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Study of Cu (II), Ni (II) and CO (II) coordination compounds with nitrogen and oxygen

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Abstract
In this paper the calculation of the edifices have been explained in the light of molar mass, natural investigation, IR, electronic Spectra, molar conductance and attractive powerlessness. The deliberate molar conductance esteem shows that the buildings are non-electrolytic in nature. The above perception shows that Schiff bases EHPQH carry on as bidentate ligand and coordination proposes through azomethine N and oxygen particle of alcoholic gathering of ligand. The calculation of the Co (II) and Ni (II) were proposed to be octahedral in math while Cu (II) edifices were proposed to be misshaped octahedral. The Schiff bases and its edifices have been assessed for their antibacterial movement. The edifices show improved antibacterial movement than ligand. We have promoted us synthesized complexes of CO(II),Ni(II) and Cu(II) with Schiff base ligand, 2-propyl-thioquinazolin 4(3H) Semicarbazones are used as ligands in coordination chemistry and are biologically active compounds.

Keywords: coordination, complexes, compounds, oxygen, Ni (II)

Introduction

The direct use to transition metal salts as antimicrobial agent cannot be recommended as they are very toxic to host human being. It has been provide from the survey of literature that the biologically active compound show greater activity when administered as metal complexes than as a free organic compounds. Semicarbazones are used as ligands in coordination chemistry and are biologically active compounds [1, 3].

Their complexation with different metal enhances the bioactivity of these molecules. These metal based complexes have attached considerable interest in chemical and biological studies due to their potentially beneficial biocidal activity which may be attributed to formation of their chelates with metal ion [4, 10]. Such promising biological potentials of Schiff base and its metal complexes as well as in continuation of our earlier research work [11] in this field we have prompted as synthesized complexes of Co(II), Ni(II) and Cu(II) with Schiff base ligand, 2-proply-thioquinazolin 4(3H) semicarbazone.

Materials and Methods

All reagents were of analytical reagent grade. The metal contents of all the complexes were analysed using standard procedure. The infrared spectra of the ligand and metal complexes in the region 200-4000cm^{-1} were recorded on Perking Elmer -577 spectrophotomer. The electronic spectra were recorded on Cary-2390 spectrophotometer in the 10000-25000 cm^{-1} and magnetic susceptibility was measured using Gouy balance using mercury tetraisothiocyanto cobaltate as a calibrant. The molar conductivity was measured on Systronics Conductivity Meter model 303 using DMF as a solvent.

Preparation of the Ligand: A mixture of 2-propyl thioquinazoline 4(3H) one (5m mol) and semicarbazide hydrochloride (5m mol) was refluxed for 1 h. After cooling, the mixture was poured into distilled water (200 ml) white precipitate were filtered and rescrystallised from ethanol. m.p.; 311±1^{0}C.

Synthesis of Metal Complexes: The complexes were prepared by reacting respective halide/nitrate of Co (II), Cu (II) and Ni (II) in ethanoic medium with the ethanolicsolution of the ligand, 2-propyl thioquinazoline 4(3H) Semucarbazone in molar ratio 1:2. The resulting reaction mixture was refluxed on water bath for 3-4h. The procedure carried out in each case was similar with slight variation of timing of reflux. On cooling solid coloured complexes separated out which were litered, washed with ethanol, dried and recrystallised.

Result and Discussion

Infrared Spectra: The mode of band formation in complexation between ligand and metal ions can be effectively determined by the Infrared spectral data (Table 2).

The IR spectrum of the ligand PTQS exhibit strong and broad band at 3200 cm^{-1} assigned to V_{N-H}. In the spectra of the complexes, this band is unaffected which indicates non-involvement of either primary amino or secondary amino group in the coordination IR spectrum of the ligand exhibit strong and broad band at 1640 cm^{-1} assigned$^{1-5}$ $V_{C=O}$. In the spectra of the complexes, this band has shifted to a lower frequency region with slightly reduced intensity. The shift of the band and change in intensity proposes co-ordination of the carbonyl oxygen with metal ions. This is further confirmed on the basis of occurrence of a far IR region band of the complexes at 540-510 cm^{-1} assigned to$_{M-O}$. The absorption bands around 1460cm^{-1} are designated to the azomethine group. In the complexes, the frequencies of azomethine group appear mostly towards the lower region. The linkage of azomethine nitrogen with metal ion is further supported by the appearance of another far IR band at 440-

405 cm^{-1} assigned to V_{M-N}. The above IR spectra data indicates that ligand coordinate to the metal through the carbonyl oxygen and azomethine nitrogen. The evidence of metal halogen linkage is confirmed by the appearance of a band in the region 320-270 cm^{-1} assigned to V_{M-X} (X=CI, Br and I). The evidence of metal halogen linkage is further confirmed by the low value of molar conductance of the complexes on the range 1.8-7.9 ohm^{-1} cm^2 mol^{-1}. Nitrate complexes show bands in the region 1340-1375 cm^{-1} and 800-825 cm^{-1} due to ionic nitrate and bands at 1025-1040 cm^{-1} can be assigned to coordinated nitrate group. Appearance of bands at 1360-1440 cm^{-1} confirms the monodentate coordination mode of the nitrate group.

Electronic Spectra and Magnetic Susceptibility of the Complex: The electronic spectra of all the complexes have been recorded in the region 10000-25000cm^{-1}. The electronic spectral and magnetic susceptibility data as shown in Table-2 suggest octahedral geometry of the complexes.

Conductivity measurement: Mole conductance values of the complexes of Co (II), Ni (II) and Cu (II) were found to be in the range. 1.8-7.9 ohm^{-1} cm^2 mol^{-1} in DMF proposes their non-electrolytic nature. The molar conductance value also supported the structure assigned on the basis of physiochemical and spectroscopic measurement.

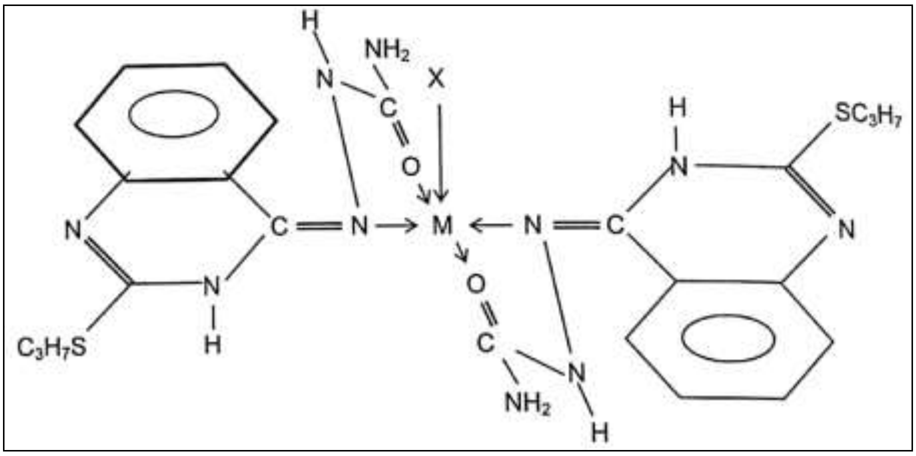
Table 1: Analytical, electronic and molar conductance measurements

Compounds (Colour)	**Molar Mass**	**% Analysis found (Calculated)**				**μ_{eff} B.M.**	**Ωmohm^{-1} cm^2 mol^{-1}**	**DT ^{0}C**	**λmax electronic cm^{-1}**
		M	C	N	H				
PTQS Colourless	278		51.62 (51.79)	25.04 (25.17)	5.69 (5.75)				
$[Co(PTQS)_2Cl_2]$ Brown	685.93	8.50 (8.59)	40.79 (41.98)	20.28 (20.41)	4.61 (4.66)	5.1	3.3	1.89	20800
$[Co(PTQS)_2Br_2]$ Brown	774.75	7.51 (7.60)	36.98 (37.17)	17.96 (18.07)	4.07 (4.13)	4.96	3.1	193	20730
$[Co(PTQS)_2I_2]$ Brown	868.73	6.70 (6.78)	32.97 (33.15)	16.02 (16.11)	3.64 (3.68)	4.92	2.6	198	21080
$[Co(PTQS)_2(NO_3)_2]$ 20300 Brown		738.93 (7.97)	7.89 (38.97)	38.71 (18.94)	18.82 (4.33)	4.29	4.99	1.8	201
$[Ni(PTQS)_2Cl_2]$ Yellowish red	685.71	8.50 (8.56)	41.83 (42.00)	20.28 (20.41)	4.60 (4.66)	3.04	4.7	204	11600. 15400, 23100
$[Ni(PTQS)_2Br_2]$ Yellowish red	774.53	7.49 (7.58)	36.96 (37.18)	17.98 (18.07)	4.08 (4.13)	3.08	4.9	211	11200, 15100, 23600
$[Ni(PTQS)_2I_2]$ Yellowish red	868.51	6.69 (6.75)	32.94 (33.16)	15.97 (16.11)	3.60 (3.65)	3.02	5.3	217	11480, 15300, 2800
$[NI(PTQS)_2(NO_3)_3]$ Yellowish red	738.71	7.87 (7.94)	38.70 (38.98)	18.80 (18.95)	4.28 (4.33)	3.11	6.8	223	12060, 15600, 23100
$[Cu(PTQS)_2Cl_2]$ Yellowish red	690.54	9.13 (9.20)	41.52 (41.70)	20.14 (20.27)	4.58 (4.63)	1.98	7.3	179	13080, 18900
$[Cu(PTQS)_2Br_2]$ Yellowish red	7798.36	8.08 (8.15)	36.86 (36.95)	17.85 (17.96)	4.06 (4.10)	1.93	7.7	186	13400, 18200
$[Cu(PTQS)_2\ (NO_3)_2]$ 13380, 18600 Yellowish red		743.54 (8.54)	8.48 (38.73)	38.60 (18.82)	18.17 (4.30)	4.25	1.89	7.9	189

Table 2: Analytical, electronic and molar conductance measurements

Compounds	**$V_{C=O}$**	**$V_{C=N}$**	**V_{M-O}**	**V_{M-N}**	**V_{M-X}**
PTQS	1440 s,b	1480 s,b	530 m	225 m	285 m
$[Co(PTQS)_2Cl_2]$	1620 m.b	1460 m.b	540 m	420 m	295 m
$[Co(PTQS)_2Br_2]$	1615 m.b	1455 m.b	535 m	435 m	305 m
$[Co(PTQS)_2I_2]$	1610 m.b	1450 m.b	530 m	440 m	310 m
$[Co(PTQS)_2(NO_3)_2]$	1620 m.b	1455 m.b	535 m	430 m	275 m
$[Ni(PTQS)_2Cl_2]$	1610 m.b	1455 m.b	540 m	440 m	280 m
$[Ni(PTQS)_2Br_2]$	1620 m.b	1455 m.b	525 m	410 m	275 m
$[Ni(PTQS)_2I_2]$	1610 m.b	1450 m.b	510 m	420 m	280 m
$[NI(PTQS)_2(NO_3)_3]$	1610 m.b	1455 m.b	520 m	415 m	270 m
$[Cu(PTQS)_2Cl_2]$	1610 m.b	1460 m.b	525 m	410 m	280 m
$[Cu(PTQS)_2Br_2]$	1610 m.b	1460 m.b	530 m	405 m	300 m
$[Cu(PTQS)_2\ (NO_3)_2]$	1620 m.b	1450 m.b	530 m	425 m	320 m

s = trong; m = medium; b = broad



M = Co (II), Ni (II); X = Cl$^-$, Br$^-$, I$^-$ and No$_3^-$
M= Cu (II); X = Cl–, Br$^-$ and No$_3^-$

Fig 1: [M (MTQS)$_2$]

Conclusion

Thus on the basis above studies it is concluded that the ligand PTQ S acts in a bidentate manner and coodination is proposed through azornethine N and carbonyl oxygen of Semicarbozone moiety. The remaining centre of the metal ion is satisfied by negative ions such as Cl, Br, I or NO_3. The geometry of the Co (II), Cu (II) and Ni (II) complexes are proposed to be octahedral in nature as shown in Fig.1

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