

Spectral Studies of the Mixed Ligand Organometallic Complexes Derived From Schiff Base

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Abstract: A number of dinuclear Co(II), Ni(II), Cu(II), Mn(II) and Zn(II) complexes have been isolated by reacting bis (Salicylaldehyde) 1:2-propane diamine with metal salts and phenyl/p-tolyl mercury thiocyanate under varied reaction conditions. Structures of the complexes have been assigned on the basis of elemental analysis, molecular weights, molar conductances, magnetic moments, UV-visible, Infrared and electronic spectral studies. The physicochemical data suggest that bis (Salicylaldehyde) 1:2- propane diamine behave as dibasic tetradentate (ONNO) donor and the isolated complexes have distorted octahedral geometry.

M^I (salpn) i.e. N,N'-1,2-propane bis (salicylidineiminato) metal(II) coordinates to transition^(1,2) and non transition^(3,4) metal ion. Ni(salpn) has been used as ligand in the formation of trinuclear heterometal^(5,6) complexes. Here we study on a new series of trimetallic complexes prepared from M(salpn) and (RHgSCN)₂ M(NCS)₂ [M=Co(II), Ni(II), Cu(II), Zn(II), Mn(II), M^I = Co(II), Ni(II), Cu(II), Zn(II), R=C₆H₅-, P-tolyl].

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I. EXPERIMENTAL

Preparation Of Phenyl Mercury Thiocyanate (C₆H₅Hgscn):

Phenyl mercury thiocyanate was prepared by stirring an ethanolic solution of phenyl mercury acetate (BDH) with ethanolic solution of KNCS (BDH) in 1:1 molar ratio. Phenyl mercury thiocyanate was immediately formed which was filtered, washed with solvent, recrystallized from acetone and dried in vacuum. The purity of the compound was tested by elemental analysis, melting point and infra-red spectra. Cobalt and nickel thiocyanates were prepared by reacting their respective nitrates with potassium thiocyanate in ethanol.

Preparation of Lewis Acid [C₆H₅HgSCN)₂ M(NCS)₂]:

1.75 gram of M(NCS)₂ [M=Co(II), Ni(II), Cu(II), Zn(II), Mn(II) (1 mole) and C₆H₅HgSCN (2 m mole) were dissolved in 25 ml of ethanol and 100 ml of ethyl acetate in two separate flasks. Both solution were mixed and stirred for 36 hours. A precipitate appeared in each case which was filtered, washed with ethyl acetate and dried in vacuum. These compounds melt with decomposition in the range 165-200°C.

Preparation Of [(C₆H₅Hgscn)₂ Co(NCS)₂(Py)₂]:

3.32 gram of Co(NCS)₂ 2Py (1 m mole) and 6.7 gram of C₆H₅HgSCN were separately dissolved in 50 ml of ethanol. The two solutions were mixed and stirred for 48 hours. A pink precipitate appeared, which was filtered, washed with solvent, recrystallized from acetone and dried in vacuum. The analytical results show that it has a molecular formula (C₆H₅HgSCN)₂ Co(NCS)₂ (Py)₂.

The compound was prepared by heating (C₆H₅HgSCN)₂ Co(NCS)₂ (Py)₂ under vacuum 50-60°C for about two hours, until the pink colour changed to blue m.p. 192°C.

Preparation Of P-Tolyl Mercury Chloride [P-CH₃C₆H₄HgCl]:

17.0 grams (0.1 m mole) of P-toluidine was added to a mixture of 50 ml of concentrate hydrochloric acid and 400 ml of water. The mixture was cooled by adding 400 grams of ice and stirred vigorously. The temperature of the reaction was maintained between 0-5°C and solid sodium nitrite (8.0 grams) was added in small fraction. After stirring for about half an hour, the whole mass was filtered. To the clear filtrate a cooled solution of (27.0 g 0.1 mole) mercuric chloride in 300 ml of concentrated hydrochloric acid was slowly added with vigorous stirring. The stirring was continued for 15-minutes more and precipitate was filtered, washed with water, followed by ether and dried in air. The p-CH₃C₆H₄N₂HgCl₂ so obtained was mixed with 12 gm of copper powder in 100 ml of cold water in fractions with stirring. The mixture was stirred for one hour and allowed to stand overnight and filtered. The residue was extracted with xylene, which on cooling gave white crystals of p-CH₃C₆H₄HgCl.

Preparations of P-Tolyl Mercury Thiocyanate:

Para tolyl mercury chloride was converted into its thiocyanate derivative by reacting with potassium thiocyanate in 1:1 molar ratio in acetone. The potassium chloride was filtered off and the filtrate was concentrated by vacuum evaporation. On addition of water to the concentrate solution, p-tolyl mercury thiocyanate separated, which was filtered, washed with water followed by ether and dried in air. The compound was recrystallised from acetone. The purity of the thiocyanate derivative was tested by elemental analysis and infrared spectral measurements.

p-CH₃C₆H₄HgSCN m.p. 187°C
 %Found C - 27.32; H - 1.89; N - 3.87; S - 9.0; Hg - 57.10
 % Calculated C - 27.46; H - 2.0; N - 4.0; S - 9.15; Hg - 57.37
 Infra-red spectral band positions:
 ν(C-N) 2175 cm⁻¹, ν(C-S) 756 cm⁻¹, δ(NCS) 436 cm⁻¹

Preparation Of M^I(Salpn) And Lewis Acids [(RHgscn)₂ M(NCS)₂]:

[M = Co(II), Ni(II), Cu(II), Zn(II), Mn(II); R=C₆H₅- and P-CH₃C₆H₄]

Preparation Of Trimetallic Complexes [(RHgscn)₂ M(NCS)₂ M^I(Salpn)]: [R = P-CH₃C₆H₄ - and C₆H₅-]

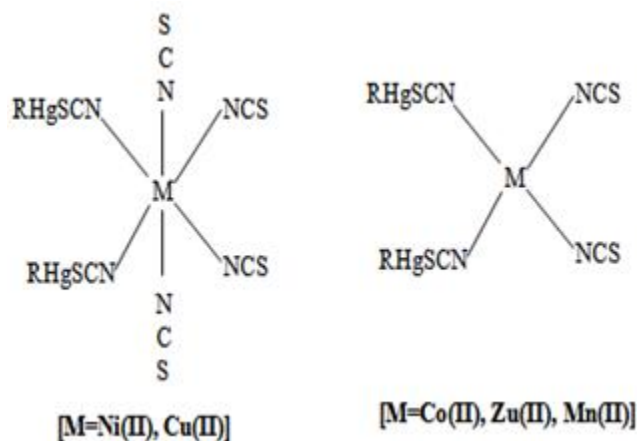
These complexes were prepared by mixing a solution of the Lewis acid in methanol with a solution of M^I(salpn) in the same solvent in 1:1 molar ratio. The mixture was refluxed for 4 hours and then stirred for 24 hours. The complex formed in each case was filtered, washed with methanol followed by ether and dried in vacuum. The complexes were recrystallized from DMSO. (Table 1-4)

II. RESULTS AND DISCUSSION

The IR spectra of phenyl mercury thiocyanate and P-tolyl mercury thiocyanate were recorded in solid and in solution phases. The solid phase spectra shows the presence of three bands at 2190 cm⁻¹, 2120 cm⁻¹ in ν(C-N) region, two bands at 730 cm⁻¹ and 720 cm⁻¹ in ν(C-S) region and two band at 460 cm⁻¹ & 410 cm⁻¹ in δ(NCS) region^(7,8). In solution phase only two bands at 2120 cm⁻¹ and 2100 cm⁻¹ are observed and the band at 2190 cm⁻¹ disappears. It shows that P-tolyl-mercuric thiocyanate is probably dimer like CH₃HgSCN in Solid phase^(9,10) through bridging. In solution phase the bridge is ruptured and it becomes a monomer (fig. 1).

Lewis Acids [(RHgSCN)₂ M(NCS)₂]:

On reaction with M(NCS)₂ the RHgSCN form the complex of general formula formula (RHgSCN)₂ M(NCS)₂. These complexes have been referred to as Lewis acids. The infra-red spectra indicate that the ν(C-N) stretching bands move from 2120 cm⁻¹ in RHgSCN to 2190 cm⁻¹ in the Lewis acid (Table 5-7). The ν(C-N) and δ(NCS) bands change their position to 790 cm⁻¹ and 480 cm⁻¹ respectively. The position of these bands are indicative of the presence of bridging thiocyanate group⁽¹¹⁻¹²⁾. A band is also observed in region 2070 cm⁻¹ which is assigned to N-bonded terminal thiocyanate arising from M-NCS⁽¹³⁻¹⁵⁾. These changes indicate that the thiocyanate of RHgSCN becomes bridging by coordination through its free N-end to M of M(NCS)₂.



The electronic spectra of cobalt Lewis acid shows the presence of two intense bands due to d-d transitions in the region 16000-16200 cm⁻¹ and 8170-8230 cm⁻¹, which are assigned to ⁴A₂→⁴T₁ (P) ν₃ and ⁴A₂→⁴T₁ (F) ν₂ transitions respectively. The Dq value is calculated from ν₂ and ν₃ band positions⁽¹⁶⁾ and is found to be 541 cm⁻¹. The electronic spectral data and the magnetic moment values (table 7) indicate that cobalt is in tetrahedral geometry in its Lewis acid. In case of nickel Lewis acid three bands are observed in the region 26320-27790 cm⁻¹, 16120-16650 and 10040-10400 cm⁻¹ which are assigned ³A_{2g}→³T_{1g}(P) ν₃, ³A_{2g}→³T_{1g}(F) ν₂ and ³A_{2g}→³T_{2g}(F) ν₁, respectively. The position of these bands various spectral parameters and the magnetic moment values indicate that nickel is in octahedral coordination geometry^(17,18). The octahedral geometry is perhaps acquired through axial coordination in its Lewis acid (fig. 2).

III. ADDUCTS

The coordination number of M[M=Co(II), Zn(II), Mn(II)] in the Lewis acid is four against the maximum of six, hence they can be reacted with bases to raise their coordination number to six. The Lewis acids where M is Ni(II) or Cu(II) the weak axial bonding can be replaced by stronger ligands. Accordingly both types of the Lewis acids have been reacted with M^I(salpn) [M=Co(II), Ni(II), Cu(II), Zn(II)]. these bases form adducts of general formula (RHgSCN)₂ M(NCS)₂ M^I(salpn) which is evident from the positive shift in ν(C-O) band in the spectra of Co(salpn) from 1540 cm⁻¹ to 1560 cm⁻¹.

The IR spectra of these adducts shows that there is no significant change in the position of $\nu(\text{C-S})$ and $\delta(\text{NCS})$ on adduct formation⁽¹⁹⁾. There is however, negative shift in the position of $\nu(\text{M-NCS})$ when M is cobalt and zinc or manganese. This change in $\nu(\text{M-NCS})$ is probably on account of change in geometry of the metal ions from tetrahedral to octahedral⁽²⁰⁾. The geometry around nickel and copper remains the same on the adduct formation hence the change in the positions of $\nu(\text{M-NCS})$ in these cases are insignificant. This shows that the basis structure of the Lewis acid is retained and the change is only in coordination environment.

The electronic spectra of the adducts have been recorded in DMSO and the result are given in table 8-9. The observed bands of cobalt in the region $21000\text{-}22200\text{ cm}^{-1}$, $15165\text{-}18000\text{ cm}^{-1}$ and $9500\text{-}10650\text{ cm}^{-1}$ are assigned to to ${}^4\text{T}_{1g} \rightarrow {}^4\text{T}_{1g}(\text{P})$ ν_3 , ${}^4\text{T}_{1g} \rightarrow {}^4\text{A}_{2g}(\text{F})$ ν_2 and ${}^4\text{T}_{1g} \rightarrow {}^4\text{T}_{1g}(\text{F})$ ν_1 , transitions respectively⁽²¹⁾. The ν_2 band being two electrons transition is very weak. The Dq, B¹ and β have been compared with ν_1 band positions and both are very close. The band position, spectral parameters and the $\mu(\text{eff})$ values support octahedral configuration around cobalt in the adduct. Similarly, nickel adducts also show the presence of three bands in the region $24240\text{-}27500\text{ cm}^{-1}$, $16260\text{-}17000\text{ cm}^{-1}$ which are assigned to to ${}^3\text{T}_{2g} \rightarrow {}^3\text{T}_{1g}(\text{P})$ ν_3 , ${}^4\text{T}_{2g} \rightarrow {}^3\text{T}_{1g}(\text{F})$ ν_2 and ${}^3\text{T}_{2g} \rightarrow {}^3\text{T}_{2g}(\text{F})$ ν_1 , transitions respectively⁽²²⁾. Thus the spectral band positions, spectral parameters and $\mu(\text{eff})$ values support octahedral geometry around nickel. Since the infrared spectra of the complexes of zinc and copper have close similarity with cobalt and nickel complexes, it has been presumed that they to have octahedral geometry around M.⁽²³⁻²⁷⁾

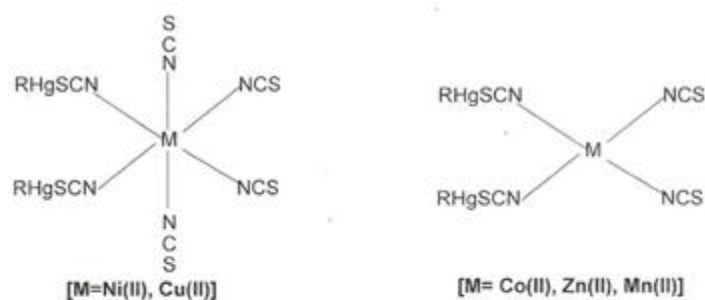


Fig. 2

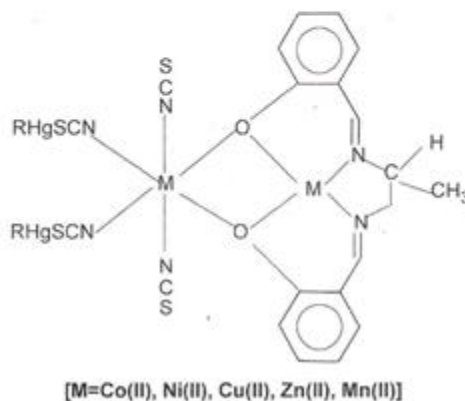


Fig. 3

TABLE 1: Analytical Data Of Complexes

S. No.	Complex	Colour	M.P. (°C)	% Sulphur Cal (obs)	% Nitrogen Cal (obs)	% Mercury Cal (Obs)	%M Cal (obs)	%M Cal (obs)
1	$[\text{C}_6\text{H}_5\text{Hg}(\text{SCN})]_2 \text{Co}(\text{NCS})_2 \text{Co}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	Dirty Green	196	10.80 (10.0)	7.08 (6.90)	33.85 (33.68)	9.94 (9.80)	-
2	$[\text{C}_6\text{H}_5\text{Hg}(\text{SCN})]_2 \text{Co}(\text{NCS})_2 \text{Ni}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	Pale Yellow	172	10.80 (9.85)	7.08 (6.92)	33.85 (33.68)	4.97 (4.80)	4.95 (4.80)
3	$[\text{C}_6\text{H}_5\text{Hg}(\text{SCN})]_2 \text{Ni}(\text{NCS})_2 \text{Co}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	Pale Yellow	222	10.80 (9.85)	7.08 (6.92)	33.85 (33.68)	4.97 (4.80)	4.95 (4.80)
4	$[\text{C}_6\text{H}_5\text{Hg}(\text{SCN})]_2 \text{Ni}(\text{NCS})_2 \text{Ni}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	Brown	213	10.60 (10.0)	7.09 (6.76)	33.86 (33.70)	9.91 (9.80)	-
5	$[\text{C}_6\text{H}_5\text{Hg}(\text{SCN})]_2 \text{Zn}(\text{NCS})_2 \text{Co}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	Brown	192	10.74 (10.0)	7.05 (6.76)	33.67 (33.50)	5.48 (5.35)	4.54 (4.40)
6	$[\text{C}_6\text{H}_5\text{Hg}(\text{SCN})]_2 \text{Zn}(\text{NCS})_2 \text{Ni}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	Pale Yellow	227	10.74 (10.0)	7.05 (6.80)	33.67 (33.50)	5.48 (5.30)	4.92 (4.80)
7	$[\text{C}_6\text{H}_5\text{Hg}(\text{SCN})]_2 \text{Co}(\text{NCS})_2 \text{Co}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	Pink	182	10.60 (10.45)	7.08 (6.90)	33.07 (32.93)	9.71 (9.53)	-

TABLE 2: Analytical Data Of Complexes

S. No.	Complex	Colour	M.P (°C)	% Sulphur Cal (obs)	% Nitrogen Cal(obs)	% Mercury Cal(Ob s)	%M Cal (obs)	%M Cal (obs)
8	(p-CH ₃ C ₆ H ₄ HgSCN) ₂ Co(NSC) ₂ Ni(C ₁₇ H ₁₆ N ₂ O ₂)	Pink	162	10.55 (10.40)	6.92 (6.80)	33.07 (32.90)	4.85 (4.70)	4.84 (4.69)
9	(p-CH ₃ C ₆ H ₄ HgSCN) ₂ Ni(NSC) ₂ Co(C ₁₇ H ₁₆ N ₂ O ₂)	Sky Blue	223	10.55 (10.40)	6.92 (6.80)	33.07 (32.90)	4.85 (4.70)	4.84 (4.69)
10	(p-CH ₃ C ₆ H ₄ HgSCN) ₂ Ni(NSC) ₂ Ni(C ₁₇ H ₁₆ N ₂ O ₂)	Green	260	10.55 (10.40)	6.92 (6.80)	34.76 (34.60)	10.17 (10.0)	-
11	(p-CH ₃ C ₆ H ₄ HgSCN) ₂ Zn(NSC) ₂ Co(C ₁₇ H ₁₆ N ₂ O ₂)	White	245	10.49 (10.38)	6.88 (6.70)	32.89 (32.72)	5.36 (5.20)	4.83 (4.65)
12	(p-CH ₃ C ₆ H ₄ HgSCN) ₂ Zn(NSC) ₂ Ni(C ₁₇ H ₁₆ N ₂ O ₂)	White	248	10.49 (10.38)	6.88 (6.70)	32.90 (32.70)	5.36 (5.20)	4.81 (4.70)
13	(p-CH ₃ C ₆ H ₄ HgSCN) ₂ Mn(NSC) ₂ Co(C ₁₇ H ₁₆ N ₂ O ₂)	White	242	10.58 (10.45)	6.94 (6.80)	33.18 (33.02)	4.54 (4.40)	4.87 (4.70)
14	(p-CH ₃ C ₆ H ₄ HgSCN) ₂ Mn(NSC) ₂ Ni(C ₁₇ H ₁₆ N ₂ O ₂)	Yellow	222	10.58 (10.45)	6.94 (6.80)	33.18 (33.02)	4.54 (4.40)	4.85 (4.69)

Table 3: Racah's Parameter: Magnetic Moment Molecular Weight And Molar Conductance Of The Complexes

S. No.	Complex	μ-eff (B.M.)	Molar Conductance cm ² mhos/mole	Molecular Weight		β
				Cal.	Obs.	
1	[(C ₆ H ₅ Hg(SCN)) ₂ Co(NCS) ₂ Co(C ₁₇ H ₁₆ N ₂ O ₂)	6.40	60.0	1185.04	1170	0.75
2	[(C ₆ H ₅ Hg(SCN)) ₂ Co(NCS) ₂ Ni(C ₁₇ H ₁₆ N ₂ O ₂)	4.76	62.48	1184.82	1165	0.93
3	[(C ₆ H ₅ Hg(SCN)) ₂ Ni(NCS) ₂ Co(C ₁₇ H ₁₆ N ₂ O ₂)	3.24	50.49	1184.82	1162	0.84
4	[(C ₆ H ₅ Hg(SCN)) ₂ Ni(NCS) ₂ Ni(C ₁₇ H ₁₆ N ₂ O ₂)	3.16	48.32	1184.60	1160	0.90
5	[(C ₆ H ₅ Hg(SCN)) ₂ Zn(NCS) ₂ Co(C ₁₇ H ₁₆ N ₂ O ₂)	4.20	56.46	1191.48	1170	-
6	[(C ₆ H ₅ Hg(SCN)) ₂ Zn(NCS) ₂ Ni(C ₁₇ H ₁₆ N ₂ O ₂)	3.25	58.03	1191.26	1167	-
7	[p-CH ₃ C ₆ H ₄ Hg(SCN)) ₂ Co(NCS) ₂ Co(C ₁₇ H ₁₆ N ₂ O ₂)	5.02	66.66	1185.04	1160	1.01

TABLE 4: RACH'S PARAMETER; MAGNETIC MOMENT MOLECULAR WEIGHT AND MOLAR CONDUCTANCE OF THE COMPLEX

S. No.	Complex	ν (C-N) cm^{-1}	ν (C-S) cm^{-1}	νM (NCS) cm^{-1}	νM (NCS) cm^{-1}	(C-O) cm^{-1}	ν (imino gp) cm^{-1}
1	[(C ₆ H ₅ Hg(SCN)) ₂ Co(NCS) ₂ Co(C ₁₇ H ₁₆ N ₂ O ₂)]	2180 (s)	760(s)	480(s)	290(m)	1560(s)	1380(s)
		2150 (w)	740(s)	450(s)	265(m)	1535(m)	1340(s)
2	[(C ₆ H ₅ Hg(SCN)) ₂ Co(NCS) ₂ Ni(C ₁₇ H ₁₆ N ₂ O ₂)]	2185(s)	760(s)	480(s)	280(s)	1560(s)	1380(s)
		2120 (sh)	735(w)	440(s)	260(s)	1540(s)	1340(s)
3	[(C ₆ H ₅ Hg(SCN)) ₂ Ni(NCS) ₂ Co(C ₁₇ H ₁₆ N ₂ O ₂)]	2170 (s)	765(s)	475(s)	270(s)	1560(s)	1380(s)
		2100 (sh)	740(w)	435(w)	265(s)	1535(s)	1340(m)
4	[(C ₆ H ₅ Hg(SCN)) ₂ Ni(NCS) ₂ Ni(C ₁₇ H ₁₆ N ₂ O ₂)]	2175 (s)	770(s)	470(s)	275(s)	1555(s)	1380(s)
		2100 (sh)	735(w)	440(w)	260(s)	1535(s)	1340(m)
5	[(C ₆ H ₅ Hg(SCN)) ₂ Zn(NCS) ₂ Co(C ₁₇ H ₁₆ N ₂ O ₂)]	2180 (s)	765(s)	480(s)	270(s)	1550(s)	1380(s)
		2120 (sh)	740(w)	435(w)	255(s)	1540(s)	1340(w)
6	[(C ₆ H ₅ Hg(SCN)) ₂ Zn(NCS) ₂ Ni(C ₁₇ H ₁₆ N ₂ O ₂)]	2180 (s)	755(s)	485(s)	275(s)	1555(s)	1380(s)
		2140 (sh)	740(s)	450(w)	260(s)	1540(s)	1340(w)
7	[p-CH ₃ C ₆ H ₄ Hg(SCN)) ₂ Co(NCS) ₂ Co(C ₁₇ H ₁₆ N ₂ O ₂)]	2185 (s)	760(s)	480(s)	280 (s)	1560(s)	1380(s)
		2090 (w)	730(s)	440(w)	260(m)	1535(m)	1340(w)

TABLE 5: INFRA-RED SPECTRAL AND BAND ASSIGNMENTS OF THE COMPLEX

S. No.	Complex	ν (C-N) cm^{-1}	ν (C-S) cm^{-1}	νM (NCS) cm^{-1}	νM (NCS) cm^{-1}	ν (C-O) cm^{-1}	ν (imino gp) cm^{-1}
8	(p-CH ₃ C ₆ H ₄ Hg(SCN)) ₂ Co(NCS) ₂ Ni(C ₁₇ H ₁₆ N ₂ O ₂)	2180 (s)	760(s)	460(s)	290(m)	1560(s)	1380(m)
		2150 (w)	730(s)	445(s)	260(m)	1540(s)	1340(s)
9	(p-CH ₃ C ₆ H ₄ Hg(SCN)) ₂ Ni(NCS) ₂ Co(C ₁₇ H ₁₆ N ₂ O ₂)	2160(s)	755(s)	490(s)	275(s)	1555(s)	1380(s)
		2100 (sh)	720(s)	470(sh)	265(s)	1535(m)	1340(w)
10	(p-CH ₃ C ₆ H ₄ Hg(SCN)) ₂ Ni(NCS) ₂ Ni(C ₁₇ H ₁₆ N ₂ O ₂)	2160 (s)	760(s)	490(sh)	270(s)	1560(s)	1380(s)
		2100 (sh)	720(w)	450(s)	265(m)	1535(m)	1340(w)
11	(p-CH ₃ C ₆ H ₄ Hg(SCN)) ₂ Zn(NCS) ₂ Co(C ₁₇ H ₁₆ N ₂ O ₂)	2160 (s)	760(s)	470(s)	275(s)	1560(s)	1380(w)
		2100 (s)	720(s)	445(s)	260(s)	1540(s)	1340(s)
12	(p-CH ₃ C ₆ H ₄ Hg(SCN)) ₂ Zn(NCS) ₂ Ni(C ₁₇ H ₁₆ N ₂ O ₂)	2180 (s)	750(s)	465(s)	275(s)	1560(s)	1380(s)
		2190 (sh)	730(w)	440(s)	250(s)	1540(m)	1340(w)
13	(p-CH ₃ C ₆ H ₄ Hg(SCN)) ₂ Mn(NCS) ₂ Co(C ₁₇ H ₁₆ N ₂ O ₂)	2150(s)	750(s)	465(s)	275(s)	1550(s)	1380(s)
		2090 (s)	720(w)	440(w)	260(m)	1535(s)	1340(m)
14	[p-CH ₃ C ₆ H ₄ Hg(SCN)) ₂ Mn(NCS) ₂ Ni(C ₁₇ H ₁₆ N ₂ O ₂)	2100 (s)	760(s)	460(s)	270 (s)	1555(s)	1380(s)
		2000 (sh)	730(w)	440(w)	260(m)	1540(m)	1340(w)

TABLE 6: INFRA-RED SPECTRAL AND BAND ASSIGNMENTS OF THE COMPLEX

S. No.	Complex	ν (C-N) cm^{-1}	ν (C-S) cm^{-1}	δM (NCS) cm^{-1}	Molar Conductance $\text{cm}^2\text{mohs/mole}$	μ_{eff} (B.M.)
1	(C ₆ H ₅ HgSCN) ₂ Co(NCS) ₂	2180 (sh)	7810(sh)	460(s)	48.65	5.12
		2160 (s)	740(s)			
2	(C ₆ H ₅ HgSCN) ₂ Ni(NCS) ₂	2160(s)	820(sh)	460(sh)	53.65	3.22
			735(s)	460(s)		
3	(C ₆ H ₅ HgSCN) ₂ Zn(NCS) ₂	2160 (s)	780(m)	470(s)	49.05	4.25
		2100 (s)	730(s)			
4	(p-CH ₃ C ₆ H ₄ HgSCN) ₂ Co(NCS) ₂	2110 (sh)	780(sh)	460(w)	62.40	5.10
		2080 (s)	760(s)	450(m)		
5	(p-CH ₃ C ₆ H ₄ HgSCN) ₂ Ni(NCS) ₂	2150 (s)	780(s)	470(s)	58.54	3.10
			750(sh)	460(sh)		
6	(p-CH ₃ C ₆ H ₄ HgSCN) ₂ Zn(NCS) ₂	2140(sh)	800(m)	460(m)	56.42	4.20
		2100 (s)	760(m)	440(m)		
7	(p-CH ₃ C ₆ H ₄ HgSCN) ₂ Mn(NCS) ₂	2155 (sh)	760(sh)	480(w)	48.54	7.86
		2100 (s)				

TABLE 7: INFRA-RED SPECTRAL AND BAND ASSIGNMENTS, MAGNETIC MOMENT AND MOLAR CONDUCTANCE OF THE COMPLEX

S. No.	Complex	μ -eff (B.M.)	Molar Conductance $\text{cm}^2\text{mhos/mole}$	Molecular Weight		β
				Cal.	Obs.	
8	$(p\text{-CH}_3\text{C}_6\text{H}_4\text{HgSCN})_2\text{Co}(\text{NCS})_2\text{Ni}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	5.07	63.40	1212.82	1190	0.94
9	$(p\text{-CH}_3\text{C}_6\text{H}_4\text{HgSCN})_2\text{Ni}(\text{NCS})_2\text{Co}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	2.96	57.52	1212.82	1190	0.86
10	$(p\text{-CH}_3\text{C}_6\text{H}_4\text{HgSCN})_2\text{Ni}(\text{NCS})_2\text{Ni}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	3.06	44.54	1212.60	1195	0.84
11	$(p\text{-CH}_3\text{C}_6\text{H}_4\text{HgSCN})_2\text{Zn}(\text{NCS})_2\text{Co}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	4.18	48.00	1219.40	1190	-
12	$(p\text{-CH}_3\text{C}_6\text{H}_4\text{HgSCN})_2\text{Zn}(\text{NCS})_2\text{Ni}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	3.16	57.08	1219.26	1192	-
13	$(p\text{-CH}_3\text{C}_6\text{H}_4\text{HgSCN})_2\text{Mn}(\text{NCS})_2\text{Co}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	8.02	64.63	1209.05	1190	-
14	$(p\text{-CH}_3\text{C}_6\text{H}_4\text{HgSCN})_2\text{Mn}(\text{NCS})_2\text{Ni}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	7.88	59.10	1208.33	1195	-

s= strong, sh=shoulder, m=medium, w=weak

TABLE 8: SELECTED ELECTRONIC BANDS AND SPECTRAL PARAMETERS OF THE COMPLEX

S. No.	Complex	$\nu_3 \text{ cm}^{-1}$	$\nu_2 \text{ cm}^{-1}$	$\nu_1 \text{ cm}^{-1}$	Dq	B'	β
1	$(\text{C}_6\text{H}_5\text{HgSCN})_2\text{Co}(\text{NCS})_2$	16050	8179	-	483	649	0.68
2	$(\text{C}_6\text{H}_5\text{HgSCN})_2\text{Ni}(\text{NCS})_2$	27730	16646	10406	1017	904	0.86
3	$(p\text{-CH}_3\text{C}_6\text{H}_4\text{HgSCN})_2\text{Co}(\text{NCS})_2$	16246	8238	-	486	595	0.69
4	$(p\text{-CH}_3\text{C}_6\text{H}_4\text{HgSCN})_2\text{Ni}(\text{NCS})_2$	26363	16127	10047	1005	822	0.80

TABLE 9: SELECTED ELECTRONIC BANDS AND SPECTRAL PARAMETERS OF THE COMPLEXES

S. No.	Complex	$\nu_3 \text{ cm}^{-1}$	$\nu_2 \text{ cm}^{-1}$	$\nu_1 \text{ cm}^{-1}$	Dq	B'	β
1	$(\text{C}_6\text{H}_5\text{HgSCN})_2\text{Co}(\text{NCS})_2\text{Co}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	22245	15182	9963	881	731	0.72
2	$(\text{C}_6\text{H}_5\text{HgSCN})_2\text{Co}(\text{NCS})_2\text{Ni}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	21836	15912	10408	721	863	0.85
3	$(\text{C}_6\text{H}_5\text{HgSCN})_2\text{Ni}(\text{NCS})_2\text{Co}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	24272	16363	10670	951	690	0.68
4	$(\text{C}_6\text{H}_5\text{HgSCN})_2\text{Ni}(\text{NCS})_2\text{Ni}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	25540	16155	10532	1051	847	0.81
5	$(p\text{-CH}_3\text{C}_6\text{H}_4\text{HgSCN})_2\text{Co}(\text{NCS})_2\text{Co}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	22073	18023	9534	892	996	1.01
6	$(p\text{-CH}_3\text{C}_6\text{H}_4\text{HgSCN})_2\text{Co}(\text{NCS})_2\text{Ni}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	21064	18022	9708	891	896	0.90
7	$(p\text{-CH}_3\text{C}_6\text{H}_4\text{HgSCN})_2\text{Ni}(\text{NCS})_2\text{Co}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	27247	17066	10210	993	897	0.85
8	$(p\text{-CH}_3\text{C}_6\text{H}_4\text{HgSCN})_2\text{Ni}(\text{NCS})_2\text{Ni}(\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2)$	27533	16902	10252	1040	857	0.81

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