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Simulation of IR Spectra of Some Organic Compounds-A Review

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Abstract: *In the present review a discussion of simulation of IR spectral studies of some organic compound is presented. This review contains 80 references.*

I. Introduction

Infrared spectroscopy (IR spectroscopy) is the branch of spectroscopy that deals with the infrared region of the electromagnetic spectrum, that is light with a longer wavelength and lower frequency than visible light. It covers a range of techniques, mostly based on absorption spectroscopy. As with all spectroscopic techniques, it can be used to identify and study chemicals. A common laboratory instrument that uses this technique is a Fourier transform infrared (FTIR) spectrometer.

The infrared portion of the electromagnetic spectrum is usually divided into three regions; the near-, mid- and far- infrared, named for their relation to the visible spectrum. The higher-energy near-IR, approximately 14000–4000 cm^{-1} (0.8–2.5 μm wavelength) can excite overtone or harmonic vibrations. The mid-infrared, approximately 4000–400 cm^{-1} (2.5–25 μm) may be used to study the fundamental vibrations and associated rotational-vibrational structure. The far-infrared, approximately 400–10 cm^{-1} (25–1000 μm), lying adjacent to the microwave region, has low energy and may be used for rotational spectroscopy. The names and classifications of these sub regions are conventional, and are only loosely based on the relative molecular or electromagnetic properties.

Infrared (IR) spectroscopy is one of the most common spectroscopic techniques used by organic and inorganic chemists. Simply, it is the absorption measurement of different IR frequencies by a sample positioned in the path of an IR beam. The main goal of IR spectroscopic analysis is to determine the chemical functional groups in the sample. Different functional groups absorb characteristic frequencies of IR radiation. Using various sampling accessories, IR spectrophotometers can accept a wide range of sample types such as gases, liquids, and solids. Thus, IR spectroscopy is an important and popular tool for structural elucidation and compound identification.

It is useful to divide the infra red region into three sections; near, mid and far infra red;

Region	**Wavelength range (mm)**	**Wave-number range (cm^{-1})**
Near	7.78-2.5	12800-4000
Middle	2.5-50	4000-200
Far	50-1000	200-10

Computational chemistry may be defined as the application of mathematical and theoretical principles to the solution of chemical problems. Molecular modeling, a subset of computational chemistry, concentration on predicting the behavior of individual molecules within a chemical system. The most accurate molecular models use an initio or (first principles) electronic structure methods, based up on the principles of quantum mechanics, and generally vary computer- intensive. However, due to advances in computer storage capacity and processor performance, molecular modeling has been a rapidly evolving and expanding field, to the point that it is now possible to solve relevant problems in an acceptable amount of time. Electronic structure calculations provide useful estimates of the energetic properties of chemical systems, including molecular structures, spectroscopic features and probable reaction pathways.

II. IR Spectral Study Related To Schiff Bases

A Schiff base, named after Hugo Schiff, is a compound with a functional group that contains a carbon-nitrogen double bond with the nitrogen atom connected to an aryl or alkyl group, not hydrogen. Schiff bases in a broad sense have the general formula $R_1R_2C=NR_3$, where R is an organic side chain. In this definition, Schiff base is synonymous with azomethine. Some restrict the term to the secondary aldimines (azomethines where the carbon is connected to a hydrogen atom), thus with the general formula RCH=NR'.

Raafal et.al have been reported the IR spectra of Schiff Bases derived from 2- Amino-3 Hydroxypyridine and 2- Amino- 3 Hydroxypyridine in organic solvent of different polarities and disscissed the result by some molecular orbital calculation using the ASED- MO Theory for Schiff bases(1). A.Kulandaismy

et.al have been prepared low molecular weight low symmetric complex of blue copper protein and characterized by H-NMR, IR, EPR Spectral study and indicated that the ligand act as monovalent tridentate chelating agent (2). A. Nagajothi et.al have been synthesized tetra-dentate CO(II) Schiff base complexes add predict octahedral geometry for all complexes and the metal complexes have been screened for their antibacterial and antifungal activity(3). S Priyarega et.al have been Synthesized six different ruthenium(III) complexes of Schiff bases characterized by infrared, electronic, electron paramagnetic resonance spectroscopy .Spectroscopic investigation reveals coordination of Schiff base ligand through ONO/ONS donor atoms and octahedral geometry around ruthenium metal(4).

Iran Sheikhshoaie were synthesized multifunctional Schiff base ligands :-2-{(E)-[(2-hydroxypropyl)imino]methyl}phenol L1, 3-{(E)-[(2-hydroxypropyl)imino]methyl}-2-naphthol L2, 2-[(E)-{[(2R)-2-hydroxypropyl]imino}methyl]-4-[(E)-phenyldiazenyl]phenol L3,2-[(E)-{[(2R)-2-hydroxypropyl]imino}methyl]-4-[(E)-(4-nitrophenyldiazenyl)]phenol L4 These Schiff base compounds have been characterized by C, H, N elemental analysis, FT-IR, UV-Vis, and 1H NMR spectroscopy(5).

Beata Cristovao has been synthesized mononuclear copper(II) and nickel(II) complexes as microcrystalline powders and characterized by IR spectroscopy The magnetic susceptibility of the Cu(II) complexes changed with temperature according to the Curie–Weiss law. The magnetic moment values do not change with lowering the temperature(6). Jimmy S. Hwang have been Synthesiszed and EPR characterization of a vanadyl complex salicylaldehyde Schiff base in methylene chloride. The magnetic parameters for this system are determined from computer simulation. A good correlation is found between g| and A| of the system studied when compared with other model compounds of vanadyl complexes(7). A.S.P. Azzouz eight Schiff bases , derived for salicylaldehyde and o-methoxybenzaldehyde with aromatic amines. The presence of hydrogen bondings in imines , are identified by using UV and IR spectra. The study led to a conclusion that imines under investigation , are exist as an equilibrium mixtures of enol and keto forms in 1,2- dichloro ethane (8).

Adnan dib synthesized schiff bases derived from acetylacetone and characterized by IR, ^{1}H NMR , ^{13}C NMR and element analysis. Hyper Chem-6 program has been used to predict structural geometries of compounds in gas phase. The heat of formation (ΔHf °) and binding energy (ΔEb) at 298 ºK for the free ligand was calculated by PM3 method(9-10).

A. M. Hamil synthesized a new Schiff base 2-[2-(E)-(2-hydroxyphenyl)ethylidene]aminoethyl) ethan-imidoyl]phen was via the reaction of 2-hydroxyacetophenone with ethylene-diamine and investigated by CHN elemental analyses, infrared, proton nuclear magnetic resonance, ultraviolet and mass spectroscopy(11). Salem Et. Ashoor synthesized Schiff bases complexes and characterized using elemental study IR and UV spectroscopy. Electric conductivity also did prove to be useful use for conductively of these complexes via using Ohm`s equation also optimization of these complexes were tested by using Hyper-Chem. release 7.5 for simulation the complexes were shown the total energy of them. These complexes were tested in antibacterial studies(12).

Mendu Padmaja synthesized a series of Cu(II) , Ni(II) , Co(II) , Mn(II) and Zn(II) complex. The nature of bonding and geometry of the transition metal complexes as well as ligand L have been deduced from elemental analysis, FT-IR, UV-Vis, ^{1}HNMR, ^{13}CNMR. The biological activity of the ligand and its complex. and found that the metal chelates are more active than the free schiff base ligand(13). S. Ali Beyramabadia synthesized three N,N_-dipyridoxyl Schiff bases and characterized by IR, ^{1}H NMR, mass spectrometry. The theoretical results and experimental evidence confirms suitability of the optimized geometries for the synthesized Schiff bases(14). A. Nagajothi et.al have been derived Fe(III) complexes from Schiff base ligands. The complexes were characterized by elemental analyses, molar conductance, magnetic susceptibility, IR, UV-Vis spectral data.The possible geometries of metal complex were evaluated using 3D molecular modelling picture. The metal complexes have been screened for their antibacterial and antifungal activity(15). A. Nagajothi et.al have been synthesized Tetradentate N2O2 type complexes of Co(II). The complexes were characterized by elemental analyses, molar conductance, magnetic susceptibility, IR, UV-Vis spectral data, From the spectral datas an octahedral geometry has been proposed for all the complexes and have been screened for their antibacterial and antifungal activity (16).

Muhanned Jawad, Kadhim Al-Assadi have been synthesized Schiff base ligand and their Ni^{2+} and Cu^{2+} complexes .The ligand and their complexes were identified by FTIR, UV and CHN. The electrical properties for preparing compounds were studied before and after doping with I_2 (17). Bulent Dede et.al have been synthesized homo- and hetero polynuclear copper(II) complexes of N,N″-bis[1-biphenyl-2-hydroxyimino-2-(4-acetylanilino)-1-ethylidene]-diamines. and characterized by different physical techniques. The free ligands were also characterized by ^{1}H- and ^{13}C-NMR spectra. Elemental analyses, stoichiometric and spectroscopic data of the metal complexes indicated that the metal:ligand ratio of dinuclear copper(II) complexes were found to be 2 : 1 while this ratio was 3 : 2 in trinuclear copper(II) complexes(18). N RAMAN et.al have been synthesized a new Schiff base chelates of Cu(II), Co(II), Ni(II) and Zn(II) derived from benzil-2,4-dinitrophenylhydrazone with aniline .Microanalytical data, molar conductance, and magnetic susceptibility values have been obtained, and

IR, ^{1}H NMR, ^{13}C NMR, UV-Visible, and EPR spectral studies have been carried out to suggest tentative structures for the complexes (19).

H. S. SELEEM et.al have been synthesized three Schiff-base hydrazones (ONN – donors). The structures of these ligands were elucidated by elemental analysis, UV, IR, ^{1}H-NMR and mass spectra(20). V. K. SHARMA, have been prepared a series of octahedral Ru(III), Rh(III) and Ir(III) complexes with tetradentate Schiff bases derived by condensing isatin with 1,2-diaminoethane, 1,3-diaminopropane, 1,4-diaminobutane, 1,2-diaminobenzene and 1,3-diaminobenzene. The IR spectral data revealed that all the Schiff bases behave as tetradentate and are co-ordinated to Ru(III), Rh(III) and Ir(III) via nitrogen and oxygen. Antifungal studies of the ligands as well as their complexes were carried out by the agar plate method(21).

Suman Malik et.al have been synthesized a Schiff base of 5-acetamido-1,3,4-thiadiazole--2-sulphonamide, Using a bidentate ligand, complexes of transition metals having the general formula ML2,where M = Mn(II), Fe(II), Ni(II) and Cu(II), were synthesized. The complexes were characterized by elemental analysis, molar conductivity, magnetic moment, electronic, ESR and IR spectroscopy revealed an octahedral geometry for all the complexes(22). K. Mounika, et.al have been synthesized Metal complexes of the Schiff base from nitrate/chloride salts of Ni(II), Co(II), Cu(II) and Zn(II) in an alcoholic medium. The chemical structures of the Schiff-base ligand and its metal complexes were confirmed by various spectroscopic studies like IR, UV-Visible , ^{1}H NMR, and suggested ligand acts as neutral and tridentate. The free Schiff base and its complexes have been tested for their antibacterial as well as antifungal activity(23).

K. Krishnankutty et.al have been synthesized two new Schiff bases containing olefinic linkages by condensing ortho-substituted aromatic amines with dicinnamoylmethane under specified conditions. The existence of these compounds predominantly in the intramolecularly hydrogen bonded keto-enamine form has been well demonstrated from their IR, ^{1}H NMR and mass spectral data(24). Nabil M. El-Halabi was prepared Schiff base by condensation reaction of salicylaldehyde with 4-amino-2-(4-chlorophenyl)-5-methyl-2H-1,2,3,6-oxatriazine 3 in refluxing ethanol. Square planar complexes of Ni(II), Pd(II) and Cu(II) 6a-c of Schiff base were obtained from their reaction with $M(OAc)_2$ in a 2:1 mol ratio in refluxing ethanol for 4 hours. The new compounds were characterized by elemental analysis, IR, ^{1}H NMR, ^{13}C NMR spectra(25).

Abdalla M. Khedr were derived New mono- and binuclear copper(II) complexes with Schiff bases from the condensation of 2-amino-5-substituted-aryl-1,3,4-thiadiazole with substituted aryl aldehydes The conductivity data of the complexes confirmed their non-electrolytic nature. An octahedral,square planer & pyramidal square planer geometry was suggested for complex. The 3D molecular modeling of a representative complex was carried out on a CS Chem 3-D Ultra Molecular Modeling and Analysis Program (26). Muneerah M. Al-Mogren was prepared novel dioxocyclodiphosph(V)azane of o-aminopyridine and their coordinating behavior towards the transition metal ion Cu(II) was studied (27).

K. Krishnankutty et.al have been yield a new series of polydentate Schiff base ligands. In the metal complexes of the Schiff base of p-phenylenediamine, the intramolecularly hydrogen bonded hydrazone protons are replaced by the metal ions(28). Aurel PUI, deals with the synthesis and characterization of some complex compounds of uranium (VI) with different symmetrical Schiff bases The obtained results suggest the fact that the coordination number of uranium (VI) in these complexes is 7. The formation of the U(VI) complexes with such Schiff bases opens new ways for the extraction of uranium from ores or different solutions in order to use it as nuclear fuel(29). Thavuduraj Kavitha1,et.al have been Synthesized and characterized Neutral tetradentate N_2O_2 complexes of Cu(II), Ni(II), Co(II), Zn(II) and VO(II). The IR, UV-Visible., magnetic susceptibility measurements and EPR spectral data of the complexes suggest that all the complexes are square planar geometry around the central metal ion except VO(II) complex which has square pyramidal geometry (30). K. P. Srivastava et.al developed Schiff bases as new ligands using condensation of 2-aminonicotinic acid with salicyldehyde, 5-nitrosalicyldehyde, 5-bromosalicyldehyde and 5-methoxysalicyldehyde All the Schiff bases were tridentate (NNO donor) ligands that were used for complexation with $CO^{2+,}$ Ni^{2+} and Zn^{2+} ions their metal complexes were characterized by analytical and spectral methods (31). Zeynep Munteha Sahin et.al successfully synthesized two-armed poly(-caprolactone) (TAPCL) polymers via the ring opening Polymerization. The synthesized TAPCL polymers were characterized by GPC, FTIR, UV–visible, and electron paramagnetic resonance (EPR) (32).

Rishipal Singh et.al have been Synthesized a schiff base from the condensation of coumarin derivative and α-amino acids. The prepared Schiff base react with La(III) ,Ce (III) and Pr (III) nitrate to give the complexes with steoichiometric ratio (1:1) .The complexes have been characterized by elemental analysis, molar conductance, electronic , IR and NMR spectral techniques ,Which indicates ligand show tridentate nature on co-ordination with metal ions (33). Islam A Patel & Bharat T Thakar have been prepared Mn(III) Schiff bases complexes and studied their physic-chemical properties. They behave as monoelectrolyte in solution,indicating non coordinating nature of anion.On the basis of analytical and physical data tetragonally distorted octahedral structure is suggested for all complexes (34). Averi Goha et.al have been synthesized and characterized Schiff

base complexes of Zn(II) & Cd(II).Electronic and Photoluminescence spectral property of complex as well as the free ligand have been investigated and DFT study has been perform to rationalize the spectral behaviour (35).

Taghreed H. Al-Noor, synthesized and characterized the tridentate Schiff base containing (N and O) as donor atoms type (ONO). Products were found to be solid crystalline complexes. The magnetic moment coupled with the electronic spectra suggested an octahedral geometry for all the complexes (36). Najia A. El-hassy1 et.al have been synthesized Schiff base of salicylaldehyde and 2-aminobenzothiazol and its chelates with TiO(IV), Cr(III) and Fe(III) ions were investigated by IR spectroscopy. On basis of these studies, it is proposed that the geometry of the chelates is an octahedral (37). Didarul A. et.al have been prepared Several new dioxouranium(VI) complexes of Schiff bases and characterized on the basis of their elemental analyses, IR and electronic absorption spectra.The results suggest that each Schiff base is a bivalent anion with tridentate ONS donors from the phenolic oxygen, azomethine nitrogen and thiophenolic sulfur. and a six-coordinate dimeric structure has been proposed for the complexes(38).

Guo-Bi Li et.al have been performed Efficient synthesis and characterization of the low dimensional heteronuclear complexes with a N_2O_2-donor Schiff base ligand (39). P Viswanathamurthi et.al have been synthesized Ru(II) complexes containing bidentate Schiff bases and triphenylphosphine or triphenylarsine The products were characterized by analytical, IR, electronic and ^{1}H-NMR spectral studies and proposed an octahedral geometry (40). Ahmad Fauzi Abu Bakar et.al have been synthesized two ligands and eight complexes by reacting 1,8-diaminonapthelene with aldehyde/ketone derivatives in 1:2 ratio for ligand formation and 1:1 ratio for complex formations. The compounds are characterized through CH IR spectroscopy, ^{1}H NMR spectroscopy, melting point and magnetic susceptibility determination. The neurotoxicity of compounds is evaluated using neuroblastoma SH-SY5Y cell lines and it was indicate the cells were non-toxic either for ligands and complexes after 24 hours exposure (41).

Dije I. Dehari, et.al have been synthesized new complexes of nickel(II) in the reaction mixture of nickel(II) acetate, ethanolamine and 5-X salicylaldehyde (X= Br, Cl). Diaquabis(2-hydroxyethylimino)methyl)-4-bromophenolato)nickel(II) and Diaquabis(2-hydroxyethylimino)methyl)-4-chlorophenolato)-nickel(II) were characterized by IR spectroscopy. Elemental analysis and mass spectrometry data of the complexes suggests the stoichiometry is 1:2 (metal-ligand) (42). Shanmugavel Sujarania et.al have been prepared a new series of biocompatible compounds by Schiff base condensation reaction. The solid derivatives have been isolated and characterized by using IR, NMR and UV-Visible spectral techniques. The primary reason behind the effort for their utility in biomedicine and therapy is their unique plasmonic properties and easy surface chemistry for a variety of functionalizations (43). Ti Feng Jiao et.al have been prepared the chitosan-based Schiff base copper (II) complexes through the reaction of relative Schiff bases with copper acetate. FTIR analysis indicated that Schiff base and coordination reaction take place in Schiff base skeleton. and chitosan-based Schiff base derivatives can be altered by modifying the molecular structures of objective compounds with proper substituent groups (44).

TAO WU,et.al were asymmetrically synthesized Novel copper(II) coordination compounds with chiral macrocyclic imine ligands derived from R-/S-camphor and characterized with the aid of chiroptical spectroscopies. The complex formation was evidenced by spectral shifts of the characteristic bands in the CD and VCD spectra (45). Carlos Kubli-Garfias perform an analysis of the photo-isomerization of the protonated Schiff base of retinal from 11-cis to 11-trans rotating the C_{10}-C_{11}=C_{12}-C_{13} dihedral angle from 0° (cis) to -180° (trans). and find that the retinal molecule shows the lowest rotational barrier (0.22 eV) when its charge state is zero as compared to the barrier for the protonated molecule which is ~0.89 eV (46). Selen Bilge et.al have been studied the UV-vis spectra of the Schiff bases in organic solvents of different polarity, acidic and basic media and found useful in understanding of tautomeric equilibria. The molecular structure of these compound has been determined crystallographically, and observed that the compound is in the form of phenol-imine, defined by the strong intramolecular hydrogen bonds (47). Emadeddin Tajkhorshid et.al were studied the planarity of the polyene chain of the retinal chromophore in bacteriorhodopsin is using molecular dynamics simulation techniques and applying different force-field parameters and starting crystal structures (48).

S. Arunachalam et.al have been synthesized stable Ru(II) carbonyl complexes The new complexes were characterized by elemental analysis, Mass spectra, IR, UV-Vis and ^{1}H, ^{13}C and ^{31}P -NMR spectral data. The redox property of the complexes were studied by cyclic voltammetric technique. An octahedral geometry has been assigned tentatively for all the complexes These complexes were also subjected to study their biocidal activity. DNA (Herring Sperm) binding behaviour of the complex has been studied by electronic spectra, cyclic voltammetric, differential pulse voltametric, circular dichorism and gel electrophoresis technique (49).

Singh Rajeev has been subjected S-2-picolyl-β-N-(2-acetylpyrrole) dithiocarbazate Schiff base to theoretical studies by using Semi-empirical AM1 and PM3 quantum chemical methods. The molecular geometry, vibration frequencies, HOMO-LUMO energy gap, molecular hardness (η), ionization energy (IE),

electron affinity (EA), total energy and dipole moment were analyzed. A good correlation has been observed between experimental and calculated values for vibration modes (50).

The optimized structural parameters (bond lengths and bond angles) of S-2-picolyl-β-N-(2-acetylpyrrole) dithiocarbazate have been obtained by semi empirical AM1 and PM3 methods shown in fig.1. Comparison for the calculated bond lengths and angles for the S-benzyldithiocarbazate with those of experimentally available x-ray8 diffraction data are listed in the table 1& 2 respectively. The calculated bond lengths are in good agreement with experimental values. For bond length, the correlation coefficient obtained for AM1 and PM3 are 0.958 and 0.966 respectively. It is evident that PM3 method gives most satisfactory correlation (CC=0.966) between experimental and calculated bond lengths. In the case of bond angle, correlation coefficients are 0.506 and 0.474 for AM1 and PM3 methods respectively. For bond angles none of the methods produce excellent correlation but out the two methods AM1 method gives slightly better results than PM3 methods (correlation coefficients, cc=0.506). The graph between experimental versus calculated bond length and bond angle are given in figure-2 and 3 respectively. Calculated and experimental Fundamental vibration frequency of S-2-picolyl-β-N-(2-acetylpyrrole) dithiocarbazate have been obtained by semi empirical AM1 and PM3 methods are listed in table 3.

Kishor Arora et.al examined the vibration modes of the 2N-(3,4,5-Trimethoxy benzalidine) amino pyridine (TMBAPy)* , 2N-(4- hydroxy-3-methoxy benzalidene) amino pyridine (HMBAPy)* and 2N-(4-chloro benzalidine) amino pyridine(p-ClBAPy)* experimentally and theoretically using the Semi-empirical AM1 and PM3 computational methods are listed in table-4, 5 and 6 respectively..The graph between experimental versus calculated fundamental vibration frequency of title compounds(listed above *) are represented in fig. 4, 5, 6. PM3 method provides most satisfactory correlations between experimental and calculated fundamental vibration modes.(51)

III. IR Spectral Study Related To Pyrazolones

Pyrazolone, a five-membered-ring lactam, is a derivative of pyrazole that has an additional keto (=O) group. It has a molecular formula of $C_3H_4N_2O$.

Jianping Hu synthesized five novel pyrazolone derivatives containing a furoyl group and characterized by elemental analysis, IR, ^{1}H NMR spectra. Photo-isomerization properties have been studied by UV–vis and fluorescence spectra. Based on theoretical calculation and crystal structural analysis, the compounds undergo photoisomerization from the enol form to the keto form(52). Alok K. Pareek et.al have been synthesized N1-(2, 5-dichloro benzoyl)-3-methyl-4-(substituted phenyl hydrazono)-5-pyrazolone derivatives. The structural assignment are based on their melting point, colour, elemental analysis, spectral data (IR) and chemical properties (53).

Angela Antochi synthesized 1-[2'-(theophyllin-7-yl)sulfonyl-4-chlor-phenoxyacetyl]-3-methyl -5-pyrazolone starting from 4-chlor-2-(theophyllin-7'-yl)sulfonyl-phenoxyacetyl hydrazide. To establish the reaction conditions it was used a planned factorial experiment of 2nd order (54).

Kishor Arora and Veena Nathani were performed Quantitative Structure Activity Relationship (QSAR) studies on selected pyrazolone compounds as antimicrobial agent. The compounds has been established on the basis of analytical methods and advanced spectroscopic techniques. Three compounds viz. 4-Amino antipyrine thiosemicarbazone (C-8), 1-(2-Chloro-5-sulfophenyl)-3-methyl-5-pyrazolone (C-9) and 1-(4-Sulfoamido phenyl)-3-methyl-5-pyrazolone (C-10) recorded significant antifungal activity against Macrophomina phaseolina (55).

Krishna Naik synthesized a series of new {4-[3-Methyl-5-oxo-4-(4|-substituted phenyl hydrazono)-4,5-dihydro-pyrazol-1-yl]-phenoxy}-acetic acid (2-oxo-1-piperidine-1- -ylmethyl-1,2-dihydro–indol-3-ylidene)-hydrazides by the Mannich reaction & were characterized by elemental analysis, IR, ^{1}H NMR and mass spectral data. Electrochemical behavior of these compounds were studied by two techniques namely polarography and cyclic voltammetry (56).

N. P. Moorjani were synthesized a series of tridentate pyrazolone-based Schiff bases by the interaction of 4-acyl/aroyl pyrazolones with 2-Amino Phenol in an ethanolic medium. All of these ligands were characterized on the basis of elemental analysis, infrared (IR) and ^{1}H-NMR data.Copper Schiff-base complexes $[Cu_2I_2]$ have been prepared by the interaction of the aqueous solution of copper acetate monohydrate with hot ethanolic solution of the appropriate ligand. The resulting complexes have been characterized by elemental analysis, IR and electronic spectral studies. Suitable square planar structure is proposed for these complexes.(57)

Rajeev Verma et.al synthesized a series of 4-arylidene-3-methyl-1-phenyl-5-pyrazolone derivative by reacting various substituted aromatic aldehydes with 3-methyl-1-phenyl-5-pyrazolone through Knoevenagel condensation by conventional as well as by exposure to microwave irradiations. Structures of all new synthesized compounds were characterized on the basis of spectral data (58) . Kishor Arora and veena nathani were evaluated some novel synthetic pyrazolone compounds for their in-vitro antimicrobial activity viz. antifungal activity against Gibberella fujikuroi. The compounds were characterized by elemental and spectral

analysis. Quantitative Structure Activity Relationship (QSAR) studies were applied to find correlation between different calculated molecular descriptors of the synthesized compounds and biological activity(59).

Subrata Kumar Dey presented the synthesis, structure, and physical properties of a series of mononuclear complexes viz. $[Cu(L)_2]$, $[CuL_2(CH_3O)_2]$ and $[Zn(L)_2]$ (where L = 1-Phenyl-3-methyl-4-benzoyl-5-pyrazolone (PMBP). The complexes were characterized by elemental analysis, IR and electronic spectroscopy, magnetic measurements at room temperature and thermogravimetric analysis. The structures of all the three complexes were determined by single crystal X-ray diffraction studies(60) WANG Jun Hua et.al were synthesized three new photoisomeric compounds: 1,3-diphenyl-4-benzal-5-pyrazolone 4-methylthiosemicarbazone (DPBP-MTSC), 1,3-diphenyl-4-(4′-methylbenzal)-5-pyrazolone 4-methylthiosemicarbazone (DP4MBP- MTSC), and 1,3-diphenyl-4-(4′-bromobenzal)-5-pyrazolone 4-methylthiosemicarbazone (DP4BrBP-MTSC) by direct condensation of pyrazolones and 4-methylthiosemicarbazone. Their structures were confirmed using ^{1}H NMR, IR, elemental analyses, and X-ray crystallographic analyses(61).

Mustafa Sacmaci et.al giving the proponohydrazide derivatives 4-(4-Methoxybenzoyl)-5-(4-methoxyphenyl)-2,3-furandione reacted with N-aryl substituted phenylhydrazone via the p,p'-dimethoxydibenzoylketene intermediate. In addition, compounds of these were converted into corresponding pyrazolone derivatives by the reactions of hydrolysis in acidic solution. The structures of these new synthesized compounds were determined by ^{13}C NMR, ^{1}H NMR and IR spectroscopic data and elemental analysis(62). Venelin Enchev calculated the heats of formation, dipole moments, polarizabilities and ionization potentials of 96 compounds, eight theoretically possible tautomeric forms of N-unsubstituted pyrazolones (hydroxypyrazoles) and 11 of their C-substituted derivatives, by means of the MNDO method, with and without configuration interaction (CI). The MNDO+ CI results for the relative stabilities are in agreement with the available experimental data(63). Sergio Zamorano et.al described the synthesis of complexes from copper (II) and vanadyl (VO^{2+}) with pyrazolone ligands Pir-C_6 , Pir-C_8 and Pir-C_{12} . The EPR spectra of this compounds are interpreted and the physical and spectroscopic measurements were made(64).

Hui Chai et.al have been synthesized a new photochromic compound 1,3-diphenyl-4-(4_-fluro)benzal-5-pyrazolone-4-ethyl thiosemicarbazone. The product was characterized by elemental analysis, IR and ^{1}H NMR spectra. The photochromic properties of the compound were studied using time-dependent fluorescence emission spectra(65). Lang Liu et.al have been synthesized a new organic photochromic compound containing pyrazolone-ring photochromic functional unit: 1-phenyl-3-methyl-4-benzoylpyrazole-5-one methyl thioesmicarbazone (1A), and some analogous non-photochromic derivatives and characterized by elemental analyses, MS, IR spectra, ^{1}H NMR spectra(66). Bang-hua Peng et.al performed analysis of the time-dependent UV–vis reflection spectra of the compound 1-phenyl-3-methyl-4-(4-methylbenzal)-5-pyrazolone 4-ethylthiosemicarbazone (PM4MBP-ETSC) undergoes a solid-state photochromism. The reaction rate constant was studied by the first-order kinetics curves. X-ray single crystal structural analysis shows that the pyrazolone-ring stabilizes in the keto form(67).

Alok K. Pareek et.al were synthesized some of the pyrazolones and pyrazoles bearing different functional groups, substituted pyrazolones by the condensation reaction of newly synthesized substituted thiosemicarbazide with substituted ethyl aceto hydrazone in the presence of glacial acetic acid as a catalyst The constitution of the newly synthesized substituted pyrazolones and substituted pyrazoles are characterized by their physical properties, elemental analysis, spectral studies like IR (68). Shilpi Gupta et.al synthesized some novel pyrazolinones by the condensation of aryl hydrazones of ethyl aceto acetate with N-(2-chloro-4-nitro) phenyl malonamic acid hydrazide by conventional as well as microwave induced synthesis. All the compounds were characterized on the basis of I.R. spectra and elemental analysis(69). Lang Liu and Dianzeng Jia have been prepared 1-Phenyl-3-methyl-4-benzoylpyrazole-5-one semicarbazone and its complexes have been prepared and characterized on the basis of elemental analyses, IR spectra, ^{1}H NMR spectra, mass spectra, molar conductivity, thermal analyses and X-ray powder diffraction(70).

Bharat Kumar et.al have been deals with the synthesis of some bromo-benzothiazolopyrazolines from substituted pyrazolines. The synthesized bromo benzothiazolopyrazolines were characterized by elemental analyses, IR, NMR and mass spectra. The fragmentation pattern of one of the compound has also been suggested(71). Abdullah M. Asiri et.al have been prepared new chromophores of the Donor-conjugated-acceptor types containing 4-N,N-dimethylaminobenzene as the donor-conjugated group with different types of acceptors. The electronic spectra were investigated in ethanol and acetonitrile to assess the effect of solvatochromic properties of these new dyes. The relative strength of the acceptor in producing large bathochromic shift was illustrated. Tricyanovinyl is the best acceptor used in this study to produce a larger bathochromic shift of the visible absorption, where as the least acceptor used is diethyl malonate (72). Bang-hua Peng studied the crystal structure of the compound 1-phenyl-3-methyl-4-benzal-5-pyrazolone 4-ethyl thiosemicarbazone (PMBP-ETSC), as determined by X-ray analysis, shows that the pyrazolone moiety stabilizes in the keto form and the

molecule is found to be in three dimensional arrangement in the unit cell linked by intermolecular hydrogen bonds. The important bands in IR spectra, as well as the main signals of the ^{1}H NMR spectra are assigned (73).

Juanjuan Lu. Et.al studied fluorescence properties of four 4-acyl pyrazolone derivatives N-(1,3-diphenyl-4-propylene-5-pyrazolone)-salicylidene hydrazone (1),1,3-diphenyl-4-ethylene-5-pyrazolone)-salicylidene hydrazone (2), 1,3-diphenyl-4-benzylidene-5-pyrazolone)-salicylidenehydrazone(3) 1,3-diphenyl-4-phenylethylene-5-pyrazolone)-salicylidene hydrazone (4), and their Zn (II) complex were studied at room temperature. It was revealed that these compounds show different fluorescence properties both in the solid state and in solution. Density functional theory (DFT) calculations on ligands 1–4 were also performed to further understand their emission properties(74). P.Nagarjuna Reddy et.al synthesized Novel mannich bases N-(2- ((R) -1- ((Z) -2- (1-((4-methyl piperazin-1-yl) methyl) -2-oxoindolin-3-ylidene) hydrazinyl) -1-oxopropan -2-ylamino) -2-oxoethyl) -4-(5–oxo –4-(2-phenyl hydrazono) -3-(trifluoromethyl) -4, 5-dihydro -1H –pyrazol -1-yl) benzamide. The structure of these newly synthesized compounds were characterized by ^{1}HNMR, Mass, IR & Elemental analysis (75).

Rahat Khan et.al synthesized derivatives of 5-methyl-2,4-dihydro-pyrazol-3-one , 5-methyl-2-phenyl-2,4-dihydro-pyrazol-3-one and 2-(2,4-dinitro-phenyl)-5-methyl-2,4-dihydro-pyrazol-3-one & have been brominated in various ways. The above compound were synthesized by condensation reaction between the ethylacetoacetate and hydrazine derivatives. All the products have been characterized by extensive use of IR, ^{1}H-NMR, ^{13}C-NMR and Mass spectral analysis(76). D. Ravi Sankar Reddy et.al have been synthesized 2-amino benzothiazoles from 3-chloro-4-fluoro aniline and further condensed with 3-methyl-1-phenyl-5-Pyrazolone to yield the corresponding Schiff's base. The Schiff's base was cyclised with chloroacetyl choride in triethylamine to yield 2-azetidinones. The formed 2-azetidinones were further condensed with different primary and secondary amines. The synthesized compounds were confirmed by spectral analysis such as IR, ^{1}H-NMR, Mass and were screened for Anti-inflammatory, Anti-diabetic, Anti-oxidant and Anti-microbial activity(77). Ram K. Agarwal describe the isolation of some lanthanide(III) chlorides coordination compounds with 4[(furan-2-ylmethylene)amino]-1,5-dimethyl-2-phenyl pyrazol-3-one (FDPPO) and isonicotinic acid(3,4,5-trimethoxybenzylidene)hydrazide All the isolated compounds were characterized through various physico-chemical studies(78). Salem Ahmed Basaif Studied heating of 3-methyl-1-(pyrid-2-yl / 4-chlorophenyl)-2-pyrazolin-5-ones (1) and some aromatic aldehydes at 150 – 160^0 C affords the corresponding 4-arylidene-2-pyrazolin-5-ones (2) as colored products with high yields. These new products were characterized by UV-visible, FT-IR and ^{1}H NMR spectroscopic techniques and elemental analysis (79).

Kishor Arora et.al have been studied the vibration modes of some pyrazolone compounds ,experimentally and theoretically using Semi-empirical AM1 and PM3 methods. Apart from giving the comparison of the significant part of the spectra, the statistical correlation was also calculated for the theoretical spectra and methods to establish the use of these methods as alternative and supportive tool in analytical chemistry. Vibration modes for the compounds under study show a perfect correlation between theoretically and experimentally observed values(80).

In this paper they wish to report the vibration modes analysis of some selected pyrazolone compounds using AM1 and PM3 methods and their comparison with their real spectra. Compounds taken for the studies here are (i) Methyl phenyl – 5- pyrazolone (MPP); (ii) Antipyrine (Antipy); (iii) 4- Amino antipyrine (4-Amantipy); (iv) Amino pyrine (Ampy) and (v) 4- Nitrosoantipyrine (4-Nitantipy).

Computational details:- The AM1 and PM3 methods in MOPAC package were used to calculate the bond lengths, bond angles, heat of formations, core-core repulsion energies, ionization potentials etc.. The calculations for vibration modes of the pyrazolone compounds under study were also done using same package. Structures of the compounds were drawn on the PCMODEL package of Serena software and then were optimized which were then used as input to MOPAC . All these calculations were done on the Pentium – III machine with configuration: P-III/866Mhz/20GB/52X/SCROLL MOUSE/ 56 KBPS.

The computed heat of formation, total energy, electronic energy, core-core repulsion energy, ionization potential and other computed results are of theoretical interest. The computed vibration modes along with their experimental values are given in the tables 7 & 8. It has also been tried to match the computed spectral peaks with their experimental values.

Correlation coefficient between computed and experimental vibration modes for the different pyrazolone compounds under study using AM1 and PM3 methods respectively are computed and are given here:

(i) Methyl phenyl – 5- pyrazolone (MPP)-- 0.99995 (AM1) and 0.99747(PM3) ;
(ii) Antipyrine (Antipy) --0.99997 (AM1) and 0.998748 (PM3) .

These correlation coefficient values among computed and experimental vibration modes for the pyrazolone compounds under study clearly indicates that computed values are approximately in correlation with the experimental values.

IV. Conclusion-

This is clear from this discussion given in this review article that workers are using software for simulation of spectra and spectral studies. Whether in semi-empirical ,Abinitio or by DFT methods. And these are proved to be important tools for this purpose and spectral analysis of organic compounds.

In conclusion, This can be mentioned that enormous possibilities are there for scientists to work in this and related field.

Table-1

Calculated and experimental selected bond lengths (Å) for S-2-picolyl-β-N-(2-acetylpyrrole) dithiocarbazate by AM1 and PM3 method

BOND LENGTH (IN A^0)	**EXPERIMENTAL**	**CALCULATED**	
		AM1	**PM3**
S2-C7	1.751	1.717	1.777
S2-C8	1.815	1.761	1.821
S1-C7	1.699	1.595	1.643
N4-C10	1.389	1.345	1.315
N4-C9	1.422	1.355	1.357
N3-C7	1.308	1.389	1.391
N2-N3	1.382	1.334	1.388
N2-C1	1.314	1.318	1.314
C8-C9	1.504	1.494	1.494
C1-C2	1.426	1.462	1.448
C1-C6	1.474	1.497	1.493
Correlation Coefficient (cc)	-	0.958	0.966

Table-2

Calculated and experimental selected bond angles (°) for S-2-picolyl-β-N-(2-acetylpyrrole) dithiocarbazate by AM1 and PM3 method

BOND ANGLE (°)	**EXPERIMENTAL**	**CALCULATED**	
		AM1	**PM3**
C7-S2-C8	104.6	103.2	103.6
C1-N2-N3	124.3	121.9	122.6
C7-N3-N2	112.4	122.7	121.4
N4-C9-C8	120.1	120.5	120.5
N3-C7-S1	127.5	119.1	118.4
C9-C8-S2	114.0	103.2	118.2
N2-C1-C2	124.8	118.0	116.4
N2-C1-C6	115.1	126.5	126.4
C1-C2-C6	120.1	115.4	117.2
Correlation coefficient (cc)	-	0.506	0.474

Table-3
Experimental and calculated fundamental vibration frequencies of S-2-picolyl-β-N-(2-acetylpyrrole) dithiocarbazate by AM1 and PM3 methods

IR Bands	Experimental (cm^{-1})	Calculated	
		AM1	PM3
ν(N-H)	3084	3290	3113
ν(C=N)	1524	1617	1714
ν(N-N)	1050	1103	1043
ν(C=S)	1046	1036	1022
ν(CSS)	996	1005	969
Correlation coefficient (cc)	-	0.999	0.995

Table 4:
Experimental and Calculated fundamental vibrational modes of 2N-(3,4,5-Trimethoxy benzalidine) amino pyridine (TMBAPy) by AM1 and PM3 Semi-empirical methods.

EXPERIMENTAL	CALCULATED	
	AM1	PM3
465.4	481.03	477.60
522.1	530.75	542.33
592.9	611.45	597.67
626.5	626.82	618.56
676.8	678.42	662.83
730.4	733.36	748.65
769.8	797.19	786.59
845.3	856.34	883.53
892.8	888.25	886.75
989.8	979.68	993.61
1038.0	1016.92	1039.84
1127.6	1102.71	1130.44
1186.4	1183.62	1173.34
1234.5	1227.56	1221.95

Table 5:
Experimental and Calculated fundamental vibrational modes of 2N-(4- hydroxy-3-methoxy benzalidene) amino pyridine (HMBAPy) by AM1 and PM3 Semiempirical methods

EXPERIMENTAL	CALCULATED	
	AM1	PM3
615.6	605.73	591.04
67503	676.81	663.01
711.3	710.86	702.69
764.6	734.83	785.64
833.6	827.86	843.35
1057.2	1016.81	1048.06
1140.7	1164.57	1146.03
1352.6	1364.29	1363.26
1383.3	1394.29	1386.97
1425.6	1429.45	1413.16
1461.3	1464.33	1487.29
1492.3	1524.80	1526.32
1594.3	1583.26	1573.36
2366.2	1921.64	1825.53
2819.9	3062.06	3060.13
3428.9	3449.17	3425.20
Correlation Coefficient (cc)	0.986742	0.98184

Table-6:
Experimental and Calculated fundamental vibrational modes of 2N-(4-chloro benzalidine) amino pyridine(p-ClBAPy) by AM1 and PM3 Semi-empirical methods

EXPERIMENTAL	CALCULATED	
	AM1	PM3
479.5	485.64	478.74
512.2	501.58	491.13
559.3	535.67	525.74
593.2	547.03	605.33
625.8	665.95	637.91
719.0	735.17	709.05
773.0	781.99	786.00
822.6	827.33	845.37
901.3	923.38	918.82
985.5	981.28	980.39
1011.9	1020.08	1011.81
1087.2	1100.33	1105.48
1135.7	1118.99	1127.85
1179.3	1182.66	1164.60
1199.5	1205.80	1207.21
1284.9	1285.88	1245.12
1322.9	1319.16	1325.27
1354.6	1355.78	1349.00
1386.2	1396.52	1397.15
1522.5	1549.30	1529.19
1598.8	1614.65	1600.30
3091.2	3061.16	3070.38
3222.5	3211.88	3182.20
Correlation Coefficient (cc)	0.999646	0.999714

Table-7
Computed and observed vibration modes values (cm-1) for Methyl phenyl-5- pyrazolone (MPP) compound.

EXPERIMENTAL	CALCULATED	
	AM1	PM3
------	488.21	474.48
499	508.36	496.39
------	553	551.54
570	593.35	569
616	650.11	626.38
689	657.07	642.52
757	726.06	673.7
800	806.55	774.89
------	884.71	812.14
917	916.53	845.39
-----	945.08	901.58
------	954.93	933.27
------	984.9	945.02
------	1003.29	976.49
1025	1044.47	994.47
------	1049.11	1005.32
1076	1089.63	1015.29
------	1109.55	1043.62
------	1131.54	1050.62
------	1196.33	1111.18
1198	1197.69	1123.59
------	1248.52	1155.52
------	1280.74	1171.79
------	1304.47	1205.69
------	1338.62	1215.08
------	1364.62	1233.17
------	1378.12	1340.38
1394	1387.52	1364.85
1397	1408.99	1385.47
------	1430.45	1386.84
1457	1474.08	1392.44
1522	1553.86	1475.41

1610	1578.08	1544.97
------	1674.82	1587.7
------	1745.91	1771.46

Table-8

Computed and observed vibration modes values (cm-1) for Antipyrine (Antipy) compound.

EXPERIMENTAL	CALCULATED	
	AM1	**PM3**
----	476.13	461.64
-----	526.75	484.82
575	595.73	559.85
-----	633.81	581.28
665	655.14	594.68
-----	677.92	634.44
-----	698.54	645.61
750	713.28	684.1
-----	814.5	773.33
-----	848.84	777.72
-----	891.1	874.95
920	952.7	889.9
-----	979.51	910.35
-----	988.88	948.19
-----	1046.96	983.38
-----	1054.66	989.61
-----	1073.07	1007.89
1115	1110.41	1016.89
-----	1134.22	1035.42
1178	1178.51	1075.74
------	1196.39	1106.7
1250	1252.97	1163.07
1350	1365.59	1247.80
------	1372.81	1349.14
-----	1378.3	1368.77
-----	1410.39	1376.68
1444	1453.82	1388.65
-----	1487.49	1392.53
-----	1503.02	1453.83
1594	1566.00	1538.81
1649	1639.06	1584.44
-----	1746.23	1769.37
-----	1774.38	1782.66
-----	1793.32	1823.82
------	2074.67	1982.65

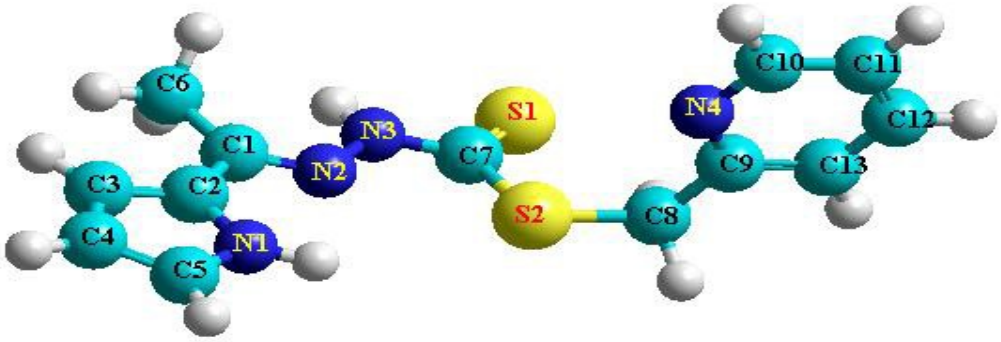

Fig. 1 PM3 Optimized geometry of S-2-picolyl-β-N-(2- acetylpyrrole) dithiocarbazate

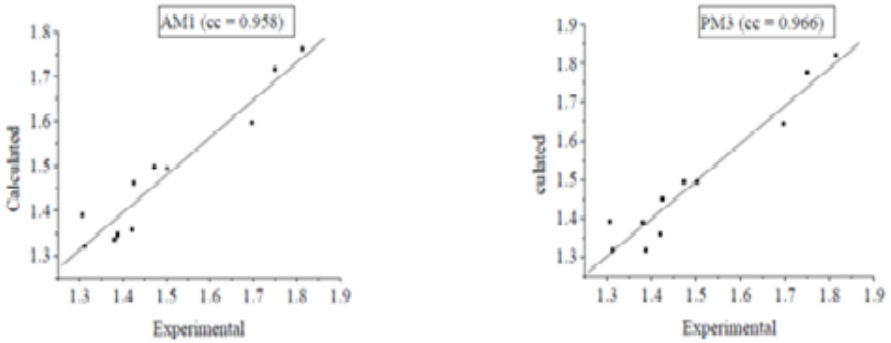

Fig-02 -Graphical correlation between the experimental and calculated bond lengths of S-2- Picolyl –β-N-(2-acetylpyrrole) dithiocarbazate obtained by AM1 and PM 3 methods.(cc=Correlation cofficient).

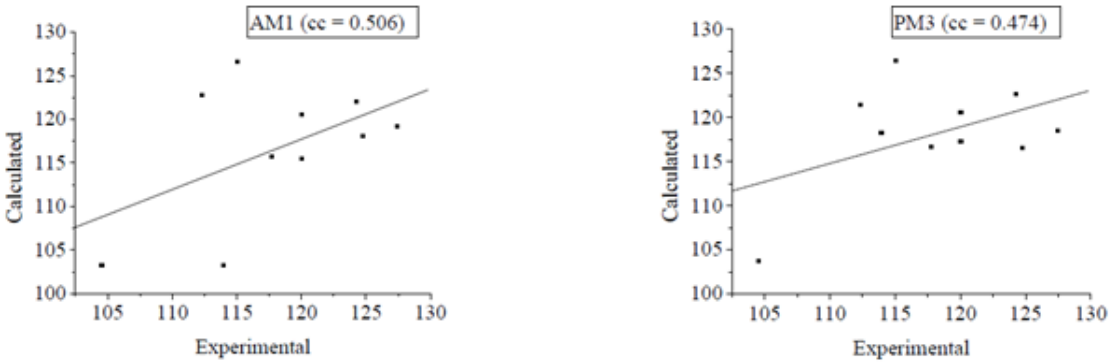

Fig-03- Graphical correlation between the experimental and calculated bond angles of S-2-Picolyl –β-N-(2-acetylpyrrole) dithiocarbazate obtained by AM1 and PM 3 methods.(CC=Correlation cofficient)

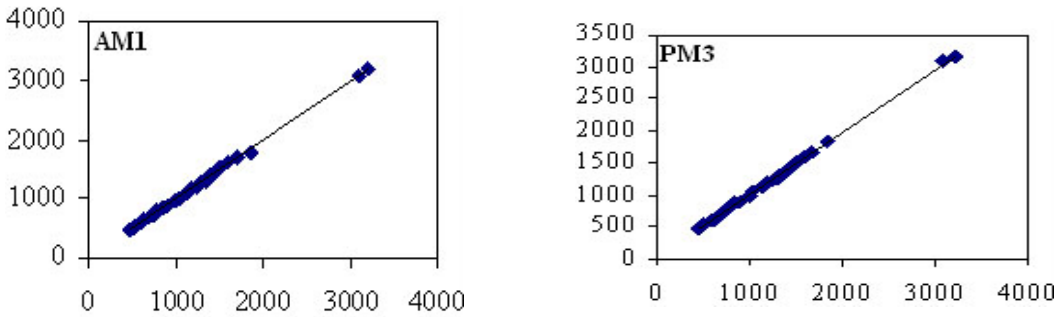

Fig 4- Graphical correlation between experimental and calculated fundamental vibration modes obtained by AM1 and PM3 Semi-empirical methods for 2N-(3, 4, 5,Trimethoxy benzalidine) amino pyridine (TMBAPy).

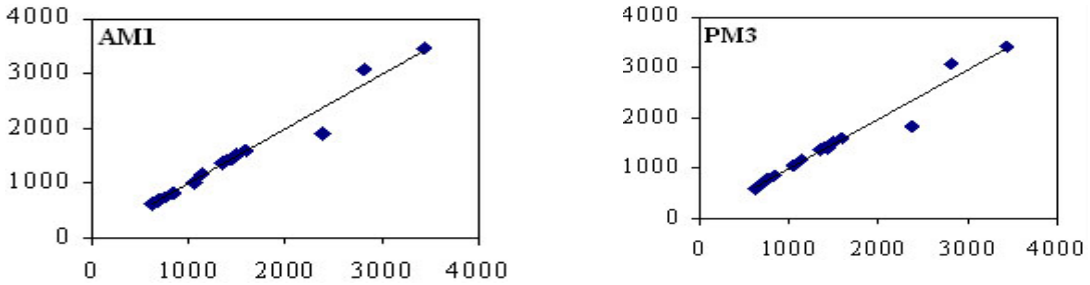

Fig. 5 Graphical correlation between experimental and calculated fundamental vibration modes obtained by AM1 and PM3 Semi-empirical methods for 2N-(4-hydroxy-3-methoxy benzalidene) amino pyridine (HMBAPy).

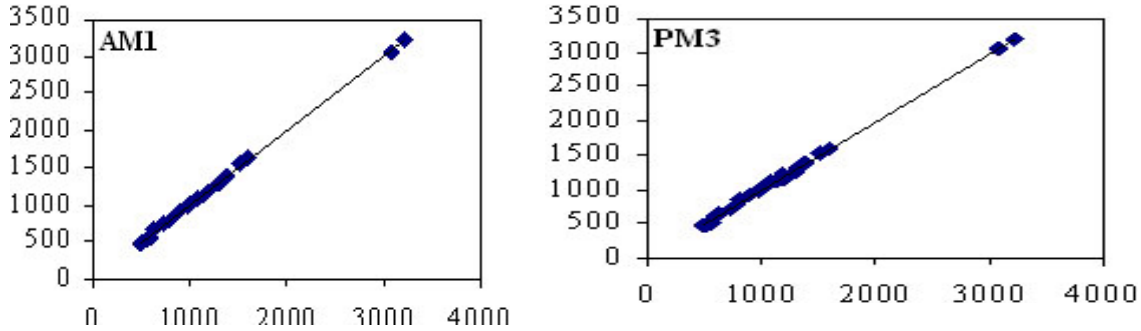

Fig 6 Graphical correlation between experimental and calculated fundamental vibration modes obtained by AM1 and PM3 Semi-empirical methods for 2N-(4-chloro benzalidine) amino pyridine (p-ClBAPy) (CC=Correlation Coefficient).

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