw	216vw	210s
δ(NMN)$_L$		176[d]	160[d]			148vs	148vs	140vs	149vs

[a] Taken from Ref. [22]. [b] Hofmann type clathrates $M(NH_3)_2Ni(CN)_4.2G$ where G is either zero (host lattice) or the guest molecule (benzene or thiophene) taken from Refs.[21,22]. [c,d,e] Taken from Refs. [17,23,13], respectively.vs: very strong, s: strong, m: medium, w: weak, vw: very weak and sh: shoulder.

cyano bridges, and the six coordination of M(II) is satisfied by four N terminals of the cyano groups and pyrimidine ring nitrogen of two 6-aminouracil molecules. Comparison of the vibrational wavenumbers of tetracyananickelate sheet of isostructural compounds lead us to express a tentative assignment for metal ligand vibrational modes.

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