4-NN-Bis-2'- Cyanoethyl Amino Benzaldehyde And 2-Methyl-4-Nn-Bis-2'- Cyanoethyl Amino Benzaldehyde And Aniline

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Abstract:
Schiff bases formed by different aldehydes are in wide use for the synthetic purpose in both organic synthesis and in co-ordination chemistry of metal complexes. These are reported as stable compounds which are in use as a ligand for synthesis of various complexes. Schiff bases formed by Aniline and Aldehydes (4-NN-BIS 2'-cyanoethylaminobenzaldehyde and 2-Methyl-4-NN-BIS 2'-cyanoethylaminobenzaldehyde) have been reported to form stable complexes with metals. Experimental data for some of these Schiff bases are available. The theoretical studies were done for Schiff bases formed by is Aldehydes with varying amines to locate and confirm the site for co-ordination of the compounds to metal on the basis of electronics structure of the Schiff bases. In the recent years it has been shown that Ab initio quantum chemical methods[1-2] which utilize the SCF approach within the Hartee - Fock- Roothan[3] approximation are limited in their practical approach as they require calculation of a very large number of many centre integrals. It is the most common requirement is to locate the bonding site, with which the metal ion will react. In this regard, the net atomic charge and the atomic electron density become useful parameter to look for the co-ordination site of a ligand and the stability of the complex. Schiff base ligands (I-II) used for complex formation were synthesized in laboratory.

Key words : Aldehyde, Aniline

I. 4-NN-bis-2'-cyanoethylaminobenzylideneaniline [4-CABAB]
II. 2-Methyl-4-NN-bis-2'-cyanoethylaminobenzylideneaniline. [2-MCABAB]

Preparation of Schiff bases :[4]
The structures of Schiff bases are shown in Fig. 1.
Physical characteristics of the Schiff base ligands are listed in Table1.

Table 1: Physical Characteristics of the Schiff bases

Schiff bases	State	Melting point (°C)	Colour	Yield
I	Solid	160	Yellow	90%
II	Solid	140	Yellow	80%

Mass spectral studies of the Schiff base ligands chosen and prepared for complex formation, were performed successfully. Molecular weight of the ligands have been confirmed from the parent peaks in their mass spectra. Parent peaks in the mass spectra of the ligands appearing at m/e 317 and 250 for 4CABAB and 2MCABAB respectively. Infra red absorptions of the Schiff bases used in this investigation have been assigned by the comparison of the spectra with those already reported by others [5] along with mono-substituted benzene ring system . The observed bands and their corresponding assignments are listed in Table2.

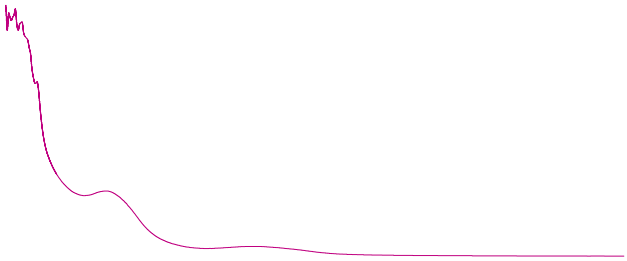
Table2. Infrared absorption frequencies (cm^{-1}) of (2MCABAB) and (4CABAB)

Assignments	2MCABAB	4CABAB
C = N stretching azomethine	1597_s	1593_s
Ring stretching N – Phenyl stretching	1367_s 1319_{sh}	1351.6_m 1315w
Ring breathing of benzene	1174.5_s 993_w	1158_m 933w
Ring breathing and deformation	1520_m 1013_w	1593_m 1053w
C – N – C bending	 816_m	- 820w

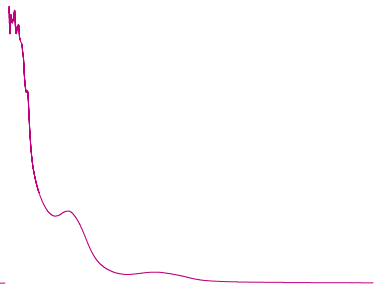
Out of plane ring deformation	763m	776_w
Out of plane bending of mono substituted benzene	603_w	602.9_w
$_V$(Th – N) Metal – ligand vibration	-	-

Electronic Spectral Studies[6-11].

Schiff base	**n π^***	**π π^***	**O-U-O absorption/ metal-N absorption**
4CABAB	230nm	327 nm	-
2MCABAB	240nm	270nm	



UV Spectra of 4CABAB



Spectra of 2MCABAB UV

N.M.R. Spectral Studies :

The N.M.R. spectral studies of some of the representative Schiff bases are done and these were compared with the NMR Spectra of corresponding ligands. N.M.R. spectra were recorded on Bruker AC 300 F NMR spectrophotometer at 300 MHz using solvents $CDfCI_3$ and $DMSOCL_6$ and were found to be in good agreement with reported observations [12]. NMR spectra of 2MCABAB contains important signals at 2.66373-2.71691, 3.84416-3.91053 (qt.), 6.50835-6.48079 (d), 6.587-6.56265 (d), 6.74529-6.71611 (d), 7.06031-6.98521 (qt), 7.28943-7.23769 (qt), 7.854827-8.0235 (t), 8.34442 (s), 9.82036 (s), and N.M.R. spectra of 4CABAB contains the important signals at 1.42853-1.3354 (pt), 2.73698-2.69401 (t), 3.93494-3.85122, 4.41757-4.30213, 6.65081-6.62248 (d), 6.76639-6.72974 (qt), 7.26142-7.18877 (t), 7.88527-7.81327 (pt), 8.07951-8.05128 (d), 8.33554 (s), and 9.82996 (s).

CONCLUSION :The quantum chemical calculation can be successfully used to prodict the stability of the complex and making more active ligands, used for complex formation which may be work of interest for co-ordination and bioinorganic chemists, as it is discussed here for a schiff bases. For any ligand, to be used for stable complex formation, it is the most common requirement is to locate the bonding site, with which the metal ion will react. In this regard, the net atomic charge and the atomic electron density become useful parameter to look for the co-ordination site of a ligand and the stability of the complex.

REFERENCES

1. W.G.Richards, T.E.H. Walker, and R.K. Hinkley "A bibilography of Ab-initio molecular wave functions", Clarendon Press, Oxford (1971)
2. L.Random and J.A.Pople, *MTP International Reviews of Science, Physical Chemistry,* 1, Serie3s 1, Ed. W. Byers-Brown, Butterworths, London 71, (1972)
3. I.L. Lavine, Quantum Chemistry, 4th Ed., (1991)
4. A.R. Khan, SYNTHESIS,SPECRAL AND THERMAL STUDIES OF Th(IV)AND DIOXOURANIUM(VI) COMPLEXES WITH NITROGEN DONOR LIGANDS, Ph.D. Thesis Jiwaji University Gwalior (2003).
5. R.K. Agarwal, K. Arora, Priyanka and I. Chakravorti, Polish J. Chem. 67, 1913 (1993)
6. K. Arora, "Physico chemical investigations of some high Coordination Compounds of thorium (IV) and dioxouranium (VI) with some oxygen and nitrogen donor ligands" Ph.D. Thesis Meerut University (1992).
7. R.C. goyal, "Physico chemical investigations of some schiff base compounds of thorium (IV) and dioxouranium (VI)" Ph.D. Thesis, Jiwaji University (2000).
8. K. Arora, "Physico chemical investigations of some high Coordination Compounds of thorium (IV) and dioxouranium (VI) with some oxygen and nitrogen donor ligands" Ph.D. Thesis Meerut University (1992).
9. .K.Aruna , Sakina Bootwala, Mobashshera Tariq, Christopher Fernandes and Sachin Somasundaran IJPSR, 5, (2), 400-409 (2014).

10. Sonal Agnihotri and Kishore Arora, CODEN EC JHAO, 7 (3, 1045-1054, (2010).
11. P.K.Verma,A.Bhattacharya,A.K. Yadav,S.N.Jha New J.Chem.42, 5243-5255, (2018).
12. Narendra Sharma and Naveen Kumar Singh Volume 7 Issue 1, Page 13-271 April (2022).