



## Synthesis and Characterization of caffeine Complexes $[M(\text{caf})_4X_2]$ $M = \text{Ni(II), Cu(II), Zn(II), Cd(II)}$ $X = \text{SCN}^-, \text{CN}^-$ ; $\text{caf} : \text{caffeine}$

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Available online at: [www.isca.in](http://www.isca.in), [www.isca.me](http://www.isca.me)

Received 29<sup>th</sup> December 2013, revised 10<sup>th</sup> January 2014, accepted 17<sup>th</sup> February 2014

### Abstract

A series of complexes  $[M(\text{caf})_4X_2]$  where  $X = \text{cyano, thiocyanato}$ ,  $\text{caf} = \text{caffeine}$ , and  $M = \text{Ni(II), Cu(II), Zn(II) and Cd(II)}$  were prepared. The prepared complexes were characterized by elemental analysis, conductance measurement, UV-Visible and FT-IR spectral analysis. The conductivity measurements reveal that the complexes are nonelectrolyte. The elemental analysis showed the formation of 1,4,2 (metal, caffeine, cyano or thiocyanato) complexes. The infrared and UV-visible data indicating a monodentate coordination of the four caffeine by N9 nitrogen atom and two cyano or thiocyanato in trans and cis octahedral geometry.

**Keywords:** Cyano, thiocyanato, caffeine, cis, trans-complexes, analysis, infrared spectroscopy, UV-Visible, molar conductivity.

### Introduction

The transition metal ions and their complexes take part for of all the fundamental biologic process oxygen, nitrogen fixation and transformation, coordination of all metabolic reactions, catalysis and bio-photocatalysis, solar energy, molecular electronic etc.

Caffeine, theophylline, theobromine they are naturally occurring drugs<sup>1</sup>, Its side-effects include toxicity in excess of consumption, high adrenal stimulation<sup>2</sup>, are present in different ratios in the different plant sources for example caffeine is found in coffee, tea, cola muts, mate and guarana<sup>3</sup>. Caffeine is a planar aromatic molecule which leads to the hypothesis that it could very easily form  $\pi-\pi$  complexes with other planar aromatic molecules such as nucleobases in DNA and several types of anticancer drugs known to intercalate DNA based on their planar structures<sup>4,5</sup>.

This caffeine have the ability to form complexes with metal ions from nd series. Caffeine contains some nitrogen, oxygen atoms involved in coordinative bonds. Some caffeine complexes were found biologically active such as the complexes  $[\text{PPh}_3\text{Me}][\text{PtCl}_3(\text{caffeine})]$ ;  $[\text{Ac}_2\text{Zn}(\text{caf})\text{H}_2\text{O}]$ ;  $[\text{Mg}(\text{SCN})_2(\text{caf})_2]_7\text{H}_2$ ,  $[\text{Cu}(\text{pyridine})(\text{caf})]$  have anticancer, antifungal and antimicrobial effect, a few metal-theophylline complexes  $[\text{M}(\text{TP})_4(\text{OCN})_2]$  have shown significant antitumor activity<sup>6</sup>, the complex has a formula  $[\text{M}(\text{Th})_2(\text{caf})_2(\text{X})(\text{Y})]$ ;  $[\text{M}(\text{Th})_2(\text{Ad})(\text{X})_3]$ ;  $[\text{M}(\text{Th})_2(\text{Ad})_2(\text{X})_2]$ ;  $[\text{M}(\text{Th})_4(\text{Y})_2]$ ;  $[\text{M}(\text{caf})_4(\text{Y})_2]$ ; where Ad: adenine and Th: theophylline  $\text{M}^{2+} = \text{Vo(II); Co(II); Ni(II), Cu(II)}$  and  $\text{X} = \text{SCN}^-$ ;  $\text{Y} = \text{OCN}^-$  already prepared<sup>7</sup>.

In this paper, we prepared and characterized a serie of new complexes  $[M(\text{caf})_4X_2]$  where  $\text{X} = \text{CN}^-, \text{SCN}^-$ ,  $\text{M} = \text{Zn(II), Cd(II), Cu(II), Ni(II)}$  and  $\text{caf} = \text{caffeine}$ .

### Material and Methods

All reagents were purchased commercially and used without further purification, caffeine was purchased from Riedl-deHaen. A.G. the chloride of the appropriate metallic ion  $\text{MCl}_2 \cdot 2\text{H}_2\text{O}$   $\text{M} = \text{Cd(II), Ni(II), Cu(II), Zn(II)}$ , KCN and KSCN were obtained from BDH.

**Instrumental analysis:** The IR spectra of the complexes were recorded on a Jasco FT IR-4100 spectrometer in the (4000-400)  $\text{cm}^{-1}$  range with KBr pellet technique. UV-Visible spectra were recorded on Shimadzu UV-1800. The elemental analysis of the complexes was carried out by (flash EA 112 Thermo). The molar conductance measurements were conducted using at in DMSO with Hach HQ430d flexi at 25°C.

**Synthesis of the complexes:** An ethanolic solution of  $4.10^{-3}$  mol caffeine (caf) and  $2.10^{-3}$  mol an aqueous solution of KCN or KSCN were respectively added to an aqueous solution of  $1.10^{-3}$  mol the metal salts. After constant stirring using appropriate amounts of materials needed as decided by the molar ratio (1:4:2) (M:caf:X), the resulting precipitates were filtered off, washed several times and recrystallized with 1:3 ethanol: water. Then, it dried in an oven at 60°C, similar method was followed to prepare all complexes.

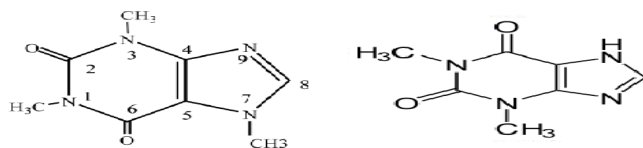
### Results and Discussion

Elemental analysis C, H and metal determination were in good agreement with general formula given for the complexes  $[M(\text{caf})_4X_2]$  as shown in table-1.

The prepared complexes were found to be solids, insoluble in water but they were soluble in some organic solvents such as dimethylsulfoxide.

The molar conductance values in DMSO obtained from 5-33  $\text{cm}^2 \text{ ohm}^{-1} \text{ mol}^{-1}$  indicates the nature of complexes is nonelectrolyte<sup>8</sup>.

**Infrared spectra:** The IR spectral data of the complexes and the free caffeine are given in table- 2-3. Caffeine and theophylline are shown in figure-1, They have a centrosymmetric  $C_s$  point group. For the caffeine the numbers of vibrations modes are as follows  $\Gamma_{\text{vib}} = 45A' + 21A''$ . Thus the vibrations of the  $A'$  species will be in plane and those the  $A''$  species will be out of plane. It is known from the literature, that the coordination of metal ions occurs the N9 nitrogen and oxygen carbonyl atoms. In coordination with the N9 nitrogen atom<sup>8,12,13</sup> which is accompanied by the elimination of the mirror plane  $\sigma_h$  and by a whole series of changes in the infrared spectrum. The changes in the spectrum of caffeine is observed in the (1700-400)  $\text{cm}^{-1}$  region corresponding of the stretching and bending vibrations of the carbonyl, imidazole, pyrimidine and methyl fragments in the caffeine<sup>9,10</sup>.



Caffeine

theophylline

Figure-1

Structure of caffeine and theophylline

Table 2-3 summarised the vibrational spectral frequencies of free caffeine ,free thiocyanato , free cyano and their complexes  $[M(\text{caf})_4X_2]$   $X = \text{CN}^-, \text{SCN}^-$ ,  $M = \text{Zn(II), Cd(II), Cu(II), Ni(II)}$ . It may be noted that the spectra of the complexes. We can raise a

band and medium intensity at the (3500-3400)  $\text{cm}^{-1}$  range which can be corresponding to stretching vibration  $\nu(\text{OH})$  of hydration water, and two less intense bands at 3100  $\text{cm}^{-1}$  and 2950  $\text{cm}^{-1}$  which can be corresponding to  $\nu(\text{CH})$  and  $\nu(\text{CH}_3)$  respectively<sup>9,10,11</sup>.

In the all complexes  $\nu(\text{SCN})$  stretching frequencies are seen between 2162  $\text{cm}^{-1}$  and 2090  $\text{cm}^{-1}$  corresponding the coordination of thiocyanato through S-atom .The frequencies of the  $\nu(\text{CN})$  are localized in both spectra in the range 2200  $\text{cm}^{-1}$  and 2124  $\text{cm}^{-1}$ , these values indicate the coordination of the cyano ligand<sup>7,12,13</sup>.

The presence of a single and two strong  $\nu(\text{CN})$  and  $\nu(\text{SCN})$  for the complexes indicate the existence of inequivalent thiocyanato and cyano in two isomers (cis + trans) in octahedral geometry.

A strong absorption bands  $\nu(\text{CO})$  for the carbonyl group in the caffeine and their complexes  $[M(\text{caf})_4X_2]$   $X = \text{CN}^-, \text{SCN}^-$  for  $M = \text{Zn(II), Cd(II), Cu(II), Ni(II)}$  are observed in the region (1700-1650)  $\text{cm}^{-1}$ . This region is a characteristic of aromatic lactones for one and two carbonyl as in the quinone<sup>9,10</sup>.

Caffeine contain two carbonyl vibration in the meta position. The very strong bands observed at 1702  $\text{cm}^{-1}$  and 1662  $\text{cm}^{-1}$  are considered to be due to  $\nu(\text{CO})$  asymmetric and  $\nu(\text{CO})$  symmetric stretching vibration in caffeine<sup>9,10</sup>. The infrared spectra of the complexes  $[M(\text{caf})_4X_2]$   $X = \text{CN}^-, \text{SCN}^-$  for  $\text{Zn(II), Cd(II), Cu(II), Ni(II)}$  are characterized by insignificant shift frequency for asymmetric  $\nu(\text{CO})$  but  $\nu(\text{CO})$  symmetric is shifted to lower frequencies by 10  $\text{cm}^{-1}$ . The band noticed in the caffeine spectrum at 1548  $\text{cm}^{-1}$  conferring to the vibrations  $\nu(\text{imidazol}) + \nu(\text{pyrimidine}) + \delta(\text{HCN})$  and appeared for the caffeine complexes at 1540  $\text{cm}^{-1}$  table-2,3<sup>6,7</sup>.

Table-1  
Elemental analysis and molar conductivity of the prepared complexes

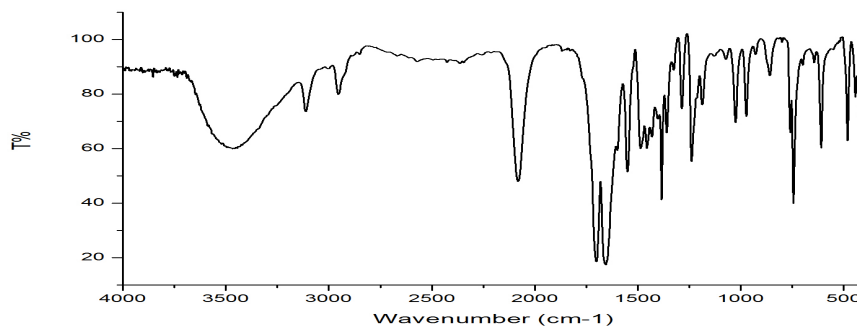
Complexes $[M(\text{caf})_4(X)_2]$ $X = \text{CN}^-, \text{SCN}^-$	Colour	Molecular weight	% Metal	% C	% H	$\Omega (\text{ohm}^{-1} \text{ cm}^2 \text{ mol}^{-1})$
$[\text{Cu}(\text{caf})_4(\text{SCN})_2]$	Brown	956.306	(6.64) 6.62	(41.4) 41.6	(4.1) 4.3	10,4
$[\text{Zn}(\text{caf})_4(\text{SCN})_2]$	white	958.169	(6.82) 6.84	(41.32) 41.41	(4.17) 4.21	14,3
$[\text{Ni}(\text{caf})_4(\text{SCN})_2]$	green	951.453	(6.16) 6.21	(41.62) 41.73	(4.2) 4.35	12,8
$[\text{Cd}(\text{caf})_4(\text{SCN})_2]$	white	1005.17	(11.18) 11.3	(39.39) 39.57	(3.97) 4.13	19,1
$[\text{Cu}(\text{caf})_4(\text{CN})_2]$	bleu	892.306	(7.12) 7.15	(44.37) 44.46	(4.48) 4.57	8.4
$[\text{Zn}(\text{caf})_4(\text{CN})_2]$	white	894.169	(7.31) 7.53	(44.28) 44.35	(4.47) 4.53	33
$[\text{Ni}(\text{caf})_4(\text{CN})_2]$	green	887.453	(6.61) 6.7	(44.62) 44.75	(4.5) 4.71	16.2
$[\text{Cd}(\text{caf})_4(\text{CN})_2]$	white	941.17	(11.9) 12.1	(42.07) 42.14	(4.25) 4.38	5.13

\*The theoretical values are in parenthesis

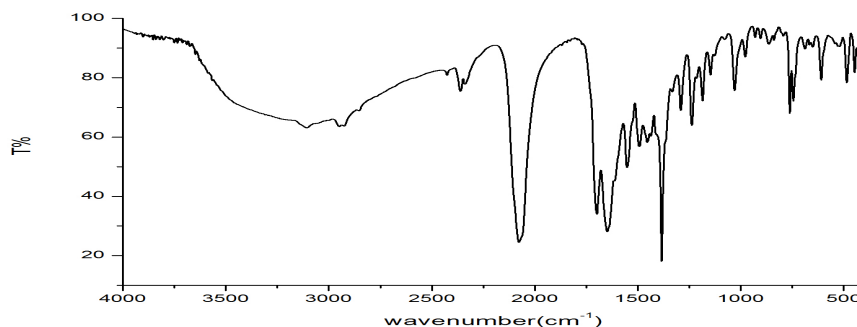
The band observed in the range  $(1480-1400) \text{ cm}^{-1}$  for the complexes  $[\text{M}(\text{caf})_4\text{X}_2]$  belong to the deformation vibrations  $\delta(\text{CH}_3) + \delta(\text{HCN})$  and  $\delta(\text{CH}_3) + \gamma(\text{CH}_3)$  are shifted to lower frequencies see table-2-3<sup>9,10</sup>.

Their frequencies noticed in  $(1445-1400) \text{ cm}^{-1}$  in the complexes binding vibrations and stretching vibrations are due to the connection from the methyl fragment. The deformation and rotation vibrations of fragment pyrimidine and imidazole are usually found at lower frequencies in non affected.

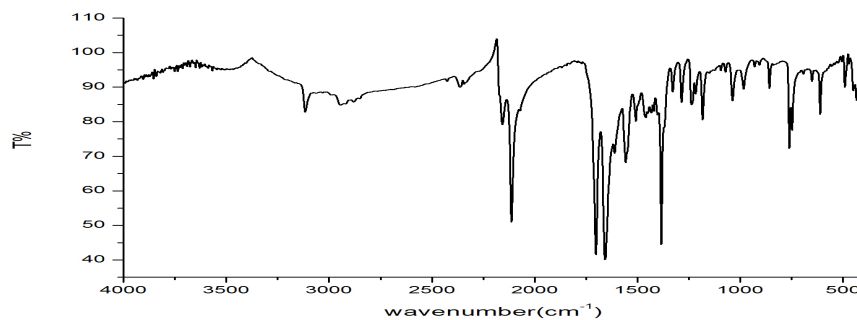
The newly vibrations appeared in the spectra of these complexes compared to the caffeine free spectrum are those due to the metal caffeine band  $\nu(\text{M-N})$  at  $520 \text{ cm}^{-1}$ <sup>9,10,11</sup>. It should be noted that in the spectra of complexes that no contain direct oxygen-carbonyl binding, were observed spectrum changes in the region corresponding for stretching and bending vibrations fragments  $\nu(\text{CO})$ ,  $\delta(\text{HCN})$ ,  $\nu(\text{pyrimidine})$ ,  $\nu(\text{imidazole})$ ,  $\delta(\text{HCN})$ ,  $\delta(\text{CH}_3)$  attributed for authors by coordination on the nitrogen N9 atoms of caffeine<sup>5</sup>.



**Figure-2**  
IR spectrum of the complex  $[\text{Zn}(\text{caf})_4(\text{SCN})_2]$



**Figure-3**  
IR spectrum of the complex  $[\text{Cd}(\text{caf})_4(\text{SCN})_2]$

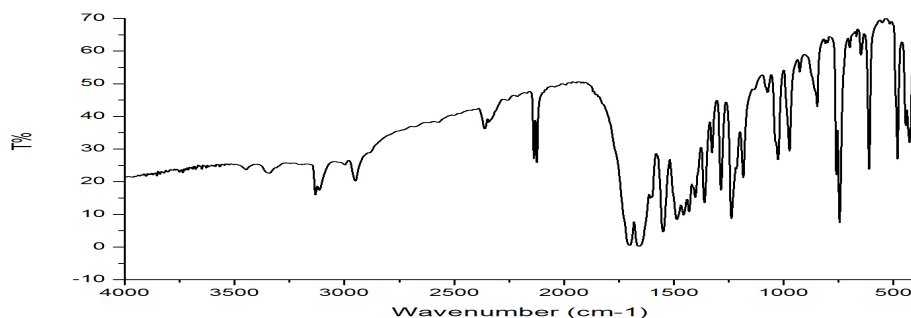


**Figure-4**  
IR spectrum of the complex  $[\text{Cu}(\text{caf})_4(\text{SCN})_2]$

**Table-2**  
**IR spectral data of the ligand and its complexes (cm<sup>-1</sup>) [ M(caf)<sub>4</sub>(X)<sub>2</sub>] X = SCN<sup>-</sup> ; M = Cu(II) , Cd(II) , Ni(II) , Zn(II) and caf = caffeine**

Free ligands		[Cd(caf) <sub>4</sub> (X) <sub>2</sub> ]	[Ni(caf) <sub>4</sub> (X) <sub>2</sub> ]	[Zn(caf) <sub>4</sub> (X) <sub>2</sub> ]	[Cu(caf) <sub>4</sub> (X) <sub>2</sub> ]	Assignment
KSCN	Caféine					
		3400 vs	3400 vs	3465 vs		$\nu(\text{OH})_{\text{H}_2\text{O}}$
	3110 m	3100 vs	3111 vs	3109 vs	3111 vs	$\nu(\text{CH}=\text{N})$
	2954 m	2950 vs	2952 vs	2948 vs	2952 vs	$\nu(\text{CH}_3)$
		2160 s	2162 s	2160 s	2158 s	$\nu(\text{SCN})$
2051 s		2100 m	2110 vs	2090 s	2111 vs	$\nu(\text{SCN})$
	1700 vs	1695 vs	1700 vs	1694 vs	1695 vs	$\nu_{\text{s}}(\text{CO})$
	1660 vs	1654 vs	1650 vs	1653 s	1650 vs	$\nu_{\text{a}}(\text{CO})$
	1600 m	1590 vs	1597 s	1596 s	1608 s	$\nu(\text{C}=\text{C})+\nu(\text{HCN})$
	1548 s	1542 vs	1540 s	1542 s	1550 s	$\delta(\text{HCN})+\nu(\text{imidazol})+\nu(\text{pyrimidine})$
	1470 m	1480 vs	1480 s	1480 s	1500 m	$\delta(\text{HCN})+\delta(\text{CH}_3)$
	1466 m	1446 vs	1448 s	1452 s	1450 m	$\gamma(\text{CH}_3)+\delta(\text{CH}_3)$
	1432 m	1422 vs	1418 s	1428 s	1430 m	
		1400 vs		1386 s	1388 s	
	1360 s	1360 vs	1360 s	1360 m	1365 m	$\delta(\text{HCN})+\nu(\text{imidazol})+\delta(\text{CH}_3)$
	1326 w	1325 s	1325 m	1326 m	1330 m	$\nu(\text{imidazol}) + \nu(\text{pyrimidine})$
	1285 s	1288 vs	1288 m	1284 m	1286 m	$\nu(\text{pyri})$
	1237 vs	1242 vs	1242 s	1240 s	1237 m	$\nu(\text{CN}) + \rho(\text{CH}_3)$
	1210 w	1216 vs	1212 m	1216 m	1218 w	$\delta(\text{CH}) + \rho(\text{CH}_3)$
	1188 m	1187 s	1187 m	1188 m	1183 m	$\delta(\text{CH}) + \rho(\text{CH}_3)$
	1130 w	1130 m	1138 m	1124 w	1130 w	$\rho(\text{CH}_3)$ out of plan
	1071 s	1070 m	1078 w	1075 w	1074 w	$\rho(\text{CH}_3) + \rho(\text{CH})$
	1025 s	1024 vs	1024 m	1024 w	1038 w	$\rho(\text{CH}_3) + \rho(\text{CH})$
	973 s	976 vs	970 w	973 w	982 w	$\nu(\text{N-CH}_3)+\rho(\text{CH}_3) + \delta(\text{imidazol})$
	923 w	924 m	924 w	928 w	930 w	$\gamma(\text{CH})$
	862 m	860 m	857 s	858 w	857 w	$\rho(\text{CH}_3)+\nu(\text{N-CH}_3)+\delta(\text{C}=\text{O})$
	800 s	797 m	797 w	797 w		$\rho(\text{pyrimidine}) + \delta(\text{C}=\text{O})$
748 m		760 s	760 w	759 w	761 w	$\nu(\text{C-S})$
	700 m	700 w	698 w	698 w	690 w	$\gamma(\text{pyrimidine})+\gamma(\text{imidazol})$
	642 s	642 w	642 w	642 w	654 w	$\delta(\text{pyrimidine})+\rho(\text{imidazol})$
	611 s	610 vs	612 w	611 m	610 vs	$\gamma(\text{imidazol})$
		549 w	549 w	551 w	549 w	$\nu(\text{M-N})$
	481 vs	482 s	482 w	478 w	494 w	$\tau(\text{caffeine})$
		443 s	443 w	440 w	440 w	$\nu(\text{M-SCN})$
	420 vs	425 s	421 w	420 w	424 w	$\rho(\text{C}=\text{O})$

vs: very strong, s: strong, m: medium, w: weak



**Figure-5**  
**IR spectrum of the complex [Cu(caf)<sub>4</sub>(CN)<sub>2</sub>]**

Table-3

IR spectral data of the ligand and its complexes (cm<sup>-1</sup>) [M(caf)<sub>4</sub>(X)<sub>2</sub>] X = CN<sup>-</sup>; M = Cu<sup>+2</sup>, Cd<sup>+2</sup>, Ni<sup>+2</sup>, Zn<sup>+2</sup> and caf = caffeine

Free ligands		[Cd(caf) <sub>4</sub> (X) <sub>2</sub> ]	[Ni(caf) <sub>4</sub> (X) <sub>2</sub> ]	[Zn(caf) <sub>4</sub> (X) <sub>2</sub> ]	[Cu(caf) <sub>4</sub> (X) <sub>2</sub> ]	Assignment
KCN	caféine					
		3500 s	3400 s	3500 s	3450 s	ν(OH) <sub>H2O</sub>
	3110 m	3102 s	3100 m	3105 s	3104 s	ν(CH=)
	2955 m	2950 s	2952 m	2950 s	2951 m	ν(CH <sub>3</sub> )
					2137 s	ν(CN)
2088 s*		2200 m	2175 s	2217 m	2124 m	ν(CN)
	1700 vs	1693 vs	1694 vs	1695 vs	1695 vs	νas(CO)
	1660 vs	1647 vs	1646 vs	1650 vs	1650 vs	νa(CO)
	1600 m	1594 s	1595 m	1598 s	1604 s	ν(C=C)+ν(HCN)
	1548	1540 vs	1540 s	1540 vs	1540 vs	δ(HCN)+ν(imidazol) + ν(pyrimidine)
		1478 vs	1478 m	1476 vs	1490 s	δ(HCN)+δ(CH <sub>3</sub> )
	1466 m	1446 s	1446 m	1446 s	1450 s	ν(CH <sub>3</sub> )+δ(CH <sub>3</sub> )
	1432 m	1426 s		1425 s	1428 s	
	1405 m	1403 s	1400 w	1403 s	1402 s	
	1360 s	1358 vs	1364 m	1357 s	1360 m	δ(HCN)+ν(imidazole)+δ(CH <sub>3</sub> )
	1326 w	1325 s	1327 w	1320 m	1324 w	ν(imidazol) + ν(pyrimidine)
	1285 s	1282 s	1254 w	1280 m	1280 w	ν(pyrimidine)
	1237 vs	1234 vs	1240 m	1235 s	1230 w	ν(CN) + pr(CH <sub>3</sub> )
	1188 m	1184 s	1185 w	1184 m	1180 w	δ(CH) + pr(CH <sub>3</sub> )
	1130 w	1125 w	1130 w	1127 w	1133 w	pr(CH <sub>3</sub> ) out of plan
	1071 s	1070 m	1080 w	1067 w	1074 w	ρ(CH <sub>3</sub> ) + ρ(CH)
	973 s	968 s	978 m	968 s	978 m	ν(N-CH <sub>3</sub> )+pr(CH <sub>3</sub> )+δ(imda)
	923 m	924 w	930 w	922 w	924 w	γ(CH)
	862 m	858 m	870 w	864 w	840 w	ρ(CH <sub>3</sub> )+ν(N-CH <sub>3</sub> )+δ(C=O)
	800 s	798 w	800 w	798 w	800 w	ρ(pyrimid) + δ(C=O)
	743 vs	740 vs	747 vs	740 vs	740 vs	γ(pyrimidine) + γ(imidazol)
	642 s	643 w	643 w	643 w	648 w	
	611 s	610 m	612 m	609 m	610 m	γ(imidazole)
		550 w	558 w	548 w	551 w	ν(M-N)
	481vs	480 m	480 m	478 s	481 m	T[(caffeine)]
		438 w	440 s	454 s	440 m	δ <sub>ring</sub> (pyrimidine)
	420 vs	420 m	425 w	420 m	426 m	pr(C=O)

vs: very strong, s: strong, m: medium, w: weak

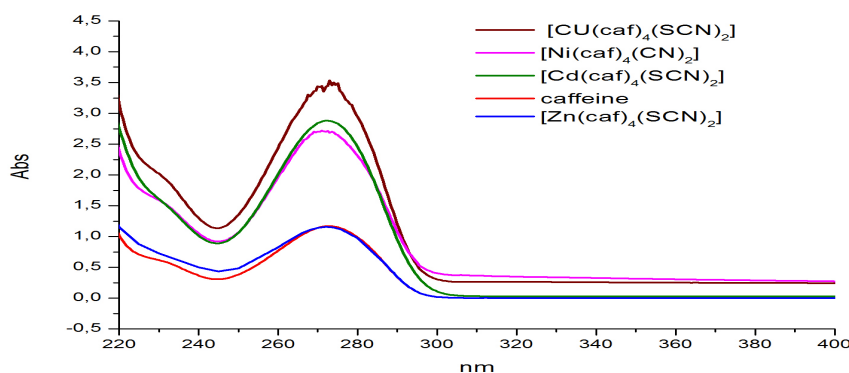
**UV-Visible electronic absorption spectra :** The electronic absorption spectral of the complexes [Zn(caf)<sub>4</sub>(SCN)<sub>2</sub>] and [Cd(caf)<sub>4</sub>(CN)<sub>2</sub>] have (d<sup>10</sup>) electronic configuration, which is confirmed absence of d-d transition<sup>15</sup>. The electronic spectra of these complexes show metal to ligand charge transfer transition (M→L) at 272 nm and 271 nm respectively and the values are shown in figure-5, table-4.

The electronic spectrum of [Cu(caf)<sub>4</sub>(SCN)<sub>2</sub>] complex shows band at 621nm and 864 nm which is attributed of the electronic

transitions <sup>2</sup>e<sub>2g(D)</sub>→<sup>2</sup>b<sub>1g(D)</sub> and <sup>2</sup>a<sub>1g(D)</sub> →<sup>2</sup>b<sub>1g(D)</sub> (v3) respectively (see figure-5). Therefore, these transitions confirmed that the [Cu(caf)<sub>4</sub>(SCN)<sub>2</sub>] complex has a cis-trans octahedral stereochemistry<sup>14</sup>.

The electronic spectra of [Ni(caf)<sub>4</sub>(CN)<sub>2</sub>] complex shows electronic transition <sup>3</sup>A<sub>2g(F)</sub> → <sup>3</sup>T<sub>1</sub>

<sup>g(F)</sup> and <sup>3</sup>A<sub>2g(F)</sub> → <sup>3</sup>T<sub>2g(F)</sub> at 865 nm and 942 nm (figure-5).



**Figure-5**  
UV-visible spectra of the complexes  $[M(\text{caf})_4(\text{X})_2]$  ( $M = \text{Ni}^{2+}, \text{Cu}^{2+}, \text{Cd}^{2+}, \text{Zn}^{2+}$ )  $\text{X} = \text{SCN}^-, \text{CN}^-$  in DMSO

**Table-4**  
U.V-visible spectra of free ligand and their complexes  $10^{-3}\text{M}$  in DMSO.

Compound	$\lambda_{\text{max}}$ (nm)	Transitions	
Caffeine	274	$\pi \rightarrow \pi^*$	
$\text{CN}^-$	426	$n \rightarrow \pi^*$	
$\text{SCN}^-$	235 360	$\pi \rightarrow \pi^*$ $n \rightarrow \pi^*$	
$[\text{Cu}(\text{caf})_4(\text{SCN})_2]$	273 317 369	Charge transference $M \rightarrow L$	
	621		${}^2b_{2g(D)} \rightarrow {}^2b_{1g(D)}$
	864		${}^2e_{2g(D)} \rightarrow {}^2b_{1g(D)}$
$[\text{Ni}(\text{caf})_4(\text{CN})_2]$	271	Charge transference $M \rightarrow L$	
	865	${}^3A_{2g(F)} \rightarrow {}^3T_{1g(F)}$	
	942	${}^3A_{2g(F)} \rightarrow {}^3T_{2g(F)}$	
$[\text{Cd}(\text{caf})_4(\text{CN})_2]$	271	Charge transference $M \rightarrow L$	
$[\text{Zn}(\text{caf})_4(\text{SCN})_2]$	272	Charge transference $M \rightarrow L$	

## Conclusion

We have been able to synthesis and characterize complexes  $[M(\text{caf})_4(\text{X})_2]$  containing caffeine, cyano or thiocyanato ion coordinated with Ni(II), Cu(II), Zn(II) and Cd(II).

From the results obtained by elemental analysis, conductance measurement, UV-Visible and infrared spectral indicate the structures of complexes are cis and trans octahedral symmetry.

## Acknowledgement

We thank the Université Moulay Ismail, faculté des sciences, Meknès, Morocco for financial supports.

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