

Vibrational Spectroscopic Study of Creatinine Hofmann-T_d-Type Complexes

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(Received: 17 March 2012;

Accepted: 17 May 2013)

AJC-13507

New Hofmann-T_d-type complexes in the form of M(creat)₂M'(CN)₄ (M = Mn and Cd; M' = Zn, Cd and Hg; creat = creatinine = 2-amino-1-methyl-5H-imidazol-4-one) were prepared in powder form and their FT-IR (4000-400 cm⁻¹), far-IR (400-50 cm⁻¹), FT-Raman (4000-50 cm⁻¹) spectra and elemental analyses are reported. Creatinine molecules are found to involve coordination through one of the imidazole ring nitrogen atoms. The spectral features of the compounds studied are found to be each other indicating that they have analogous structures.

Key Words: Creatinine, FT-IR, Far-IR, FT-Raman spectra, Tetracyanometallate.

INTRODUCTION

Creatinine (C₄H₇N₃O) is produced from creatine, a molecule of major importance for energy production in muscles. Creatinine is transported through the bloodstream to the kidneys. The kidneys filter out most of the creatinine and dispose of it in the urine¹. An abnormal level of creatinine in biological fluids is an indicator of various disease states². Creatinine has two tautomeric forms, the imine (I) and the amine (II) (Fig. 1). *Ab initio* calculations have shown that in the gas phase, the imine form is preferred but the solid state, the amine form is observed and is predicted theoretically³⁻⁵. The fundamental vibrations for the creatinine molecule have assigned using the generalized valence force field approximation⁶. More recently, the study of complexes of this bioligand are attracting considerable interest. The X-ray crystal structure and the coordination chemistry with transition metal ions of creatinine have been widely studied⁶⁻¹¹. Although the infrared spectra of Pt(creat)₂(NO₂)₂, Pt(creat)₂(ClO₄)₂ have been completely analyzed⁶, no complete spectral characterizations have been done on the other complexes. Muradlihan *et al.*¹² investigated M(creat)₂X₂ (M = Zn, Cd or Hg, X = Cl, Br or I) complexes using IR, NMR and TG. They only reported M-N and M-Cl frequencies for these complexes. In our previous study we reported the spectra of metal halogen complexes of creatinine M(creat)₂X₂ (M = Zn, Cd or Hg, X = Cl or Br) and it was concluded that coordination through imidazol ring nitrogen¹³.

We have also prepared five new complexes of the form M(creat)₂M'(CN)₄ (M = Mn or Cd; M' = Zn, Cd or Hg). These complexes are analogous to the Hofmann-T_d-type complexes¹⁴⁻¹⁸

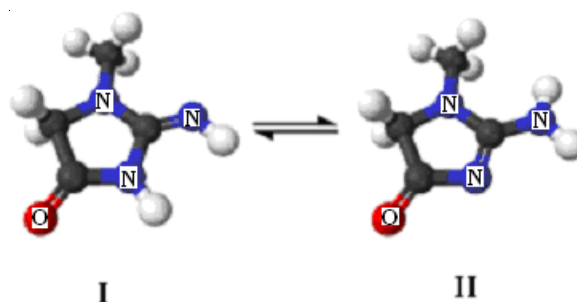


Fig. 1. Imine (I) and amine (II) tautomeric forms of creatinine

and clathrates¹⁹⁻²¹. In these structures, the host framework is formed from the infinite -Cd-L₂-Cd- chains extending along the a- and b-axes alternately and tetrahedral M'(CN)₄ ions arranged between the consecutive crossing -Cd-L₂-Cd- chains with the connections of the N-ends bound to the Cd atoms in the chains¹⁴⁻²¹. The compounds possessing this type of the host framework reported to date were confined to the Mn or Cd metal atom in an octahedral environment and to the Cd or Hg metal atom in a tetrahedral group¹⁶⁻²¹.

EXPERIMENTAL

Preparation of complexes: The complexes Mn-creat-M (M = Zn, Cd or Hg) were synthesized by adding 2 mmol of creatinine and 1 mmol of K₂M(CN)₄ solution in water. The precipitate formed was filtered, washed with water, ethanol and ether successively and kept in a dessicator. The Cd-creat-Cd and Cd-creat-Hg complexes were prepared using a method analogous to that given in the literature¹⁶⁻²¹.

The freshly prepared compounds were also analyzed for C, H and N by a LECO CHNS-932 analyzer with the following results (found %/calcd. %). $\text{Cd}(\text{C}_4\text{H}_7\text{N}_3\text{O})_2\text{Cd}(\text{CN})_4$: C = 42.73/42.94, H = 4.35/4.46, N = 14.11/14.31; $\text{Cd}(\text{C}_4\text{H}_7\text{N}_3\text{O})_2\text{Hg}(\text{CN})_4$: C = 42.73/42.94, H = 4.35/4.46, N = 14.11/14.31; $\text{Mn}(\text{C}_4\text{H}_7\text{N}_3\text{O})_2\text{Zn}(\text{CN})_4$: C = 42.73/42.94, H = 4.35/4.46, N = 14.11/14.31; $\text{Mn}(\text{C}_4\text{H}_7\text{N}_3\text{O})_2\text{Cd}(\text{CN})_4$: C = 42.73/42.94, H = 4.35/4.46, N = 14.11/14.31; $\text{Mn}(\text{C}_4\text{H}_7\text{N}_3\text{O})_2\text{Hg}(\text{CN})_4$: C = 35.78/37.34, H = 3.47/3.87, N = 12.29/12.44. The analytical results were agreement with the proposed formula.

Physical measurements: The FT-IR spectra recorded between 4000-400 cm^{-1} on Perkin Elmer 1330 and Mattson 1000 FT-IR spectrometers, which were calibrated using indene and polystyrene film. The samples were prepared as mulls in nujol and KBr pellets. Far-infrared (400-50 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 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 4000 and 50 cm^{-1} .

RESULTS AND DISCUSSION

The FT-IR, FT-Raman and far-IR spectra of $\text{Cd}(\text{creat})_2\text{Cd}(\text{CN})_4$ and $\text{Mn}(\text{creat})_2\text{Zn}(\text{CN})_4$ compounds are given in Figs. 2-4, respectively. Because of the lack of structural data on the compounds studied, the assignment was made by treating the ligand molecules and the $\text{M}(\text{CN})_4$ ($\text{M} = \text{Zn}, \text{Cd}$ or Hg) ions as isolated units. The wavenumbers and assignments made are given for ligand molecules and $\text{M}(\text{CN})_4$ ions in Tables 1 and 2, respectively, together with some relevant spectral data for comparison.

Creatinine (creat) vibrations: Creatinine (2-amino-1-methyl-5*H*-imidazol-4-one) has 15 atoms and 39 normal modes. It has methyl, methylene, amino and C=O groups. The methyl group as a united atom in the creatinine molecule considered by Trendafilova *et al.*⁶ and 30 vibrational modes discussed. Costa *et al.*⁷ reported some selected IR bands of creatinine. The detailed vibrational assignments of fundamental modes of creatinine along with the calculated at B3LYP levels using the triple split valence basis set along with diffuse and polarization functions, 6-311++G (d,p) and normal mode

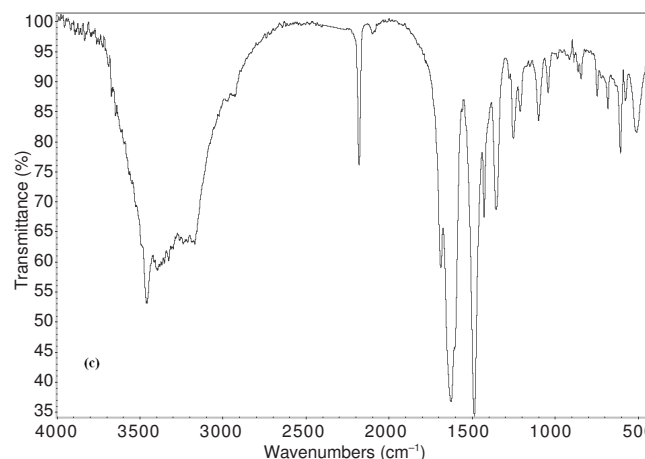
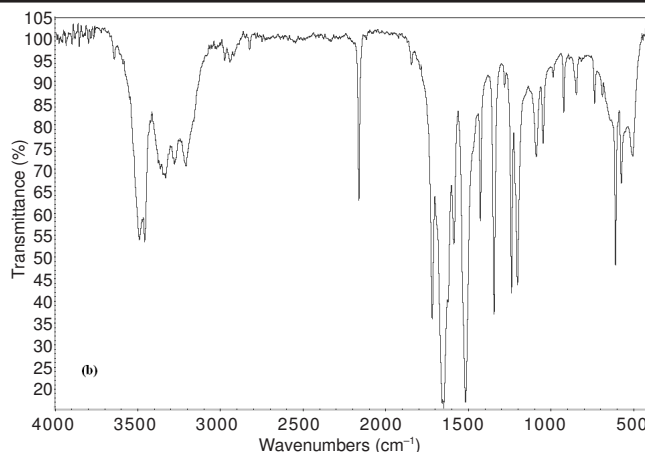
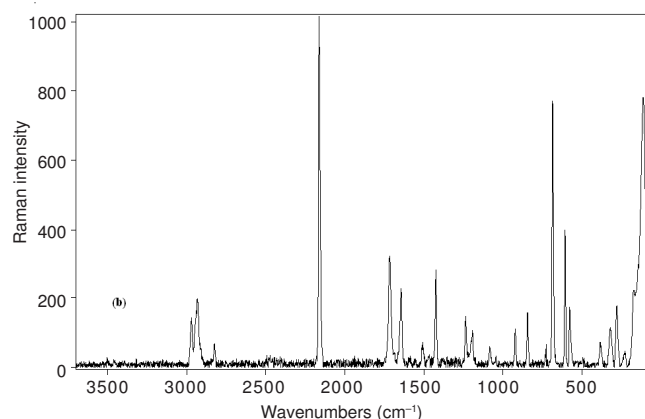
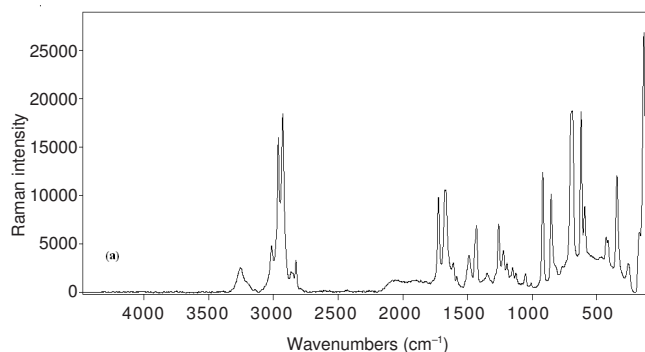
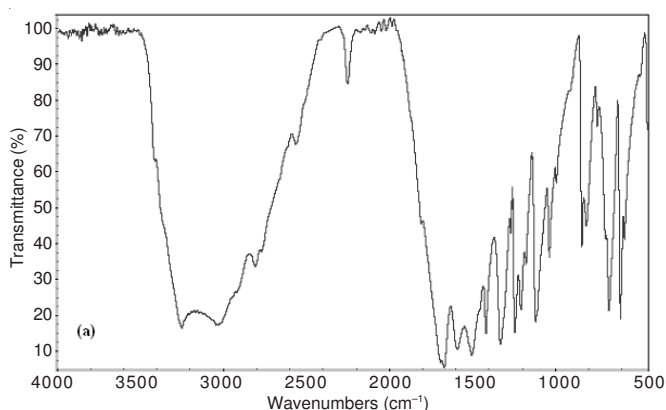


Fig. 2. FT-IR spectra of the creatinine (solid) (a), Cd-creat-Cd (b) and Mn-creat-Zn (c) complexes



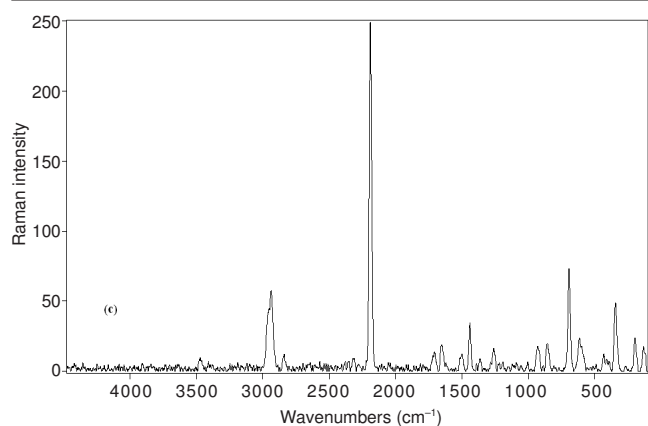


Fig. 3. FT-Raman spectra of the creatinine (solid) (a), Cd-creat-Cd (b) and Mn-creat-Zn (c) complexes

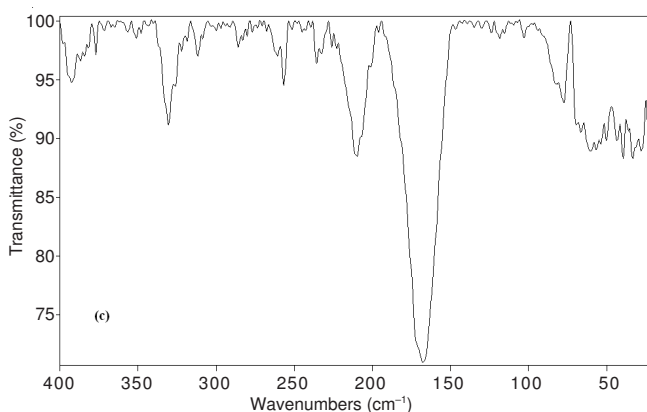
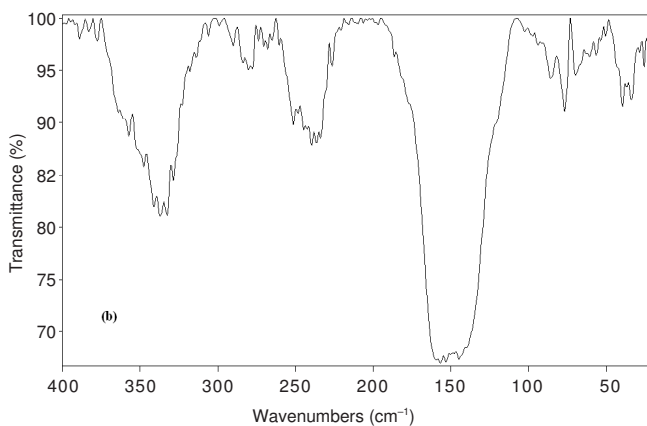
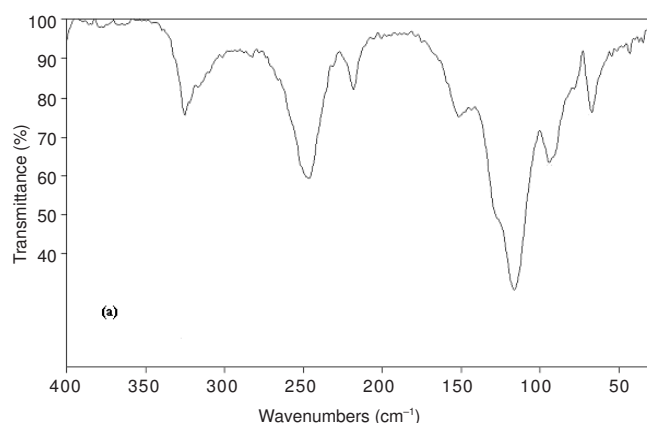


Fig. 4. Far-IR spectra of the creatinine (solid) (a), Cd-creat-Cd (b) and Mn-creat-Zn (c) complexes

descriptions (characterized by TED) based on SQM force field calculations are reported of Bayrak *et al.*¹³ The FT-IR, FT-Raman and far-IR spectra of creatinine is illustrated in Figs. 2a, 3a and 4a.

Creatinine can coordinate through the ring nitrogen, the C=O and/or -NH₂ groups. In metal complexes, creatinine typically coordinates to the metal *via* the ring nitrogen^{6-8,11,22}. The N-H stretching vibration of NH₂ group are much affected and found to shift to lower wavenumbers on coordination^{23,24}. The shifts to lower wavenumbers of the $\nu(\text{C}=\text{O})$ in the complexes can be attributed to the effect of coordination through the oxygen atoms of these groups to the metal²⁵. When the aromatic ring nitrogen coordinates to metal, the ring stretching wavenumbers shift to higher wavenumbers²⁵. In order to determine the coordination site of creatinine in $\text{M}(\text{creat})_2\text{M}'(\text{CN})_4$ ($\text{M} = \text{Mn}$ or Cd ; $\text{M}' = \text{Zn}$, Cd or Hg) complexes, the wavenumbers of creatinine in complexes are compared with those of free creatinine. Some selected fundamental modes of complexes are reported in Table-1.

We observed four broad bands corresponding to stretching vibrations $\nu(\text{NH}_2)$ and their wavenumbers are found to be higher in value than those of free creatinine. A positive shift of these absorptions is usually regarded as signifying that the ligand is not NH₂-bonded. This band indicates the presence of creatinine in the metal halogen complexes in its amine form and the rather broad character of the NH₂ vibration bands is suggestive of H bond participation²⁶. In addition, NH₂ scissoring mode of creatinine is observed at 1670 cm⁻¹ for creatinine and around 1650 cm⁻¹ in the FT-IR spectra (1645 and 1626 cm⁻¹ FT-Raman, respectively) for complexes. These results suggested that the NH₂ groups of creatinine are not involved in the coordination with the metal ions and are in good agreement with those reported in the literature^{6,7}.

The $\nu(\text{C}=\text{O})$ mode is observed at 1692 cm⁻¹ for free creatinine and around 1720 cm⁻¹ in the infrared spectra and at 1716 cm⁻¹ in the FT-Raman spectra of complexes, indicating that the ligand does not coordinate to the metal ions through (C=O) group. These bands in the FT-IR spectra at 1503, 1208, 1177, 841, 813, 677 and 608 cm⁻¹ with ring contribution exhibit intensity changes and shift to higher (1517, 1210, 1192, 923, 847, 688 and 610 cm⁻¹ FT-IR, respectively) wavenumbers in complexes. In our previous study we observed the ring stretching mode in the Raman spectra at 1151 cm⁻¹ and the ring deformation mode 852 cm⁻¹ in free creat molecules. On the other hand, these modes at 1151 and 852 cm⁻¹ are observed at 1192 and 923 cm⁻¹ in FT-Raman. The above mentioned complexes, the ring bending mode complexes at 687 (very strong band) and 610 cm⁻¹ (medium band) observed in the FT-Raman spectra (Table-1). All of these data suggest binding between the metal(II) and the ring N atom of the creatinine. Similar shifts have been observed in metal-coordinated creat compounds⁶⁻¹³.

It is clear from Table-1 that most of the vibrational modes of coordinated creatinine in the complexes have increased in wavenumbers when compared with uncoordinated creatinine. These shifts may be explained as the coupling of M-N(creat) vibrations. Similar observations have been previously for creatinine metal halogen complexes^{6,13} pyridine nitrogen complexes^{13,15,16} and imidazole nitrogen clathrate¹⁹.

TABLE-1
 VIBRATIONAL WAVENUMBERS (cm⁻¹) OF CREATININE IN METAL COORDINATION COMPLEXES

| Modes | Creatinine ^a | | | Cd-creat-Cd | | Cd-creat-Hg | | Mn-creat-Zn | | Mn-creat-Cd | | Mn-creat-Hg | | TED % |
|-------|-------------------------|-------|--------------------|-------------|--------|-------------|--------|-------------|--------|-------------|--------|-------------|--------|---|
| | v _{exp.} | | v _{calc.} | IR | Ra | IR | Ra | IR | Ra | IR | Ra | IR | Ra | |
| | IR | Ra | IR | | | | | | | | | | | |
| 39 | 3252vs | 3256w | 3565 | 3451vs | | 3491vs | | 3463vs | 3469vw | 3460vs | 3469vw | 3461vs | 3469vw | 100 v _a (NH ₂) |
| 38 | 3030vs | 3015m | 3454 | 3186vs | | | | | | 3200vs | 3189vw | 3205vs | 3189vw | 100 v _s (NH ₂) |
| 37 | 2980vw | 2963s | 2990 | | | | | | | | | | | 100 v _a (CH ₃) |
| 36 | | | 2965 | 2945vw | 2970 w | | 2972 w | | | | | 2969vw | | 100 v _a (CH ₂) |
| 35 | 2922w | 2928s | 2959 | 2907vw | 2933w | 2944vw | 2931w | 2907vw | 2938w | 2906vw | 2938w | 2907vw | 2938w | 100 v(CH ₃) |
| 34 | | 2863w | 2909 | | | | | | | | | | | 100 v _s (CH ₂) |
| 33 | 2809w | 2826w | 2875 | 2827vw | 2824vw | 2824vw | 2824vw | 2838vw | 2839vw | 2836vw | 2839vw | 2824vw | 2839vw | 100 v _s (CH ₃) |
| 32 | 1692sh | 1724s | 1730 | 1721vs | 1716m | 1718s | 1717m | 1689s | 1706w | 1685s | 1706w | 1718s | 1706w | 65 v(C=O)+11 v(CN) _{ring} |
| 31 | 1670vs | 1673s | 1664 | 1649vs | 1645w | 1655vs | 1643w | 1626vs | 1654w | 1630vs | 1654w | 1635vs | 1654w | 51 δ(NH ₂)+27 δ(HNC)+11 v(C-NH ₂) |
| 30 | 1590s | 1609w | 1581 | 1588s | | 1589vw | | 1586s | | 1587s | | 1587vw | | 37 v(CN) _{ring} +20 v(CNH ₂)+13 v(C=O)+10 δ(HNC) |
| 29 | 1503s | 1489w | 1518 | 1517vs | 1507vw | 1518vs | 1506vw | 1508vs | 1505w | 1509vs | 1506w | 1504s | 1503w | 50 v(CN) _{ring} +15 v(C-NH ₂)+10 δ(C-NH ₂) |
| 28 | 1457sh | | 1474 | 1427w | 1425m | 1427m | 1423m | 1433w | 1440w | 1435w | 1443w | 1434w | 1441w | 64 δ(CH ₂)+12 δ _{ring} +10 τ(H ₂ C-NC-CH ₃) |
| 27 | | | 1462 | | | | | | | | | | | 55 δ(CH ₃)+32 τ(CN-CH ₃) |
| 26 | 1418s | 1430m | 1443 | 1345vw | | 1345m | | 1378vw | 1364w | 1377vw | 1360w | 1374vw | 1366w | 53 δ(CH ₃)+30 τ(CN-CH ₃) |
| 25 | 1331s | 1349w | 1391 | | | | | 1322s | | 1324s | | 1321s | | 50 δ(CH ₃)+46 δ(N-CH ₃) |
| 24 | 1269w | 1259m | 1290 | 1281vw | | | | 1279vw | | 1261w | | 1259w | | 35 δ(CH ₂)+32 τ(CN-CH ₂)+17 v(N-CH ₃) |
| 23 | 1243s | 1221w | 1254 | 1240s | 1237w | 1239m | 1236w | | | | | | | 38 v _{ring} +30 v(N-CH ₃)+18 δ(N-CH ₃) |
| 22 | 1208m | 1194w | 1200 | 1210m | | 1210m | | 1219m | | 1217m | | 1221m | | 45 v _{ring} +28 δ(CH ₂)+13 δ(C=O) |
| 21 | 1177w | 1151w | 1182 | 1192w | 1193vw | 1159w | 1191vw | 1190m | 1192w | 1191m | 1193w | 1192m | 1189w | 33 v _{ring} +17 δ(C-NH ₂)+15 δ(N-CH ₃)+14 v(NCH ₃) |
| 20 | 1118s | | 1143 | 1091w | 1084vw | | 1084vw | 1082m | | 1081m | | 1083m | | 46 δ(CH ₂)+30 τ(NC-CH ₂) |
| 19 | 1036m | 1051w | 1096 | 1048w | | 1048w | | 1044w | 1004w | 1041w | 1006w | 1042w | 1005w | 72 δ(N-CH ₃)+15 τ(CN-CH ₃) |
| 18 | | | 1086 | | | | | | | | | | | 60 δ(C-NH ₂)+15 v _{ring} +10 δ(C=O) |
| 17 | | | 1015 | | | | | | | | | | | 44 δ(N-CH ₃)+35 v(CN) _{ring} |
| 16 | 992w | 917s | 979 | 988vw | | 988vw | | 988vw | 930w | 982vw | 932w | 984vw | 933w | 26 τ(C=O)+21 δ(C-CH ₂)+16 τring+13 τ(ring-CH ₂) |
| 15 | 841s | 852s | 849 | 923vw | 923w | 923vw | 920w | 907vw | 856w | 904vw | 855w | 908vw | 851w | 63 v _{ring} +16 δ _{ring} +10 δ(C-NH ₂) |
| 14 | 813m | | 801 | 847w | 845w | 856w | 848w | 834w | 807w | 838w | 805w | 835w | 806w | 40 v(CN) _{ring} +17 v(N-CH ₃)+14 δring+10 v(C-NH ₂) |
| 13 | 747mw | 689s | 733 | 736w | 727vw | 736vw | 725vw | 747vw | 794w | 743vw | 791w | 745vw | 797w | 50 ω(NH ₂)+30 τ _{ring} |
| 12 | 677vs | 662s | 661 | 688w | 687vs | 689w | 688vs | 681w | 694w | 680w | 692w | 683w | 695w | 43 δ _{ring} +15 v(C-NH ₂)+11 v _{ring} +10 v(C=O) |
| 11 | 608vs | 593m | 606 | 610m | 608s | 610m | 609s | 665m | 616w | 663m | 617w | 666m | 612w | 32δ _{ring} +18 v(N-CH ₃)+10 v _{ring} +10 δ(C=O) |
| 10 | 583mw | | 577 | 574m | 579m | 579w | 577m | 609w | | 607w | | 610w | | 30 δ(C=O)+28 τ(ring-CH ₂)+14 τ(C=O)+12 δ(NC-NH ₂) |
| 9 | 455vw | | 531 | 505m | | 507m | | 509w | 489m | 507w | 491m | 511w | 485m | 20 δ(NC-NH ₂)+17 τ(ring-NH ₂)+13 τ(ring-CH ₂)+10 τ(C=O) |
| 8 | 406m | 427w | | | | 426s | | 406vw | 411w | 404vw | 413w | 407vw | 414w | 71 τ(ring-NH ₂) |
| 7 | 325m | 344s | 350 | 328m | 322w | 387w | 321w | 330m | 343w | 332m | 345w | 333m | 345w | 87 τ(ring-NH ₂) |
| 6 | 246s | 257w | 314 | 318m | 281w | 237w | 285w | 318w | 269w | 317w | 271w | 319w | 272w | 48 δ(NC-NH ₂)+20 δ(C=O)+13v _{ring} |
| 5 | 218m | | 291 | 215w | 230w | 204m | 234w | 223 | 196w | 223 | 196w | 223 | 196w | 58 δ(CN-CH ₃)+15 τ(ring-NH ₂) |
| 4 | 151mw | 135vs | 160 | 153vs | 173w | 157m | 177w | 167s | 134w | 166s | 131w | 169s | 135w | 27 τ(ring-CH ₃)+24 τ(ring-CH ₂)+15 τ(ring-NH ₂) |
| 3 | 116vs | | 123 | | 114s | 134m | 116s | 116w | | 114w | | 115w | | 37 τ(C=O)+22 τ _{ring} +13 τ(ring-NH ₂) |
| 2 | 94mw | | 101 | 85w | | 79w | | 103w | | 108w | | 106w | | 90 τ(ring-CH ₃) |
| 1 | 67mw | | 85 | 77w | 73w | 59w | 76w | 77w | | 78w | | 79w | | 46 τ(ring-CH ₃)+28 τ(H ₃ C-ring-NH ₂) |

^aTaken from Ref.-13. (TED: The total energy distributions). vs: very strong, s: strong, m: medium, w: weak, vw: very weak, sh: shoulder.

TABLE-2
VIBRATIONAL WAVENUMBERS (cm⁻¹) OF CYANIDE GROUP FOR THE M-creat-M' COMPLEXES

| Assignment ^a | K ₂ Zn(CN) ₄ ^a | K ₂ Cd(CN) ₄ ^a | K ₂ Hg(CN) ₄ ^a | Cd-creat-Cd | Cd-creat-Hg | Mn-creat-Zn | Mn-creat-Cd | Mn-creat-Hg |
|---|---|---|---|-------------|-------------|-------------|-------------|-------------|
| v ₁ (CN) A ₁ | (2157) | (2145) | (2146) | (2163vs) | (2164vs) | (2180vs) | (2185vs) | (2187vs) |
| v ₅ (CN) F ₁ | 2152 | 2145 | 2146 | 2163vs | 2164vs | 2172vs | 2170vs | 2170vs |
| v ₂ (MC) A ₁ | (347) | (327) | (335) | (359w) | (361w) | (357w) | (358w) | (356w) |
| v ₆ [v(MC)+δ(NCM)]F ₂ | 359 | 316 | 330 | 353s | 350s | 355s | 354s | 353s |
| v ₇ [v(MC)+δ(NCM)]F ₂ | 315 | 250 | 235 | 261w | 261w | 270w | 267m | 268m |

The band observed in the Raman spectra are in given parentheses. ^a Taken from Ref.-27.

M'(CN)₄ (M = Zn, Cd or Hg) group vibrations: In assigning the bands attributable to M'(CN)₄ (M' = Zn, Cd or Hg) ions in the spectra of our compounds, we refer to the work of Jones²⁷ who presented vibrational data for the salts K₂M(CN)₄ (M = Zn, Cd or Hg) in the solid phase and assigned the infrared and Raman active fundamental vibrations of the M(CN)₄ ion on the basis of T_d symmetry. The assigned wavenumbers for the M'(CN)₄ groups in the compounds studied appear to be much higher than those for M(CN)₄ groups in K₂M(CN)₄ (M = Zn, Cd or Hg) (Table-2). Such frequency shifts have been observed for other T_d-type host complexes¹⁵⁻¹⁸ and T_d-type clathrates^{14,19-21}, in which both ends of the CN group are coordinated and explained as the mechanical coupling of the internal modes of M'(CN)₄ (M' = Zn, Cd or Hg) with the M-NC vibrations. It follows that the N-ends of the M'(CN)₄ groups are also bound to a M atom in present complexes.

ACKNOWLEDGEMENTS

The author is grateful to Prof. Mustafa Senyel, Department of Physics, Anadolu University, Eskisehir, Turkey for the far-IR and FT-Raman measurements.

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