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Spectral Simulation Studies of Organic Components– A Review

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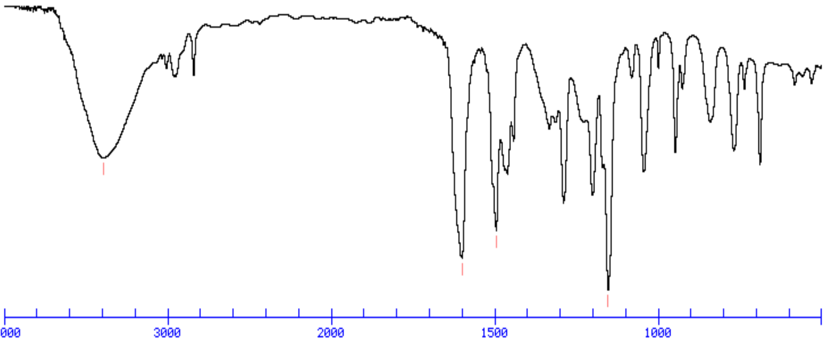
Abstract: *Spectral studies of Organic compound for the purpose of their structural establishment are one of the major tools or technique in this regards. In the modern era simulation of spectra using computational methods is becoming popular method among workers. The present review deals with such types of literature available and it contains 106 references.*

I. Introduction

An invaluable tool in organic structure determination and verification involves the class of electromagnetic (EM) radiation with frequencies between 4000 and 400 cm^{-1} (wave numbers). The category of EM radiation is termed infrared (IR) radiation, and its application to organic chemistry known as IR spectroscopy. Radiation in this region can be utilized in organic structure determination by making use of the fact that it is absorbed by inter-atomic bonds in organic compounds. Chemical bonds in different environments will absorb varying intensities and at varying frequencies. Thus IR spectroscopy involves collecting absorption information and analyzing it in the form of a spectrum -- The frequencies at which there are absorptions of IR radiation ("peaks" or "signals") can be correlated directly to bonds within the compound in question.



An Example IR Spectrum

Because each inter-atomic bond may vibrate in several different motions (stretching or bending), individual bonds may absorb at more than one IR frequency. Stretching absorptions usually produce stronger peaks than bending, however the weaker bending absorptions can be useful in differentiating similar types of bonds (e.g. aromatic substitution). It is also important to note that symmetrical vibrations do not cause absorption of IR radiation. For example, neither of the carbon-carbon bonds in ethene or ethyne absorb IR radiation.

Literature Survey and Critical Discussion on it-

A critical review of literature for the proposed project revealed that Galina A. Chmutova et.al (1) have reported that the use of IR and NMR ^{1}H spectroscopy, 3-acetylamino (II) and 3-benzoylamino-1-(2',4',6'-trichlorophenyl) pyrazoline-2-on-5 (III) in solid state, as well as in non-polar and low-polarity solvents has been established to be in CH-tautomeric form. The composition of acetylation and benzoylation products of the compounds (II) and (III) has been characterized. There has been determined pKa of acid-base equilibriums of pyrazolone acylamino derivatives in water-dioxane media (50:50). The energies and atomic charges of the investigated molecules and anions, formed while de-protonation, have been calculated by PM3 level.**(1)**

Alevtina Yu. Yegorova and Zlata Yu. Timofeyeva(2) have reported that Michael's condensation in the series of 5-alkyl(aryl)-3*H*-pyrrolin-2-ones with donor-substituted chalcones has been studied. All peculiarities of this reaction have been revealed. The reaction is shown to proceed through the formation of 1, 5-dicarbonyl compounds. The structure of the reaction products have been proved by means of IR and NMR 1H spectroscopy.**(2)**

Vasile Dinoiu and Jian-Ming (3) reported that 3,5-Dialkyl-4-hydroxybenzylhydrazine 1 reacted with hexa-fluoroacetylacetone, and trifluoro acetyl acetone yielding the pyrazoles 2 bearing trifluoromethyl and/or methyl substituents in positions 3 and 5. The same hydrazine derivatives 1 afforded the pyrazol-5-ones 3 with trifluoro acetoacetic acid ethyl ester. On oxidation with lead tetra acetate in CH_2Cl_2, some stable aroxyls were obtained and their ESR spectra are described.**(3)**

Paresh P Rathia, et.al. (4) reported that The present study was aimed to synthesize a series 2-[(1,3-benzothiazol-2-ylamino) methyl]-5-methyl-2,4-dihydro-3H-pyrazol-3-one (3 a-l) and to evaluate their in-vitro anti-inflammatory activity. The starting material (1a-l) was prepared by the application of cyclization reaction. In-vitro anti-inflammatory activity of synthesized compounds [3a-l] was evaluated using inhibition of bovine serum albumin denaturation method. 3c and 3l have shown significant in-vitro anti-inflammatory activity. The findings of present study clearly demonstrate that chloro functional group possess inhibition of bovine serum albumin denaturation capacity and has in-vitro anti-inflammatory activity. However methyl, methoxy and dimethyl derivatives show mild to moderate in-vitro anti-inflammatory activity.**(4)**

Fabio Marchetti, Claudio Pettinari, Corrado Di Nicola, Riccardo Pettinari, Alessandra Crispini, Marcello Crucianelli, Andrea Di Giuseppe (5) these were reported that Reaction of $VOSO_4 \cdot 5H_2O$ with a methanol solution of the HQ proligand (HQ = 1-R^1-4-R^2(C$=$O)pyrazol-5-one in general, in detail: HQ^{nPe}, R^1 = phenyl, R^2 = neopentyl; $HQ^{Me,Me}$, $R^1 = R^2$ = methyl; $HQ^{Me,naph}$, R^1 = methyl, R^2 = naphthalen-1-yl; HQ^{naph}, R^1 = phenyl, R^2 = naphthalen-1-yl; HQ^{Ph}, $R^1 = R^2$ = phenyl; HQ^{CF3}, R^1 = phenyl, R^2 = trifluoromethyl; $HQ^{py,CF3}$, R^1 = pyridin-2-yl, R^2 = trifluoromethyl) gave seven novel $VO(Q)_2(H_2O)$ complexes which have been characterized by elemental analyses, IR, ESI-MS, electronic spectroscopy and magnetic susceptibility measurements and, in the case of derivative $VO(Q^{CF3})_2$, also by EPR spectroscopy. The X-ray diffraction study, carried out on derivative $VO(Q^{nPe})_2(H_2O)$, evidenced a distorted octahedral environment with the two pyrazolonates in anti configuration and the vanadium atom 0.2914(7) Å away from the least-squares plane defined by the four equatorial oxygen atoms. The catalytic activity of these new oxovanadium (IV) complexes has been exhaustively tested for the oxidation of styrene, α-methylstyrene and cis-β-methylstyrene, in the presence of H_2O_2 as primary oxidant. The effects of oxidant to substrate molar ratio, catalyst amount, solvent and temperature have been studied. Overall, the vanadium complexes showed high activity and high to moderate selectivity toward the benzaldehyde (acetophenone) formation, depending from both the type of starting substrate and experimental reaction times.**(5)**

It has been reported by Chunhui Huang, Fuyou Li, Li Shen, Mei Shi, Dengqing Zhang, Xianghong Li, Enxian Shi, Tao Yi, Yukou Du, that A series of novel dendritic β-diketone ligands, 1-phenyl-3-[G-n]-4-phenylacetyl-5-pyrazolone (n = 0−3, G stands for polyaryl ether), were synthesized by introducing Fréchet-type dendritic branches. The corresponding Tb^{3+}-cored dendritic complexes were characterized by X-ray crystallography, elemental analysis, ESI mass spectra, and FT-IR spectra. These dendritic complexes, prepared from aqueous solution, exhibit high stability. Interestingly, the study of photophysical properties shows that the luminescence quantum yields of the dendritic Tb-complexes increase from 0.1 to 2.26% with an increase of the dendritic generation from 0 to 3. Importantly, an “energy-reservoir effect” was observed in the dendritic system using the method based on the resonance energy transfer from these complexes to rhodamine 6G. With the increase of the dendritic generation, the metal-centered luminescence quantum yield was almost the same, and the energy transfer ($\varphi_{transfer}$) from the ligand to Tb^{3+} increased. Further measurements of the triplet state and oxygen quenching of these dendritic complexes verify that this enhancement of the energy transfer ($\varphi_{transfer}$) is attributed to both an “antenna effect” and a “shell effect.**(6)**

Yasuro Shinohara, Jun-ichi Furukawa, Naoki Fujitani, Kayo Araki, Yasuhiro Takegawa, Kota Kodama reported that Post-translational modifications (PTMs) of serine and threonine occur by diverse mechanisms, including phosphorylation, sulfation, and various types of sugar chain modifications, making characterization of the resulting structures very labor-intensive. Moreover, to fully understand the biological functions of PTMs, both the sites of modification and the modified structures must be analyzed. The present work describes a novel, versatile strategy in which the released O-glycan and the formerly.**(7)**

It has been reported by Kishor Arora and Anu Parmar, In the present review a discussion of simulation of IR spectral studies of some organic compound is presented. This review contains 80 references.**(8)**

Mohamed Jawed Ahsan Jeyabalan Govinda Samy, et.al. reported that, In search of potential therapeutics for tuberculosis, we describe herewith the synthesis, characterization and ntimycobacterial activity of 1,5-dimethyl-2-phenyl-4-([5-(arylamino)-1,3,4-oxadiazol-2-yl]methylamino)-1,2-dihydro-3H-pyrazol-3-one analogues. Among the synthesized compounds, 4-[(5-[(4-fluorophenylamino]-1,3,4-oxadiazol-2-yl)methylamino]-1,2-dihydro-1,5-dimethyl-2-phenylpyrazol-3-one (4a) was found to be the most promising compound active against Mycobacterium tuberculosis $H_{37}Rv$ and isoniazid resistant M. tuberculosis with minimum inhibitory concentrations, 0.78 and 3.12 μg/mL, respectively, free from any cytotoxicity (>62.5 μg/mL).**(9)**

These have been reported by Julio Belmar, a, Fredy R. Pérezb, Joel Alderetea and Celia Zúñigaa that(10) 1-(n-Hexyl)-3-methyl-2-pyrazolin-5-one was acylated with acid chlorides. Condensation of acyl derivatives with primary amines afforded enamines. According to the 1H and 13C NMR data, the acyl derivatives have mainly a 4-acylpyrazol-5-ol structure with intramolecular hydrogen bond, and the 4-

aminomethylene derivatives exist predominantly in the enamine form stabilized by the same type of interaction.**(10)**

B. A. Uzoukwu, V. C. Ekeka, C. Ayozie & J. O. Onwuatu reported that the effect of sulphate ions in a buffered medium on the extraction of manganese(II) (Mn(II)) into 1-phenyl-3-methyl-4-butyryl-pyrazolone-5 (HBuP) in chloroform and benzene solutions has been studied. It showed that extraction at lower pH values is more favorable with solvents that have lower dielectric constants. It is also shown that an increase in sulphate ion concentration in the buffered medium leads to a decrease in Mn(II) extraction and a shift of the extraction process to higher pH values. Slight synergism occurred in the distribution of the metal ion into the benzene-butanol phase and data showed that pH was further shifted to lower values on the addition of butanol into either of the organic phases studied. The slope analysis indicated that $Mn(BuP)_2$ species were extracted during all the extraction processes. The extraction patterns from solutions of mineral acids, salting out, and auxiliary complexing agents were reported. The pH, log K and log K of all the extraction systems were determined and used for explaining the various extraction processes observed.**(11)**

Xingchen Yan, Xiaojing Wu et.al. These were reported, A potassium coordination polymer $[K_2(PMBP)_2(H_2O)_3]_n\cdot 2nH_2O$ (1) was prepared by reaction of 4-benzoyl-3-methyl-1-phenyl-2-pyrazolin-5-one (HPMBP) with potassium hydroxide. The single crystal of the supermolecule $C_6H_{11}NH_3^+\cdot PMBP^-$ (2) was then obtained by utilizing cyclohexylamine as the proton acceptor. It is a diketonate salt with an organic base where the $PMBP^-$ anions are stabilized by the intermolecular weak interactions (including hydrogen bonding, π–π stacking interactions and Van der Waals forces), rather than by coordination to a metal centre. Geometrical parameters of the isolated $PMBP^-$ anion were optimized through quantum chemistry calculation to simulate the state without any disturbances or interactions. Comparison of geometric parameters of compound 1 with the optimized structure of $PMBP^-$provides an approach to study weak intermolecular interactions in the crystal state. The coordination sites and the proton acceptors of hydrogen bonds predicted by theoretical calculations are consistent to the experimental result.**(12)**

M. L. P. Reddy, et.al. reported that Para-substituted 4-aroyl derivatives of 1-phenyl-3-methyl-5-pyrazolones (HX), namely, 1-phenyl-3-methyl-4- (4-fluorobenzoyl)-5-pyrazolone (HPMFBP) and 1-phenyl-3-methyl-4- (4-toluoyl)-5-pyrazolone (HPMTP) were synthesized and examined with regard to the extraction behavior of multivalent metal ions such as magnesium(II), aluminum(III), titanium(IV), vanadium(V), chromium(III), manganese(II), iron(II), and iron(III) that are present in titania waste chloride liquors. For comparison, studies have also been carried out with 1-phenyl-3-methyl-4-benzoyl-5-pyrazolone (HPMBP). The results demonstrate that vanadium(V) and iron(III) are extracted into chloroform with 4-aroyl-5-pyrazolones as $VO_2X \cdot HX$ and FeX_3, respectively. On the other hand, magnesium(II), aluminum(III), titanium(IV), chromium(III), manganese(II), and iron(II) were not found to be extracted into the organic phase. The equilibrium constants of vanadium(V) and iron(III) with various 4-aroyl-5-pyrazolones follow the order HPMFBP>HPMBP>HPMTP, which is in accordance with their pKa values. The selectivity between vanadium(V) and iron(III) increases with increasing hydrochloric acid concentration. Further, it is clear from the results that iron(III) is not getting extracted above 1.0 mol dm^{-3} hydrochloric acid solution. The electronic and IR spectra of the extracted complexes of vanadium(V) and iron(III) were used to further clarify the nature of the extracted complexes. The potential of these reagents for the selective extraction and separation of vanadium(V) from titania waste chloride liquors has also been discusse.**(13)**

These were reported by Bojan Burja,Tamara Čimbora-Zovko, et.al. A series of pyrazolone-fused combretastatins and precursors were synthesized and their cytotoxicity as well as antitubulin potential was evaluated. The hydrazide 9f and the pyrazolone-fused combretastatins 12a,12b and 12c were highly cytotoxic against various tumor cell lines including cisplatin resistant cells. The same compounds were also the best inhibitors of tubulin polymerization. Molecular modeling results showed that they bind the colchicine binding site at the tubulin heterodimer. The hydrazide 9f arrested HeLa cells in the G2/M phase of the cell cycle and strongly affected cell shape and microtubule network.**(14)**

Maria Atanassova, Vanya Kurteva, Lubomir Lubenov and Sabi Varbanov reported that, Synergistic solvent extraction of selected trivalent lanthanoids (La, Nd, Eu, Ho and Lu) with mixtures of a chelating extractants (HL), either 4-(4-fluorobenzoyl)-3-methyl-1-phenyl-pyrazol-5-one (HPMFBP) or 3-methyl-4-(4-methylbenzoyl)-1-phenyl-pyrazol-5-one (HPMMBP) and 5,11,17,23-tetra-tert-butyl-25,26,27,28-tetrakis-(dimethylphosphinoylmethoxy) calix[4] arene (S) in $CHCl_3$ from chloride medium has been studied. The interaction between the extractants in deuterochloroform has been examined by ^1H, ^{13}C and ^{31}P NMR spectra. The composition of the extracted species has been established as $LnL_3\cdot HL$ (HL and L^- represent either HPMFBP or HPMMBP and their anions, respectively). It has found that, in the presence of the phosphorus-containing calix[4]arene, the lanthanoids were extracted as $LnL_3\cdot S$. On the basis of the experimental data, the values of the equilibrium constants have been calculated. The influence of the para-substituted 4-aroyl-3-methyl-1-phenyl-pyrazol-5-ones on the extraction process has been discussed. The synergistic enhancement and separation factors between metals have been evaluated.**(15)**

These have been reported by Xue-Qin Song et.al., Two new structure-related pyrazolone-type Salen ligands, N,N′-ethylamine bis[1-(4-methoxy-phenyl)-3-methyl-4-benzoylimino-2-pyrazoline-5-ol](H_2L^I) and N,N′-ethylamine bis[1-(4-methoxy-phenyl)-3-methyl-4-acetylimino-2-pyrazoline-5-ol](H_2L^{II}) have been designed and synthesized with the ultimate aim of self-assembling novel Zn(II) compounds with interesting fluorescence properties. Reactions of $Zn(OAc)_2$ with the two ligands led to the formation of two new Zn(II) complexes with the formulae of $[ZnL^I(CH_3OH)]$ (1) and $[Zn_2L^{II}_2]$ (2), which have been characterized by single-crystal X-ray diffraction, powder X-ray diffraction, elemental analysis, IR spectroscopy and thermal gravimetric analysis. Mononuclear complex 1 with the pentacoordinated zinc(II) ion hosted into the N2O3 compartment crystallized in the monoclinic space group$P2_1/c$, while the hydroxyl-bridged dinuclear $[Zn_2L^{II}_2]$ complex (2) with the pentacoordinated zinc(II) ion hosted into the N2O2 compartment crystallized in the monoclinic space group C2/c and had a Zn–O–Zn–O four-membered ring. The structure determinations show that substituted group at the 4,4′-position of the this kind of Salen ligands are important factors influencing the crystalline array. The fluorescent properties of the two compounds at ambient temperature both in solid state and solution were also investigated. The results provided interesting insights into ligand effects on the structures and fluorescent properties of zinc(II) coordination complexes.**(16)**

It has been reported by Mehdi Abaszadeh, Hassan Sheibani and Kazem Saidi The addition of (chlorocarbonyl)phenyl ketene **2** to 5-alkylpyrazol-3(4H)-ones **1** led to the formation of 3-hydroxypyrazolo[1,2-a]pyrazole-dione/pyrazolo[1,2-a]pyrazole-trione derivatives **3**. This is ascribed to hydrogen exchange in initially formed unstable, mesoionic pyrazolo[1,2-a]pyrazol-4-ium-5-olates. In contrast, condensation of the same ketene with 3-alkyl-1-phenyl-2-pyrazolin-5-ones **4** afforded 4-hydroxy-3-alkyl-1,5-diphenylpyrano[2,3-c]pyrazol-6-one derivatives **5**. The latter reaction provides a new and rapid route to 4-hydroxy-2-pyrones fused to pyrazole rings, in good to excellent yields.**(17)**

Lucy C. Emeleus, Domenico C. Cupertino, Steven G. Harris, Susan Owens et.al Potentially bidentate 4-diazopyrazol-5-one ligands carrying a range of substituents can readily be prepared by coupling arene diazonium salts on to the appropriate pyrazolones.Hydrocarbon-soluble versions are shown to be suitable reagents for the recovery of copper bysolvent extraction from ammoniacal leach solutions, and potentially have greater resistance to chemical degradation than the β-diketones which have been used. Cobalt(III), nickel(II), copper(II) and zinc(II) complexes with 4-(4-tert-butylphenylazo)-3-methyl-1-phenyl-5-pyrazolone (HL) have been characterised by X-ray crystallography. The significant deviations from planar coordination geometry which are observed in $[CuL_2]$ and $[CuL'_2]$, where HL′ is 3-methyl-1-phenyl-4-phenylazo-5-pyrazolone, arise from interligand repulsion, and account for the relatively weak complexation and ease of stripping of copper from this class of extractant. The cobalt(III) complex $[CoL_3]\cdot 3MeOH$ and the high spin nickel(II) complex $[NiL_2(MeOH)_2]\cdot 2MeOH$ both have approximately octahedral geometries, but show significantly different bite distances in the chelate rings. The zinc complex $[ZnL_2]$ has a pseudo-tetrahedral structure.**(18)**

These have been reported by B. A. Uzoukwu, V. C. Ekeka, C. Ayozie & J. O. Onwuatu The effect of sulphate ions in a buffered medium on the extraction of manganese(II) (Mn(II)) into 1-phenyl-3-methyl-4-butyryl-pyrazolone-5 (HBuP) in chloroform and benzene solutions has been studied. It showed that extraction at lower pH values is more favorable with solvents that have lower dielectric constants. It is also shown that an increase in sulphate ion concentration in the buffered medium leads to a decrease in Mn(II) extraction and a shift of the extraction process to higher pH values. Slight synergism occurred in the distribution of the metal ion into the benzene-butanol phase and data showed that pH was further shifted to lower values on the addition of butanol into either of the organic phases studied. The slope analysis indicated that $Mn(BuP)_2$ species were extracted during all the extraction processes. The extraction patterns from solutions of mineral acids, salting out, and auxiliary complexing agents were reported. The pH, log K_D, and log K_{ex} of all the extraction systems were determined and used for explaining the various extraction processes observed.**(19)**

Sergey I. Levchenkov, Igor N. Shcherbakov et.al reported that The mononuclear copper(II) complex $[CuL(CH_3COO)]$, where L is monoanion of 1-phenyl-3-methyl-4-formylpyrazol-5-one 2-quinolylhydrazone has been synthesized. The weak intermolecular antiferromagnetic exchange interaction between copper(II) ions has been determined with the data of ESR spectroscopy and cryomagnetic measurements ($2J = -3.25\ cm^{-1}$). XRD data in combination with DFT calculations of exchange parameter within broken symmetry approach indicates that intermolecular exchange coupling is going through NH···O hydrogen bonds in centrosymmetric H-bonded dimers.**(20)**

Julio Belma, Fredy R. Pérez reported that 1-(n-Hexyl)-3-methyl-2-pyrazolin-5-one was acylated with acid chlorides. Condensation of acyl derivatives with primary amines afforded enamines. According to the ^1H and ^{13}C NMR data, the acyl derivatives have mainly a 4-acylpyrazol-5-ol structure with intramolecular hydrogen bond, and the 4-aminomethylene derivatives exist predominantly in the enamine form stabilized by the same type of interaction.**(21)**

These have been reported by Andrea Mazzanti, Teresa Calbet, Merce Font-Bardia et.al The enantioselective synthesis of pyrazol-3-ones has not been extensively studied in orgasynthesis. Here in we report the first asymmetric addition of pyrazolones to maleimidescatalyzed by bifunctional thiourea catalysts.**(22)**

Natarajan Raman, Muthusamy Selvaganapathy reported that Three novel mixed-ligand complexes using pyrazolone derivative (4-chloro-benzylidene-4-aminoantipyrine) as primary ligand and L-methionine as co-ligand, were synthesized and characterized by physico-chemical analytical techniques. The DNA interaction of these complexes was investigated by electronic absorption spectroscopy, viscosity, cyclic voltammetry and gel electrophoresis measurements. The results indicate that the complexes bind to DNA through intercalation and act as efficient cleaving agents. The in vitroantibacterial and antifungal assay indicates that these complexes are good antimicrobial agents against various pathogens.**(23)**

These have been reported by Maria Atanassova, Vanya Kurteva, et.al. Synergistic solvent extraction of selected trivalent lanthanoids (La, Nd, Eu, Ho and Lu) with mixtures of a chelating extractants (HL), either 4-(4-fluorobenzoyl)-3-methyl-1-phenyl-pyrazol-5-one (HPMFBP) or 3-methyl-4-(4-methylbenzoyl)-1-phenyl-pyrazol-5-one(HPMMBP)and5,11,17,23-tetra-tert-butyl-25,26,27,28-tetrakis-(dimethylphosphinoylmethoxy)calix[4]arene (S) in $CHCl_3$ from chloride medium has been studied. The interaction between the extractants in deuterochloroform has been examined by ^{1}H, ^{13}C and ^{31}P NMR spectra. The composition of the extracted species has been established as $LnL_3{\cdot}HL$ (HL and L^- represent either HPMFBP or HPMMBP and their anions, respectively). It has found that, in the presence of the phosphorus-containing calix[4]arene, the lanthanoids were extracted as $LnL_3{\cdot}S$. On the basis of the experimental data, the values of the equilibrium constants have been calculated. The influence of the para-substituted 4-aroyl-3-methyl-1-phenyl-pyrazol-5-ones on the extraction process has been discussed. The synergistic enhancement and separation factors between metals have been evaluated.**(24)**

These have been reported by Sieglinde Ebner, Bianca Wallfisch, John Andraos, et.al. Flash vacuum thermolysis (FVT) of 1-(dimethylamino) pyrrole-2,3-diones 5 causes extrusion of CO with formation of transient hydrazonoketenes 7. The transient ketenes 7 are observable in the form of weak bands at 2130 (7a) or 2115 cm^{-1} (7b) in the Ar matrix IR spectra resulting from either FVT or photolysis of either 5 or 1,1-dimethylpyrazolium-5-oxides 8, and these absorptions are in excellent agreement with B3LYP/6-31G frequency calculations. Under FVT conditions theketenes 7 cyclize to pyrazolium oxides 8, which undergo 1,4-migration of a methyl group to yield1,4-dimethyl-3-phenylpyrazole-5(4H)-one 9a and 1,4,4-trimethyl-3-phenylpyrazole-5(4H)-one 9b. All three tautomers of 9a have been characterized, viz. the CH form 9a (most stable form in the gas phase, the solid state and solvents of low polarity), the OH form 9a′ (metastable solid at room temperature) and the NH form 9a″ (stable in aprotic dipolar solvents). The isomeric 1,4-dimethyl-5-phenylpyrazole-3(2H)-one 12 tautomerizes to the 3-hydroxypyrazole 12′. The crystal structure of the hydrochloride 14 of 9a′/9a″ is reported, representing the first structurally characterised example of a protonated 5-hydroxypyrazole.**(25)**

Khandelwal, Anderson and Pluto reported that The molecular structures and infrared spectra of Co, Ni, Cu and Zn complexes of two schiff base ligands, viz N-(o-vanillinidene)sulfanilamide (oVSaH) and N-(o-vanillinidene)sulfamerazine (oVSmrzH) are studied in detail by PM3 method. It has been shown that the proposed structures for the compounds derived from microanalytical, magnetic and various spectral data were consistent with the IR spectra simulated by PM3 method. Coordination effects on ν(C[illegible]N) and ν(C–O) modes in the schiff base ligands are in close agreement with the observed results.**(26)**

A Filarowski, A Koll, M Rospenk, I Krol-Starzomska, P E Hansen have reported that A series of sterically hindered o-hydroxy Schiff bases derived from o-hydroxyaceto- and benzophenones with very short intramolecular hydrogen bonds were described qualitative and quantitatively by deuterium isotope effects on C-13 chemical shift, (n)Delta C(XD), (n)Delta F(XD), (1)J(N,H) coupling constants, delta NCH3 chemical shifts and UV spectra. All the investigated compounds are found to be tautomeric. The tautomeric character is described by the signs of the deuterium isotope effects on the C-13 chemical shifts. For the 3-nitro-5-chloro derivatives at low temperature, the equilibrium is shifted almost fully toward the proton transferred form in CD2Cl2. Intrinsic deuterium isotope effects on chemical shifts of these compounds as well as (1)J(N,H) coupling constants suggest that a zwitterionic resonance form is dominant for the proton transferred form. Structures, H-1, F-19, and C-13 chemical shifts, and deuterium isotope effects on C-13 chemical shifts are calculated by ab initio methods. The potential energy functions and the total deuterium isotope effects are calculated, and they are shown to correspond well with the experimental findings.**(27)**

These has been reported by Ganpat L. Talesara, Usha Ameta, Swati Ojha, et.al. A simple method for the synthesis of title compounds is reported, which were isolated from a series of reactions. After a nucleophilic reaction of 2-phenyl-3,1-benzoxazin-4(3H)-one (1) with thiosemicarbazide to furnish quinazolinylthiourea (2), followed by cyclisation with chloroacetic acid, 3-[(4-oxo-1,3-thiazolidin-2-yliden)amino]-2-phenylquinazolin-4(3H)-one (3) was yielded, which was converted to corresponding arylidene derivatives (5a-f) by treatment with various aldehydes (4a-f). Subsequent condensation of (5a-f) with phthalimidoxyethylbromide gave title compounds (7a-f). The structure of isolated compounds has been determined by means of IR, 1H NMR and mass spectroscopy.**(28)**

Arora Kishor and Singh Bhoop reported that The vibration modes of some synthetic compounds viz. derivatives of pyridines were examined 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. As well as, we report here frontier molecular orbitals (FMO) energy gap, molecular hardness (_), ionization energy (IE), electron affinity (EA), total energy and dipole moment of some pyridine derivatives supported by semi-empirical calculations, which properties provide the reactivity, stability and polarizabilities of the title compounds.**(29)**

Sieglinde Ebner, Bianca Wallfisch, John Andraos, Ilyas Aitbaev, have reported that Flash vacuum thermolysis (FVT) of 1-(dimethylamino)pyrrole-2,3-diones 5 causes extrusion of CO with formation of transient hydrazonoketenes 7. The transient ketenes 7 are observable in the form of weak bands at 2130 (7a) or 2115 cm_1 (7b) in the Ar matrix IR spectra resulting from either FVT or photolysis of either 5 or 1,1-dimethylpyrazolium-5-oxides 8, and these absorptions are in excellent agreement with B3LYP/6-31G frequency calculations. Under FVT conditions the ketenes 7 cyclize to pyrazolium oxides 8, which undergo 1,4-migration of a methyl group to yield 1,4-dimethyl-3-phenylpyrazole-5(4H)-one 9a and 1,4,4-trimethyl-3-phenylpyrazole-5(4H)-one 9b. All three tautomers of 9a have been characterized, viz. the CH form 9a (most stable form in the gas phase, the solid state and solvents of low polarity), the OH form 9a_ (metastable solid at room temperature) and the NH form 9a_ (stable in aprotic dipolar solvents). The isomeric 1,4-dimethyl-5-phenylpyrazole-3(2H)-one 12 tautomerizes to the 3-hydroxypyrazole 12_. The crystal structure of the hydrochloride 14 of 9a_/9a_ is reported, representing the first structurally characterised example of a protonated 5-hydroxypyrazole.**(30)**

It has been reported by Hiral S. Tailor that A large number of alkaloids, drugs, antibiotics, agrochemicals, and antimicrobial agents contains the quinazolone nucleus. They are essential component of very important naturallyoccurring substances (i.e. nucleic acids). The final product 6-Bromo-2-phenyl-3-[4-(3-substitutedphenylacryloyl)- phenyl]-3H-quinazolin-4-one is obtained from the starting reagent 2-amino benzoic acid via 4 step synthesis. All the compounds have characterized by IR & NMR spectra and elemental analysis.**(31)**

A. R. DESAI, R. U. ROY and K.R.DESAI reported that Several 2-[2-{(4-substitutedbenzylidene)-phenyl}vinyl]-4-oxo-3,4-dihydroquinazolone-6-sulfonicacid 4(a-l) and 2-[2-{4-(3-chloro-4-substituedphenylazetidin-2-one)-phenyl}vinyl]-4-oxo-3,4-dihydroqui-nazolone-6-sulfonic acid 5(a-l) were synthesized by using conventional techniques and were screened forantibacterial and antifungal activity. The compounds showed good to moderateantimicrobial activity and were characterized on the basis of spectral analysis.**(32)**

Charles R. Cornman, Katherine M. Geiser-Bush et.al. reported that [N,N‘-Ethylenebis (o-(tert-butyl-p-methylsalicylaldiminato)] oxovanadium(IV) (1), [N,N‘-propanediylbis (o-(tert-butyl-p-methylsalicylaldiminato)] oxovanadium(IV) (2), bis(N-methylsalicylaldiminato) oxovanadium(IV) (3), bis (N-isopropyl-o-methylsalicylaldiminato) oxovanadium(IV) (4), and, bis(N-methyl-o-(tert-butyl-p-methylsalicylaldiminato) oxovanadium(IV) (5) were prepared and characterized by X-ray crystallography and EPR spectroscopy. Complexes 1 and 2 are best described as square pyramids, while complexes 3−5 are distorted trigonal bipyramids, demonstrating that oxovanadium(IV) complexes can readily adopt a trigonal bipyramidal geometry. All five compounds give nearly the same parallel hyperfine coupling constant (A_z) regardless of the fact that the geometry about the vanadium changes from square pyramidal to trigonal bipyramidal. Crystal data for 1: space group $P\bar{1}$, a = 7.9382(3) Å, b = 12.6749(7) Å, c = 13.8353(7) Å, α = 109.608(5)°, β = 96.552(5)°, γ = 96.589(5)°, Z = 2. Crystal data for 2: space group $I4_1/a$, a = 16.1895(6) Å, b = 16.1895(6) Å, c = 41.117(3) Å, Z = 16. Crystal data for 3: space group C2/c, a = 18.8230(17) Å, b = 7.5118(5) Å, c = 11.7460(10) Å, β = 112.229(7)°, Z = 4. Crystal data for 4: space group $P2_1/c$, a = 9.7086(6) Å, b = 11.4554(7) Å,c = 20.866(2) Å, β = 103.943(6)°, Z = 4. Crystal data for 5: space group Pbca, a = 10.667(3) Å, b = 25.549(5) Å, c = 18.322(4) Å, Z = 8.**(33)**

These have been reported by Minoru Sugihara, Volker Buss, et.al. Density functional theory (DFT) calculations based on the self-consistent-charge tight-binding approximation have been performed to study the influence of the protein pocket on the 3-dimensional structure of the 11-cis-retinal Schiff base (SB) chromophore. Starting with an effectively planar chromophore embedded in a protein pocket consisting of the 27 next-nearest amino acids, the relaxed chromophore geometry resulting from energy optimization and molecular dynamics (MD) simulations has yielded novel insights with respect to the following questions: (i) The conformation of the β-ionone ring. The protein pocket tolerates both conformations, 6-s-cis and 6-s-trans, with a total energy difference of 0.7 kcal/mol in favor of the former. Of the two possible 6-s-cis conformations, the one with a negative twist angle (optimized value: −35°) is strongly favored, by 3.6 kcal/mol, relative to the one in which the dihedral is positive. (ii) Out-of-plane twist of the chromophore. The environment induces a nonplanar helical deformation of the chromophore, with the distortions concentrated in the central region of the chromophore, from C10 to C13. The dihedral angle between the planes formed by the bonds from C7 to C10 and from C13 to C15 is 42°. (iii) The absolute configuration of the chromophore. The dihedral angle about the C12−C13 bond is +170° from planar s-cis, which imparts a positive helicity on the chromophore, in agreement with earlier considerations based on theoretical and spectroscopic evidence.**(34)**

Abhiram Dukkipati, Anakarin Kusnetzow, Kunnel R. Babu, Lavoisier Ramos, Deepak Singh, Barry E. Knox, and Robert R. Birge have reported that The photochemical and subsequent thermal reactions of the mouse short-wavelength visual pigment (MUV) were studied by using cryogenic UV−visible and FTIR difference spectroscopy. Upon illumination at 75 K, MUV forms a batho intermediate (λ_{max} ~380 nm). The bathointermediate thermally decays to the lumi intermediate (λ_{max} ~440 nm) via a slightly blue-shifted intermediate not observed in other photobleaching pathways, BL (λ_{max} ~375 nm), at temperatures greater than 180 K. The lumi intermediate has a significantly red-shifted absorption maximum at 440 nm, suggesting that the retinylidene Schiff base in this intermediate is protonated. The lumi intermediate decays to an even more red-shifted meta Iintermediate (λ_{max} ~480 nm) which in turn decays to meta II (λ_{max} ~380 nm) at 248 K and above. Differential FTIR analysis of the 1100−1500 cm^{-1} region reveals an integral absorptivity that is more than 3 times smaller than observed in rhodopsin and VCOP. These results are consistent with an unprotonated Schiff base chromophore. We conclude that the MUV−visual pigment possesses an unprotonated retinylidene Schiff base in the dark state, and undergoes a protonation event during the photo bleaching cascade.**(35)**

These are reported Xiayan Wang, Zhaoxiang Deng, Baokang Jin, Yupeng Tian, Xiangqin Lin The mechanisms of the electron transfer of S-benzyl-N-(ferrocenyl-1-methyl-methylidene)-dithiocarbazate palladium(II)/zinc(II) complexes $[Pd(lsb)_2]$/$[Zn(lsb)_2]$ were studied by cyclic voltammetry, differential pulse voltammetry, digital simulation and in-situ subtractively normalized interfacial Fourier transform infrared (SNIFTIR) spectroelectrochemistry. The results indicate that $[Pd(lsb)_2]$, which has a square-planar configuration, involved two consecutive one-electron steps in the redox process, while the tetrahedral configuration of Zn(II) involved a two-electron step. The $[Pd(lsb)_2]$ complex exhibits a moderately strong electronic communication between the two-ferrocene moieties, which occurs through the skeleton chain of the ligand due to extensive electron delocalization of the whole molecule during the redox process, while the $[Zn(lsb)_2]$ complex shows low electron delocalization, and has two almost identical ferrocene moieties.**(36)**

Naomi Hoshino, Tamotsu Inabe, et.al. have reported that A thermochromic derivative of salicylideneaniline, N,N′-bis(salicylidene)-p-phenylenediamine (BSP), has been prepared and subjected to structural and optical studies in the crystalline state. An X-ray crystallographic analysis has shown that the molecules are planar and are stacked in a parallel fashion to form one-dimensional columns. The interplanar spacing has been found to be quite short, suggesting the existence of an intermolecular charge-transfer interaction. The molecule contains fairly short O–H··· N hydrogen bonds, the strength of which is manifested in an OH stretching absorption band in the infrared region, showing considerable broadening and a low-frequency shift. The BSP crystals are remarkably thermochromic, and visible absorption and emission spectral changes with temperature have been interpreted in terms of an intramolecular proton transfer from the hydroxyl oxygen to imine nitrogen through the O–H··· N hydrogen bond. The emission spectra have also been examined under high pressures.**(37)**

Matthias Georg Schwab, Birgit Fassbender, Hans Wolfgang Spiess, Arne Thomas, Xinliang Feng and Klaus Müllen have reported that Recently, the synthesis of organic materials with high porosity has received considerable scientific interest, and various chemical approaches have been applied to the build-up of microporous polymer networks. In a novel catalyst-free process using Schiff base chemistry, melamine has been reacted with various di- and trivalent aldehydes to form a series of highly cross-linked microporous aminal networks with BET surface areas as high as 1377 m^2/g and a NLDFT micropore volume of up to 0.41 cm^3/g. It was shown that through the proper choice of the starting compounds the porosity of the final material can be fine-tuned. The materials contain up to 40 wt % of nitrogen and were also found to exhibit high thermal stability. Owing to the cheap and abundant monomers used in this study these networks are promising candidates for large-scale applications in gas storage, gas separation, catalysis, and sensing.**(38)**

Perla Elizondo Martínez, Blanca Nájera Martínez reported that Our interest in Environmental Chemistry has prompted us to design new materials containing polyfunctional units able to bind certain metallic ions. These materials can be used as modifying agents to produce chemically modified electrodes. We expect to facilitate the detection of organic pollutants in water by binding these materials to an electrode surface. We report a Ni(II) and Co(II) complexes prepared from the Schiff base macroligand N,N´-bis(2-nitrobenzyl)ethylendiimine (L_1) with Ni(II) salt and L_1 with Co(II) salt. The nature of the complex was established by common spectroscopic techniques. A thermal gravimetric analysis of the complex showed that it is thermodynamically stable. Its formation constant was obtained by conductimetric analysis ($K_f = 1.25x10^6$). The affinity of L towards Ni(II) and Co(II) was determined by atomic absorption. The electrochemical study of the complex [Ni(II)-L_1]SO_4 was also performed by the cyclic voltammetry technique. The results showed that, under certain conditions, this complex is capable of polymerizing on the electrode surfaces made of vitreous carbon and indium tin oxide. The chemical modification on the surface was probed by exploring the cyclic voltammograms, which showed oxidation and reduction peaks that are characteristic of the Ni(II)/Ni(III) pair. The sensing capability towards 2,4-dichlorophenol of these modified electrodes is currently under study.**(39)**

It has been reported by Esin İspir Three novel Schiff base ligands containing the azo group, 2-((E)-(4-((E)-phenyldiazenyl)phenylimino)methyl)phenol, 3-((E)-(4-((E)-phenyldiazenyl)phenylimino)methyl)benzene-1,2-diol and 4-((E)-(4-((E)-phenyldiazenyl)phenylimino)methyl)benzene-1,2,3-triol, were synthesized from the reaction of p-aminoazobenzene with salicylaldehyde, 2,4-dihydroxybenzaldehyde and 2,3,4-trihydroxybenzaldehyde, respectively. The mononuclear Co(II) and Cu(II) complexes of the Schiff base ligands were prepared and characterized using elemental analyses, IR, UV–visible spectroscopy, magnetic susceptibility and conductance measurements; ^{1}H NMR and mass spectra of the ligands were also recorded. The Co(II) and Cu(II) metal complexes are formed by the coordination of the N and O atoms of the ligands. The electrochemical properties of the metal complexes were investigated at 100 mV s^{-1} scan rate in DMSO; the oxidative C–C coupling properties of the Co(II) and Cu(II) complexes were investigated on the sterically hindered 2,6-di-tert-butylphenol (DTBP). In addition, the Schiff base ligands and their complexes were evaluated for both their in vitro antibacterial activity using the disc diffusion method.**(40)**

Constantinos G. Neochoritis[a], Tryfon Zarganes-Tzitzikas[a], Constantinos A. Tsoleridis[a], et.al reported that The synthesis of a number of benzimidazole Schiff bases 3 and 3-oxo-pyrimido[1,2-a]benzimidazoles 4 in excellent yields by a one-step sequence from the reaction of 2-aminobenzimidazole under green chemistry conditions is described. Structural assignments of the new compounds as well as complete assignment of ^{1}H and ^{13}C NMR signals have been unambiguously achieved based on the analysis of their ^{1}H and ^{13}C NMR (1D and 2D), IR, MS and elemental analysis data. To the synthesized Schiff bases the E-configuration was assigned on the basis of comparison of experimental and calculated (DFT) ^{13}C NMR chemical shifts. Compounds 3 and 4 were evaluated as inhibitors of lipoxygenase (LOX) and of lipid peroxidation (LPO). All the tested derivatives showed inhibition of lipid peroxidation, whereas most of them were found to have higher activation than the reference compound trolox; The Schiff bases 3e, 3h, and 3i, and the pyrimidobenzimidazoles 4a, 4e and 4f were found to be the most potent. The most potent LOX inhibitor within the subset of Schiff bases was found compound 3i, followed by 3f, whereas compounds 4a and 4gwere found the most potent of the 3-oxo-pyrimido[1,2-a]benzimidazole group. Moreover, some cytotoxicity assessments were undertaken, whereupon it was found that Schiff base 3i and pyrimidobenzimidazoles 4eand 4f did not exhibit cytotoxicity at similar concentrations resembling thus the inhibitory activity of lipid peroxidation. The most cytotoxic Schiff base and pyrimidobenzimidazole were found to be 3d and 4c, respectively.**(41)**

Those were reported by Yann Pellegrin Dr., Annamaria Quaranta Dr. et.al. synthesis and characterisation of the heteroditopic ligand N,N′-bis(3,5-di-tert-butylsalicylidene)-5, 6-(1,10-phenanthroline)diamine ($DPSalH_2$) bearing a phenanthroline and a bis(salicylidene)diimine cavity are reported. This versatile ligand combines two of the most widely used ligands in coordination chemistry. Sequential metallation of the phenanthroline end with Ru^{II} and the salophenic cavity with Cu^{II} is described. Electrochemical behaviour of the supramolecular complexes $[Ru(bpy)_2(DPSalH_2)]^{2+}$ and $[Ru(bpy)_2(DPSalCu)]^{2+}$ are analysed in connection with UV/Vis and EPR spectroscopy. The data for the one-electron-reduced species and the singly oxidised species of the binuclear Ru^{II}–Cu^{II} complex confirmed the formation of metalloradical complexes. Density functional calculations on the free ligand and the copper-only complex indicate in both cases that the HOMOs and LUMOs are developed on the Schiff base cavity with minor contributions on the bipyridine end. These findings support a bichromophoric character for our ruthenium complexes in the ground state, a necessary condition in the design of supramolecular systems for the study of electron transfer. Photophysical studies indicate fast quenching of the triplet excited state in both complexes, which suggests strong intercomponent excited-state interactions. Evidence is presented that this quenching is due to intramolecular electron transfer, at least in the case of $[Ru(bpy)_2(DPSalH_2)]^{2+}$, for which a charge-separated state with a remarkable lifetime of about 30 μs was observed.**(42)**

It has been repoted by Lallan Mishra', Kumari Bindu, and Subarto Bhattacharya, Tetradentate Schiff bases N,N′-bis(salicylidene)-p-phenylenediamine (LH_2) and N,N′-bis(salicylidene)-benzidine, ($L'H_2$) are exploited for the syntheses of Cu(II) and Zn(II) based macrocyclic skeletons and it is found that four phenol molecules bind with a representative Zn(II) complex of LH_2.**(43)**

These have been reported by Partha Roy, Koushik Dhara, Mario Manassero and Pradyot Banerjeea that Three Schiff-base compounds, 4-methyl-2,6-bis(1-(2-piperidinoethyl)iminomethyl)-phenol (HL^1), 4-methyl-2,6-bis(1-(2-pyrrolidinoethyl)- iminomethyl)-phenol (HL^2) and (4-methyl-2,6-bis(1-(2-morpholinoethyl)iminomethyl)-phenol) (HL^3), have been synthesized and characterized by elemental analysis, FT-IR, ^{1}H NMR, UV–Vis, electrospray ionisation mass and fluorescence spectroscopy. The emission quantum yield of the compounds increases by ca. 10–17 times by the addition of Zn^{2+} ion. Introduction of other metal ions of biological and environmental relevance either keeps unaltered or quenches the emission intensity of the ligands. This happens because of large binding constant ($\sim 10^4$ M^{-1}) of the ligand with Zn^{2+} ion in acetonitrile. Each of the three ligands forms 1: 2 (ligand:metal) complexes which are characterized by single crystal X-ray diffraction analyses. This imposes rigidity to the ligand due to the complexation and, as a result, the radiative decay constant increases and the corresponding nonradiative decay parameter decreases. All of the ligands react with zinc chloride in acetonitrile to form dinuclear complexes which have been characterized by the elemental analysis, FT-IR, UV–Vis, electrospray ionisation mass spectroscopies and single crystal X-ray structural determinations.**(44)**

J.Costa Pessoa, I. Cavaco, et.al have reported that A range of mostly new oxovanadium(IV) complexes is described. They contain coordinated Schiff bases, made from natural amino acids (glycine, alanine, valine, leucine, isoleucine, methionine, phenylalanine, threonine, aspartic acid, and histidine) and salicylaldehyde or such derivatives as 3-, 4-, or 5-methoxy-salicylaldehyde. The coordination sphere is completed by simple ligands like water, 2,2′-bipyridyl or pyridine. The compounds are characterised and the nature of their coordination spheres shown by analysis, TLC, and by appropriate spectroscopy (EPR, IR, electronic and circular dichroism of solution and solids). In a few cases, magnetic properties are described to establish oxidation state. In several cases, the solubility of the compounds from racemic amino acids differs markedly from those containing the single enantiomer. The crystal and molecular structure of the related (and novel) compound with N-pyridoxylidene-D,L-isoleucinate, $[VO(pyr\text{-}D,L\text{-}Ile)(bipy)]\cdot H_2O$ is described. It contains two diastereomers. Denoting the chiral vanadium centres as **A** or **C**, these are and [**A**(pyr-L-Ile)(bipy)] [**C**(pyr-D-Ile)(bipy)].**(45)**

These have been reported by Adeola A. Nejo, Gabriel A. Kolawole, Andy R. Opoku, and Joanna Wolowska, A series of oxovanadium (IV) symmetrical tetradentate Schiff base complexes have been isolated from the reaction of $VOSO_4$ with Schiff bases obtained from the condensation of 2-hydroxybenzophenone or 2-hydroxy-5-chlorosalicylaldehyde with various aliphatic diamines. The compounds were characterized by elemental analyses, ^1H NMR, infrared, electron paramagnetic resonance, electronic spectral, cyclic voltammetry and room temperature magnetic susceptibility measurements. The solution EPR spectra are consistent with square pyramidal complexes with C_{4v} symmetry. The IR spectra confirmed that the complexes are all monomeric except for $[VO(Clsal)_2tn]$ which polymerizes via $O{=}V\cdots V{=}O$ linkages. The electronic spectra indicate a square pyramidal geometry in both non-coordinating and coordinating solvents except for $[VO(bp_2\text{-}pn)]$ which appears to be octahedral in DMSO. The room temperature magnetic moments of 1.7–1.8 B.M. are normal for V(IV) d^1 configuration. Evidence for electrochemical pseudo-reversibility is presented for four of the complexes. In vitro studies revealed that two of the compounds, $[VO(bp_2\text{-}en]$ and $[VO(bp_2\text{-}tn)MeOH]$, significantly increased glucose uptake when compared to the basal glucose uptake in transformed and sensitized C1C12 cells, but not at the same level as insulin.**(46)**

Ag. Stamatis, P. Doutsi, and Ch. Vartzouma, reported that Two new symmetrical acetylacetone-based Schiff bases, herein called L_A and L_B, have been synthesized. The complexes formed by their association with Mn(II) have been evaluated for catalytic alkene epoxidation with H_2O_2. The catalytic efficiency of $Mn(II)/L_A$ and $Mn(II)/L_B$ systems were shown to be switched on by ammonium acetate with remarkable effectiveness and selectivity towards epoxides. EPR spectroscopy for $Mn(II)/L_A$ shows that the catalytic centre is a mononuclear Mn complex. Additives that allow easier oxidation of Mn(II) to higher oxidation states, i.e. such as acetate and bicarbonate, can promote decisively the catalytic function. Additives that do not allow oxidation of Mn(II) to higher oxidation states, i.e. such as formate and oxalate, inhibit severely the catalytic function. Monocarboxylate ions, i.e. acetate, bicarbonate and formate do not disturb considerably the first coordination sphere of Mn(II). Dicarboxylate additives, i.e. such as oxalate, form strong complex with the Mn(II). Based on the catalytic and EPR data, a double role is suggested for ammonium acetate. This is to promote Mn(II) oxidation, and to function as a dual acid-base system, participating into the catalytic cycle.**(47)**

These have been reported by R.I Kureshy, N.H Khan, S.H.R Abdi, et.al. Some symmetrical and non symmetrical square planar Ni(II) chiral Schiff base complexes derived from 1S,2S(+)diaminocyclohexane, S(+)1,2-diaminopropane and 1R,2R(-)diphenyldiamino ethane with 3-acetyl-4-hydroxy-6-methyl-2-pyrone have been prepared. The characterization of the complexes was done by physico–chemical methods viz. microanalysis, conductance measurement, IR-, UV/visible-, ^1H-, $^{13}C\{^1H\}$NMR, CD spectral studies, optical rotation and cyclic voltammetry. These complexes catalyses the epoxidation of non-functionalized olefins viz. 1-hexene, 1-octene, trans-4-octene and indene with molecular oxygen as terminal oxidant in presence of the sacrificial reductant. Excellent chemical yield was obtained by GC with middle and terminal long chain alkenes than indene although the enantiomeric excess is good for indene with catalyst 3 and evaluated by ^1H NMR using chiral shift reagent $Eu(hfc)_3$ or by chiral capillary column on GC.**(48)**

C Topacli', and A Topacli have reported that The molecular structures and infrared spectra of Co, Ni, Cu and Zn complexes of two schiff base ligands, vizN-(o-vanillinidene)sulfanilamide (oVSaH) and N-(o-vanillinidene) sulfamerazine (oVSmrzH) are studied in detail by PM3 method. It has been shown that the proposed structures for the compounds derived from microanalytical, magnetic and various spectral data were consistent with the IR spectra simulated by PM3 method. Coordination effects on ν(C▒N) and ν(C–O) modes in the schiff base ligands are in close agreement with the observed results.**(49)**

Oleg N. Kadkin, Haksoo Han, and Yuri G. Galyametdinov reported that Rotationally fixed [3]ferrocenophane extends the variety of possible molecular geometries in its derivatives in comparison with unbridged ferrocenes. In this respect molecular geometry–liquid crystalline properties relationship studies in [3]ferrocenophane mesogens are of considerable interest. Different positional isomers of mono- and di-substituted [3]ferrocenophanes which are obtained by incorporating one or two promesogenic building blocks into the cyclopentadienyl rings are reported in this article. A series of mono-substituted [3]ferrocenophane-containing Schiff's bases was synthesized by condensing isomeric p-aminophenyl [3]ferrocenophanes with appropriate aldehydes. Isomers of di-substituted [3]ferrocenophane amines gave rise to a series of azomethines with two promesogenic substituents in the cyclopentadienyl rings. Besides, a β-enaminoketone was prepared from 3-(p-aminophenyl)[3]ferrocenophane. Nematic and smectic mesophases were observed in the synthesized compounds under a polarizing optical microscope. The [3]ferrocenophane-containing β-enaminoketone showed complex mesomorphic behaviour connected with occurrence of the keto-enamine and imino-enol tautomeric equilibrium in this compound. On the base of computational models obtained by semi-empirical quantum chemistry calculations the molecular geometry–phase behaviour relationships were examined. It was demonstrated that mesomorphism of [3]ferocenophane azomethines depends on the spatial orientation of the substituents with respect to the propanediyl bridge in a case of mono-, and as well as to each other in a case of di-substituted derivatives.**(50)**

These have been reported by Biswarup Sarkar, Michael G.B. Drew, Marta Estrader, that Two tridentate N,N,O donor Schiff bases, HL^1 (4-(2-ethylamino-ethylimino)-pentan-2-one) and HL^2 (3-(2-amino-propylimino)-1-phenyl-butan-1-one) on reaction with Cu^{II} acetate in presence of triethyl amine yielded two basal-apical, mono-atomic acetate oxygen-bridging dimeric copper(II) complexes, $[Cu_2L^1_2(OAc)_2]$ (1), $[Cu_2L^2_2(OAc)_2]$ (2). Whereas two other similar tridentate ligands HL^3 (4-(2-amino-propylimino)-pentane-2-one) and HL^4 (3-(2-amino-ethylimino)-1-phenyl-butan-1-one) under the same conditions produced a mixture of the corresponding dimers and a one-dimensional alternating chain of the dimer and copper acetate moiety, $[Cu_4L^3_2(OAc)_6]n$ (3) and $[Cu_4L^4_2(OAc)_6]n$ (4), formed by a very rare μ_3 bridging mode of the acetate ion. All four complexes (1–4) have been characterized by X-ray crystallography. The isotropic Hamiltonian,$H = -JS_1S_2$ has been used to interpret the magnetic data. Magnetic measurements of 1 and 2 in the temperature range 2–300 K reveal a very weak antiferromagnetic coupling for both complexes ($J = -0.56$ and $-1.19\ cm^{-1}$ for 1 and 2, respectively).**(51)**

These have been reported by M. Akbar Ali, Hjh Junaidah Hj Abu Bakar, et.al. that Complexes of general formula, $[M(isa\text{-}sme)_2] \cdot n(solvate)$ [$M = Ni^{2+}$, Cu^{2+}, Zn^{2+}, Cd^{2+}; isa-sme = monoanionic form of the Schiff base formed by condensation of isatin with S-methyldithiocarbazate;n = 1 or 1.5; solvate = MeCN, DMSO, MeOH or H_2O] have been synthesized and characterized by a variety of physicochemical techniques. An X-ray crystallographic structure determination of the $[Ni(isa\text{-}sme)_2] \cdot MeCN$ complex reveals a six-coordinate, distorted octahedral geometry. The two uninegatively charged, tridentate, Schiff base ligands are coordinated to the nickel(II) ion meridionally via the amide O-atoms, the azomethine N-atoms and the thiolate S-atoms. By contrast, the crystal structure of $[Zn(isa\text{-}sme)_2] \cdot MeOH$ shows a four-coordinate distorted tetrahedral geometry. The two dithiocarbazate ligands are coordinated as N, S bidentate chelates with the amide O-atom not coordinated. The structure of the copper(II) complex $[Cu(isa\text{-}sme)_2] \cdot DMSO$ is complicated and comprises two different complexes in the asymmetric unit, one four- and the other five-coordinate. The four-coordinate copper(II) has a distorted (flattened) tetrahedral geometry as seen in the Zn(II) analogue whereas the five-coordinate copper(II) has a distorted square-pyramidal geometry with one ligand coordinated to the copper(II) ion as a tridentate (N, S, O) ligand and the other coordinated as a bidentate N, S chelate. EPR spectroscopy indicates that in solution only one form is present, that being a distorted tetrahedral complex.**(52)**

It has been reported by Huijin Liu , Wangen Miao , and Xuezhong Du The chain orientation in the monolayers of amino-acid-derived Schiff base, 4-(4-dodecyloxy)-2-hydroxybenzylideneamino)benzoic acid (DSA), at the air−water interface has been determined using infrared reflection absorption spectroscopy (IRRAS). On pure water, a condensed monolayer is formed with the long axes of Schiff base segments almost perpendicular to the water surface. In the presence of metal ions (Ca^{2+}, Co^{2+}, Zn^{2+}, Ni^{2+}, and Cu^{2+}) in the subphase, the monolayer is expanded and the long axes of the Schiff base segments are inclined with respect to the monolayer normal depending on metal ion. The monolayer thickness, which is an important parameter for quantitative determination of orientation of hydrocarbon chains, is composed of alkyl chains and salicylideneaniline portions for the DSA monolayers. The effective thickness of the Schiff base portions is roughly estimated in the combination of the IRRAS results and surface pressure−area isotherms for computer simulation, since the only two observable p- and s-polarized reflectance−absorbance (RA) values can be obtained. The alkyl chains with almost all-trans conformations are oriented at an angle of about 10° for H_2O, 15° for Ca^{2+}, 30° for Co^{2+}, 35°−40° for Zn^{2+}, and 35°−40° for Ni^{2+} with respect to the monolayer normal. The chain segments linked with gauche conformers in the case of Cu^{2+} are estimated to be 40°−50° away from the normal.**(53)**

These has been reported by Hitoshi Miyasaka Prof., Tomokura Madanbashi, Kunihisa Sugimoto Dr. et.al. that An alternated 1:1 chain compound of a Mn^{III} salen derivative and the TCNQ monoradical was synthesized: [Mn(5-TMAMsaltmen)(TCNQ)]$(ClO_4)_2$ (1) (TCNQ=tetracyano-p-quinodimethane; 5-TMAMsaltmen=N,N′-(1,1,2,2-tetramethylethylene) bis(5-trimethylammoniomethylsalicylideneiminato)). Compound 1 has a zigzag chain structure packed with adjacent chains with an interchain Mn· · · Mn distance of over 8 Å. As compound 1 contains no crystallization solvent, the void spaces between chains are occupied only by ClO_4^- counter ions. Compound 1 has a structure reminiscent of what has been observed in the family of Mn^{III}(porphyrin)-TCNE or -TCNQ compounds reported previously by Miller and co-workers and we demonstrate herein its unique single-chain magnet behavior among this family of compounds. The direct current (dc) magnetic measurements established the one-dimensional nature of compound 1 with an antiferromagnetic exchange coupling, $J/k_B \approx -96$ K, between the Mn^{III} ion and TCNQ radical and with an activated correlation length (Δ_ξ=26.5 K) at low temperatures (50–15 K). The slow relaxation of the magnetization was shown in compound **1** by the field hysteresis of the magnetization observed below 3.5 K (with a coercive field up to 14 kOe at 1.8 K). Single-crystal magnetization measurements demonstrated the uniaxial symmetry of this compound and allowed an estimation of the anisotropy field, $H_a \approx 97$ kOe. The absence of magnetic ordered phase or spin-glass behavior was established by heat-capacity calorimetry measurements that exhibit no abnormality of C_p between 0.5 K and 10 K. The study of the magnetization relaxation by combined ac (alternating current) and dc techniques showed that compound 1 possesses a single relaxation time (τ). As the consequence of the finite size of the chain, the temperature dependence ofτ presents two activated regimes above and below 4.5 K with $\tau_{01}=2.1\times10^{-10}$ s, $\Delta\tau_1$=94.1 K and $\tau_{02}=6.8\times10^{-8}$ s and $\Delta\tau_2$=67.7 K, respectively. The detailed analysis of these dynamics properties together with the correlation length, allows an unambiguous demonstration of the single-chain magnet behavior in 1.**(54)**

It has been reported by Soumen Mukherjee, Thomas Weyhermüller, Eberhard Bothe, Karl Wieghardt and Phalguni Chaudhuri et.al that A pentadentate phenol-containing ligand (H_3L) with N_2O_3 donor atoms yields Ni^{II}_2 (1), Ni^{II}_4 (2), Cu^{II}_2 (3) and Cu^{II}_4 (4) complexes, which have been structurally characterized by X-ray diffraction. Complex **1** contains a single-atom O-bridged urea. The compounds were characterized by IR, UV/Vis, mass spectrometry, electrochemistry and variable-temperature (2−295 K) magnetic susceptibility measurements. Analysis of the susceptibility data shows antiferromagnetic interactions between the metal centers indicating a diamagnetic ground state for complexes 1, 3 and 4, whereas complex 2, a tetranuclear Ni^{II} cubane, has a complicated low-lying magnetic structure with a non-diamagnetic ground state. A plot of J vs. Ni−O−Ni angles for all structurally characterized Ni_4O_4 cubane cores, including 2, irrespective of their symmetry exhibits a large variation of J values within a small range of Ni−O−Ni angles. The electrochemistry of all complexes was investigated in detail and the ligand-centered oxidation to a radical-ligand is inferred from the occurrence of oxidation processes at potentials which are similar.**(55)**

G. Leniec, S.M. Kaczmarek, J. Typek, B. Kołodziej et.al. reported that Gadolinium(III) tripodal Schiff base (tris(((5-chlorosalicylidene)amino)ethyl)amine) complex has been obtained and investigated by infrared spectroscopy (IR), magnetic susceptibility, and electron paramagnetic resonance (EPR) methods. Comparison of IR bands in ligand and gadolinium complex confirmed the formation of the gadolinium complex and allowed to propose its structure. Both electron ionization and electron spray molecular spectroscopy spectra confirmed the [1:1] proportion of a ligand to metal in gadolinium tripodal Schiff base complex sample. IR spectroscopy and TG–DTA excluded the presence of water molecule in the metal coordination sphere. X-ray powder analysis applying Fullprof computer program has shown that the investigated sample was monophase with the monoclinic symmetry of the unit cell having the lattice constants: a = 10.028(4) Å, b = 13.282(5) Å, c = 21.20(1) Å and β = 101.58(4)°. Space group P21/c, Z = 4. EPR spectra of the complex have been registered in the 4–300 K temperature range. Each spectrum has been fitted using EPR–NMR computer program and the values of the spin-Hamiltonian parameters at each temperature have been calculated. Temperature dependence of the integrated intensity of the EPR spectrum allowed revealing the magnetic interactions in the spin system of this compound. Comparison of the temperature dependence of dc magnetic susceptibility (χ) and EPR susceptibility (χ_{EPR}) showed significant differences between these quantities due to the presence of short-lived clusters with a non-magnetic ground state.**(56)**

It has been reported by Michael J. Adam, Laurance D. Hall that Metal-complexing, salicylaldimine ligands 4, 7, 8, and 9 have been synthesized from 2-amino-2-deoxy-D-glucopyranose and some of its derivatives with salicylaldehyde and 3-formyl-2-hydroxybenzoic acid. Copper(II), zinc, and cobalt(II) complexes were formed from ligand 7, whereas only copper(II) would complex with ligand 8. The sugar ligand 4 forms a water-soluble complex with copper(II) and ligand 9 forms a binuclear copper(II) complex. These products have been studied by ^{1}H nmr, visible absorption, and esr spectroscopy, mass spectrometry, and by their magnetic moment data.**(57)**

Umberto Casellato, Paolo Guerriero, Sergio Tamburini, Pietro A. Vigato and Rodolfo Graziani have reported that Mono-and homo-binuclear uranyl(VI) complexes of the type $[UO_2(H_2L^1)]\cdot$solv, $[(UO_2)_2(L^1)(\text{solv})]$, $[UO_2(H_2L^2)]\cdot$solv, and $[(UO_2)_2(L^2)(\text{solv})]$, where solv is a co-ordinatingsolvent[H_2O, dimethylformamide (dmf), or dimethyl sulphoxide (dmso)] and H_4L^1 and H_4L^2 are the potentially heptadentate dinucleating ligands derived by the condensation of 2,3-dihydroxybenzaldehyde with 1,5-diamino-3-azapentane or 1,5-diamino-3-thiapentane, have been prepared by a template procedure or by reaction of the preformed ligands with $[UO_2(CH_3CO_2)_2]\cdot 2H_2O$ and characterized by i.r., ^{1}H and ^{13}C n.m.r. spectroscopic and X-ray diffraction techniques. The crystal structures of $[UO_2(H_2L^1)]\cdot$dmf, $[(UO_2)_2(L^1)(\text{dmso})]$, and $[(UO_2)_2(L^1)(\text{dmf})]$ have been determined by X-ray crystallography and refined to conventional R values of 0.044, 0.054, and 0.039 respectively: $[UO_2(H_2L^1)]\cdot$dmf is monoclinic, space group $P2_1/n$, with a= 21.155(5), b= 11.833(8), c= 9.679(8)Å, β= 102.34(3)°, Z= 4; $[(UO_2)_2(L^1)(\text{dmso})]$ is monoclinic, space group$P2_1/c$, with a= 14.985(5), b= 16.536(5), c= 19.956(5)Å, β= 90.13(3)°, Z= 8; $[(UO_2)_2(L^1)(\text{dmf})]$ is monoclinic, space group $P2_1/c$, with a= 9.285(6), b= 16.187(5), c= 17.544(5)Å, β= 104.56(3)°, and Z= 4. In $[UO_2(H_2L^1)]\cdot$dmf the ligand behaves as a quinquedentate dianionic and, using the inner co-ordination chamber, binds equatorially to UO_2^{2+} leading to seven-co-ordinated uranium in a distorted bipyramidal co-ordination geometry. A dmf molecule is hydrogen bonded to the phenolic oxygens of the ligand. Selected bond distances for this compound are U–O(uranyl) 1.79 (mean), U–O(ligand) 2.235 (mean), and U–N (mean) 2.59 Å. In $[(UO_2)_2(L^1)(\text{dmso})]$ and $[(UO_2)_2(L^1)(\text{dmf})]$ the tetra-anionic chelating ligand co-ordinates the inner UO_2^{2+} as in $[UO_2(H_2L^1)]\cdot$dmf, while the outer UO_2^{2+} is co-ordinated by four oxygen atoms of the dinucleating ligand and by the oxygen atom of the solvent molecule. Structural details of the binuclear complexes are comparable. Comparison of the structures in the solid and in solution revealed some conformational differences.**(58)**

Those were reported by Mohammad Akbar Ali, A.H Mirza, Thahira B.S.A Ravoof, Paul V Bernhardt that New mixed-ligand copper(II) complexes of empirical formulas $[Cu(pysme)(sac)\ (CH_3OH)]$ and $[Cu(6mptsc)(sac)]_2$ have been synthesized and characterized by conductance, magnetic, IR and electronic spectroscopic techniques. X-ray crystallographic structure analyses of these complexes indicate that in both complexes the copper(II) ions adopt a five-coordinate distorted square-pyramidal geometry with an N_3SO donor environment. The Schiff bases are coordinated to the copper(II) ions as tridentate NNS chelates via the pyridine nitrogen atom, the azomethine nitrogen atom and the thiolate sulfur atom. In the monomeric [Cu(pysme)(sac)(MeOH)] complex, the saccharinate anion acts as a monodentate ligand coordinating the copper(II) ion via the imino nitrogen atom whereas in the dimeric $[Cu(6mptsc)(sac)]_2$ complex, the sac anion behaves as a bridging bidentate ligand providing the imino nitrogen donor atom to one of the copper(II) ions and the carbonyl oxygen as a weakly coordinated axial ligand atom to the other Cu(II) ion. In both complexes, the copper(II) ions have distorted square-pyramidal environments. The distortion from an ideal square-pyramidal geometry is attributed to the restricted bite angles of the planar tridentate ligand.**(59)**

Irina Cârlescu, Ana Maria Scutaru, et.al reported that The synthesis and characterization of new ferrocene-containing mesomorphous compounds is described. In order to induce mesogenic behavior, the structure of the substituent was systematically modified. Derivatives with no more than two rings in the core did not exhibit liquid crystalline properties. The synthesized products were characterized using NMR, IR and mass spectroscopy, DSC and polarized optical microscopy.**(60)**

Topacli a reported that The molecular structures and infrared spectra of Co, Ni, Cu and Zn complexes of two schiff base ligands, viz N-(o-vanillinidene)sulfanilamide (oVSaH) and N-(o-vanillinidene)sulfamerazine (oVSmrzH) are studied in detail byPM3 method. It has been shown that the proposed structures for the compounds derived from microanalytical, magnetic and various spectral data were consistent with the IR spectra simulated by PM3 method. Coordination effects on v(C=N) and v(C-O) modes in the schiff base ligands are in close agreement with the observed results.**(61)**

These have been reported by Goran Zgrablić, Kislon Voïtchovsky, Maik Kindermann, et.al that esent a comparative study of the ultrafast photophysics of all-trans retinal in the protonated Schiff base form in solvents with different polarities and viscosities. Steady-state spectra of retinal in the protonated Schiff base form show large absorption-emission Stokes shifts (6500–8100 cm^{-1}) for both polar and nonpolar solvents. Using a broadband fluorescence up-conversion experiment, the relaxation kinetics of fluorescence is investigated with 120 fs time resolution. The time-zero spectra already exhibit a Stokes-shift of ∼6000 cm^{-1}, indicating depopulation of the Franck-Condon region in ≤100 fs. We attribute it to relaxation along skeletal stretching. A dramatic spectral narrowing is observed on a 150 fs timescale, which we assign to relaxation from the S_2 to the S_1 state. Along with the direct excitation of S_1, this relaxation populates different quasistationary states in S_1, as suggested from the existence of three distinct fluorescence decay times with different decay associated spectra. A 0.5–0.65 ps decay component is observed, which may reflect the direct repopulation of the ground state, in line with the small isomerization yield in solvents. Two longer decay components are observed and are attributed to torsional motion leading to photo-isomerization. The various decay channels show little or no dependence with respect to the viscosity or dielectric constant of the solvents. This suggests that in the protein, the bond selectivity of isomerization is mainly governed by steric effects.**(62)**

P. N. Remya, D. B. Ambili Raj & M. L. P. Reddy reported that Para substituted 4 aroyl derivatives of 1phenyl 3 methyl 5 pyrazolones (HX), namely, 1 phenyl 3 methyl 4 (4 fluorobenzoyl) 5 pyrazolone (HPMFBP) and phenyl 3 methyl 4 (4 toluoyl) 5 pyrazolone (HPMTP) were synthesized and examined with regard to the extraction behavior of multivalent metal ions such as magnesium(II), aluminum(III), titanium(IV), vanadium(V), chromium(III), manganese(II), iron(II), and iron(III) that are present in titania waste chloride liquors. For comparison, studies have also been carried out with 1 phenyl 3 methyl 4 benzoyl 5 pyrazolone (HPMBP). The results demonstrate that vanadium(V) and iron(III) are extracted into chloroform with 4 aroyl 5 pyrazolones as $VO_2X \cdot HX$ and FeX_3, respectively. On the other hand, magnesium(II), aluminum(III), titanium(IV), chromium(III), manganese(II), and iron(II) were not found to be extracted into the organic phase. The equilibrium constants of vanadium(V) and iron(III) with various 4 aroyl 5 pyrazolones follow the order HPMFBP>HPMBP>HPMTP, which is in accordance with their pKa values. The selectivity between vanadium(V) and iron(III) increases with increasing hydrochloric acid concentration. Further, it is clear from the results that iron(III) is not getting extracted above 1.0 mol dm^{-3} hydrochloric acid solution. The electronic and IR spectra of the extracted complexes of vanadium(V) and iron(III) were used to further clarify the nature of the extracted complexes. The potential of these reagents for the selective extraction and separation of vanadium(V) from titania waste chloride liquors has also been discussed.**(63)**

Sieglinde Ebner, Bianca Wallfisch, John Andraos, et.al. have reported that Flash vacuum thermolysis (FVT) of 1-(dimethylamino)pyrrole-2,3-diones 5 causes extrusion of CO with formation of transient hydrazonoketenes 7. The transient ketenes 7 are observable in the form of weak bands at 2130 (7a) or 2115 cm^{-1} (7b) in the Ar matrix IR spectra resulting from either FVT or photolysis of either 5 or 1,1-dimethylpyrazolium-5-oxides 8, and these absorptions are in excellent agreement with B3LYP/6-31G frequency calculations. Under FVT conditions theketenes 7 cyclize to pyrazolium oxides 8, which undergo 1,4-migration of a methyl group to yield1,4-dimethyl-3-phenylpyrazole-5(4H)-one 9a and 1,4,4-trimethyl-3-phenylpyrazole-5(4H)-one 9b. All three tautomers of 9a have been characterized, viz. the CH form 9a (most stable form in the gas phase, the solid state and solvents of low polarity), the OH form 9a′ (metastable solid at room temperature) and the NH form 9a″ (stable in aprotic dipolar solvents). The isomeric 1,4-dimethyl-5-phenylpyrazole-3(2H)-one 12 tautomerizes to the 3-hydroxypyrazole 12′. The crystal structure of the hydrochloride 14 of 9a′/9a″ is reported, representing the first structurally characterised example of a protonated 5-hydroxypyrazole.**(64)**

A Filarowski, A Koll, M Rospenk, I Krol-Starzomska, P E have reported that the Series of sterically hindered o-hydroxy Schiff bases derived from o-hydroxyaceto- and benzophenones with very short intramolecular hydrogen bonds were described qualitative and quantitatively by deuterium isotope effects on C-13 chemical shift, (n)Delta C(XD), (n)Delta F(XD), (1) J(N,H) coupling constants, delta NCH3 chemical shifts and UV spectra. All the investigated compounds are found to be tautomeric. The tautomeric character is described by the signs of the deuterium isotope effects on the C-13 chemical shifts. For the 3-nitro-5-chloro derivatives at low temperature, the equilibrium is shifted almost fully toward the proton transferred form in CD2Cl2. Intrinsic deuterium isotope effects on chemical shifts of these compounds as well as (1)J(N,H) coupling constants suggest that a zwitterionic resonance form is dominant for the proton transferred form. Structures, H-1, F-19, and C-13 chemical shifts, and deuterium isotope effects on C-13 chemical shifts are calculated by ab initio methods. The potential energy functions and the total deuterium isotope effects are calculated, and they are shown to correspond well with the experimental findings.**(65)**

Y M Issa, H B Hassib, H E Abdelaal and I M Kenawi have reported that 3-Amino-1,2,4-triazole Schiff bases were reported to contain intramolecular charge-transfer. The enhancing and depressing effects were remarkable as the substituent was changed from electron-donating to electron-withdrawing groups. The path of the resonating delocalization was reversed in the case of the p-NO2 group. To validate these results we effectively used Weinhold et al's natural bond orbital analysis to assess the UV and FT-IR spectrophotometric monitoring of the change reflected in this phenomenon when the substituent in the benzene ring is altered. The NBO analysis was simulated by ab inito computations at the HF/6-31G(d) level of theory, in order to properly detect any possible presence of a hydrogen bond association. The changes occurring in electron occupancies of double-centered bonds, antibonding orbitals and in lone-pair orbitals appraised the results, as did the s and p character listings of the two-centered bonds and the simultaneous changes occurring in the geometric parameters of the molecules in question. Contrary to its normal preference, in these molecules the nitrogen used sp2 hybrid orbitals for its interaction, housing its electron lone-pair in the third p hybrid orbital. Furthermore, NBO analysis reflected the presence of a very soft intramolecular hydrogen association (C-H$\cdots\pi$), labelled by UV and FT-IR assignments, between the benzene and triazole rings in all Schiff bases but p-N(Me)2. The n-π stabilization energy decreased in the order: p-OH>p-OCH3>p-Cl>p-CH3>H>p-NO2>o-OH. The relation between the band position and Hammett substitution constant is interpreted in relation to the molecular structure.**(66)**

These have been reported by Harshita Sachdeva, Rekha Saroj, Sarita Khaturia,et.al that chemical one-pot multicomponent condensation reaction of substituted 1H-indole-2,3-diones (1), various amino acids (2), and thiosemicarbazide (3) is found to be catalyzed by lemon juice as natural acid using water as a green solvent to give the corresponding Schiff bases (4) in good to excellent yields. This method is experimentally simple, clean, high yielding, and green, with reduced reaction times. The product is purified by simple filtration followed by washing with water and drying process. The synthesized compounds are characterized by FT-IR, ^{13}CNMR, and ^{1}HNMR spectroscopy and are screened for their antifungal activity against Aspergillus niger, Penicillium notatum, Fusarium oxysporum, Alternaria brassicicola, Chaetomium orium, and Lycopodium sp. and antibacterial activity against Gram-positive bacteria, Bacillus licheniformis,Staphylococcus aureus, and Micrococcus luteus, and Gram-negative bacteria, Pseudomonas aeruginosa andEscherichia coli. Compounds have also been evaluated for cytotoxic effects against human colon cancer cell line Colo205.**(67)**

It has been reported by P E Hansen, J Sitkowski, L Stefaniak, Z Rozwadowski, T Dziembowska (1998) that A series of N-15 enriched Schiff bases have been investigated by means of N-15 NMR at variable temperature (300-200 K). Most realiable results are obtained below 250 K, as the exchange of the chelate proton is sufficiently slow on the NMR time scale at this temperature. The N-15 chemical shifts are found to vary linearly with the one bond N-15-H coupling constants. Deuterium isotope effects on N-15 chemical shifts, (1) Delta(15)N(D), show a characteristic S-shape, when plotted vs. the one-bond N-15-H coupling constants. From this graph the intrinsic isotope effects of the two forms can be estimated as (5) Delta(15)N(D)(int)similar to-1.5 ppm and (1) Delta(15)N(D)(int)similar to 3 ppm. The intrinsic isotope effects for the OH-form is shown to vary only little for the various substituted compounds investigated. The difference in N-15 chemical shifts of the OH-form minus the NH-form is estimated to 100-140 ppm. The dependence of (1) Delta(15)N(D) on the mole fraction is similar to that found for (2) Delta C(OD) for other intramolecularly hydrogen bonded cases, beta-diketones and Mannich bases and looks very similar to that determined for (1) Delta(15)N(D) of the organic acid-pyridine complex.**(68)**

P E Hansen, Z Rozwadowski, T Dziembowska reported that The review covers the use of chemical shifts, isotope effects on chemical shifts and coupling constants in the description of Schiff bases. o-Hydroxy Schiff bases are often tautomeric and special attention is devoted to this feature. Nuclei in question are H-1, C-13, N-15, F-19 and O-17. As well primary as secondary isotope effects are treated. Deuterium isotope effects on C-13 and N-15 chemical shifts are treated in detail and the theoretical background is dealt with. Finally, various applications of Schiff bases in biology and stereochemistry are discussed.**(69)**

P M Dominiak, A Filarowski, P E Hansen, and K Wozniak reported that we have analyzed deuterium isotope effects on C-13 chemical shifts in a series of o-hydroxy Schiff bases by applying factor analysis. Two orthogonal factors were obtained that explain about 80 and 10% of the variance of the data. The numerical values of these factors can be related to H-1 NMR chemical shifts of the proton involved in the intramolecular bonds delta(XH) (X=O or N). Such a relation allows one to identify clusters of compounds with different tautomeric forms of hydrogen bonding. Application of a similar approach to solution C-13 NMR chemical shifts produces three important factors. which have a different structure to factors describing isotope effects. This illustrates well the different nature of chemical shifts and isotope effects. the three factors explain about 54, 15, and 13% of variance. They can be rationalized and are strongly related to the electronic properties and location of substituent.**(70)**

Q T That, K P P Nguyen, P E Hansen have reported that Schiff bases of gossypol with benzylamine, methylamine, 4-aminoacetophenone and 4-fluoroaniline have been synthesized and characterized by NMR spectroscopy. All the Schiff bases of gossypol are in the enamine form according to (3)J(HC,NH) and (1)J(,H) coupling constants. The spectra are basically unchanged by change of solvent (CD2Cl2, THF-d(8) and CD3OD) and by variation of temperature. For the derivative of benzylamine, deuterium isotope effects on C-13 chemical shifts are determined. They support strongly the enamine form and serve as a reference for other tautomeric Schiff bases. Structures and NMR nuclear shieldings of model compounds (the second monomer is replaced by a 2-hydroxybenzene ring) have been calculated by density functional theory (DFT) methods. A good correlation is observed between calculated C-13 nuclear shieldings of the enamine form and observed C-13 chemical shifts.**(71)**

These have been reported by Sachdeva H., Dwivedi, D. Arya, K. Khaturia, S. and Saroj R. that The purpose of this research is to synthesize better anti-inflammatory compounds derived from 5-mercapto-3-(4′-pyridyl)-4H-1,2,4-triazol-4-yl- thiosemicarbazide (5). 2-Substituted-N-[3-(pyridin-4-yl)-5-sulfanyl-4H-1,2,4-triazol-4-yl]hydrazine carbothioamide derivatives (6a-j)/(7a-e) are synthesized by the condensation of 5 with variously substituted aromatic aldehydes/1H-indole-2,3-diones, respectively, under conventional and microwave irradiation methods. The microwave method is found to be superior with higher chemical yields, tremendous reduction in time, and is environmentally benign as compared to conventional heating method. The chemical structures of the newly synthesized compounds (6/7) have been confirmed by IR, ^{1}H NMR, and ^{13}C NMR spectra and have been evaluated for anti-inflammatory activity by carrageenan-induced acute paw edema method in rats.**(72)**

Sachdeva H., Saroj R., Khaturia S., et.al reported that Green chemical one-pot multicomponent condensation reaction of substituted 1H-indole-2,3-diones (1), various amino acids (2), and thiosemicarbazide (3) is found to be catalyzed by lemon juice as natural acid using water as a green solvent to give the corresponding Schiff bases (4) in good to excellent yields. This method is experimentally simple, clean, high yielding, and green, with reduced reaction times. The product is purified by simple filtration followed by washing with water and drying process. The synthesized compounds are characterized by FT-IR, ^{13}CNMR, and ^{1}HNMR spectroscopy and are screened for their antifungal activity against Aspergillus niger, Penicillium notatum, Fusarium oxysporum, Alternaria brassicicola, Chaetomium orium, and Lycopodium sp. and antibacterial activity against Gram-positive bacteria, Bacillus licheniformis, Staphylococcus aureus, and Micrococcus luteus, and Gram-negative bacteria, Pseudomonas aeruginosa and Escherichia coli. Compounds have also been evaluated for cytotoxic effects against human colon cancer cell line Colo205.**(73)**

Raafat M. Issa, Abdalla M. Khedr and Helen Rizk have reported that By condensing 2-aminobenzothiazole with 2-hydroxy-1-naphthaldehyde, 2-hydroxybenzaldehyde, 4-methoxybenzaldehyde, 4-hydroxybenzal-dehyde, benzaldehyde and 4-dimethylaminobenzaldehyde, and five Schiff bases Ia-Ie are prepared. Also, two Schiff bases IIa and IIb are prepared by condensation of 2-amino-3-hydroxypyridine with 2-hydroxy-1-naphthaldehyde and 2-hydroxybenzaldehyde. The^{1}H NMR, IR and UV/Vis spectra of these seven Schiff bases are investigated. The signals of the ^{1}H NMR spectra as well as the important bands in the IR spectra are considered and discussed in relation to molecular structure. The UV/Vis absorption bands in ethanol are assigned to the corresponding electronic transitions and the electronic absorption spectra of Schiff bases Ib and IIb are studied in organic solvents of different polarities. The UV/Vis absorption spectra of 2-amino-3-hydroxypyridine Schiff bases IIa and IIb are investigated in buffer solutions of different pH values containing 5% (v/v) methanol, and the results are utilized for the determination of pK_a and ΔG of the ionization of the phenolic OH-groups. The fluorescence spectra of IIa and IIb are studied in organic solvents of different polarities. The obtained spectral results are confirmed by some molecular calculations using the atom super position and electron delocalization molecular orbital theory for the Schiff base IIb.**(74)**

Ganpat L. Talesara, Usha Ameta, Swati Ojha, Dinesh Bhambi, and have reported that A simple method for the synthesis of title compounds is reported, which were isolated from a series of reactions. After a nucleophilic reaction of 2-phenyl-3,1-benzoxazin-4(3H)-one (1) with thiosemicarbazide to furnish quinazolinylthiourea (2), followed by cyclisation with chloroacetic acid, 3-[(4-oxo-1,3-thiazolidin-2-yliden)amino]-2-phenylquinazolin-4(3H)-one (3) was yielded, which was converted to corresponding arylidene derivatives (5a-f) by treatment with various aldehydes (4a-f). Subsequent condensation of (5a-f) with phthalimidoxyethylbromide gave title compounds (7a-f). The structure of isolated compounds has been determined by means of IR, ^{1}H NMR and mass spectroscopy.**(75)**

Arora Kishor and Singh Bhoop reported that The vibration modes of some synthetic compounds viz. derivatives of pyridines were examined 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. As well as, we report here frontier molecular orbitals (FMO) energy gap, molecular hardness (_), ionization energy (IE), electron affinity (EA), total energy and dipole moment of some pyridine derivatives supported by semi-empirical calculations, which properties provide the reactivity, stability and polarizabilities of the title compounds.**(76)**

These have been reported by Sieglinde Ebner, Bianca Wallfisch et.al that Flash vacuum thermolysis (FVT) of 1-(dimethylamino)pyrrole-2,3-diones 5 causes extrusion of CO with formation of transient hydrazonoketenes 7. The transient ketenes 7 are observable in the form of weak bands at 2130 (7a) or 2115 cm_1 (7b) in the Ar matrix IR spectra resulting from either FVT or photolysis of either 5 or 1,1-dimethylpyrazolium-5-oxides 8, and these absorptions are in excellent agreement with B3LYP/6-31G frequency calculations. Under FVT conditions the ketenes 7 cyclize to pyrazolium oxides 8, which undergo 1,4-migration of a methyl group to yield 1,4-dimethyl-3-phenylpyrazole-5(4H)-one 9a and 1,4,4-trimethyl-3-phenylpyrazole-5(4H)-one 9b. All three tautomers of 9a have been characterized, viz. the CH form 9a (most stable form in the gas phase, the solid state and solvents of low polarity), the OH form 9a_ (metastable solid at room temperature) and the NH form 9a_ (stable in aprotic dipolar solvents). The isomeric 1,4-dimethyl-5-phenylpyrazole-3(2H)-one 12 tautomerizes to the 3-hydroxypyrazole 12_. The crystal structure of the hydrochloride 14 of 9a_/9a_ is reported, representing the first structurally characterised example of a protonated 5-hydroxypyrazole.**(77)**

It has been reported by Hiral S. Tailor that A large number of alkaloids, drugs, antibiotics, agrochemicals, and antimicrobial agents contains the quinazolone nucleus. They are essential component of very important naturally occurring substances (i.e. nucleic acids). The final product 6-Bromo-2-phenyl-3-[4-(3-substitutedphenylacryloyl)- phenyl]-3H-quinazolin-4-one is obtained from the starting reagent 2-amino benzoic acid via 4 step synthesis. All the compounds have characterized by IR & NMR spectra and elemental analysis.**(78)**

A. R. DESAI, R. U. ROY and K.R.DESAI have reported that Several 2-[2-{(4-substitutedbenzylidene)-phenyl}vinyl]-4-oxo-3,4- dihydroquinazolone-6-sulfonicacid 4(a-l) and 2-[2-{4-(3-chloro-4-substituedphenylazetidin-2-one)-phenyl}vinyl]-4-oxo-3,4-dihydroqui-nazolone-6-sulfonic acid 5(a-l) were synthesized by using conventional techniques and were screened for antibacterial and antifungal activity. The compounds showed good to moderate
antimicrobial activity and were characterized on the basis of spectral analysis.**(79)**

It has been reported by Kishor Arora, Bhoop singh Yadav and SK Mishra that The vibration modes of some pyrazolone compounds were examined 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)**

These have been reported by Amira S. Abd El-A 1 ll, 2Fatma A.F. Ragab, 1Asmaa A. Magd El-Din,et.al that This research deals with an efficient green chemistry for synthesizing a series of Schiff bases 3a-m incorporating 4-1H-benzo[d] imidazole moiety, by microwave technique and heating conventional procedures which are used for their preparation. The newly synthesized Schiff bases are obtained by the reaction of 4-(1H-benzo[d]imidazol-2yl) aniline 1 with a series of different aromatic aldehydes 2a-m. This work aims to make a comparison between conventional and microwave irradiation methods. The design of selected newly Schiff bases is defined by molecular modeling. The evaluation of anticancer activities of synthesized Schiff bases are investigated against human cancer cell lines; Co rectal cancer cell line HCT116, human liver cancer cell line HepG2 and human ovarian cancer cell line A2780, the results show that compounds 3c,3f,3g have more activity than the comparing drug CK0106023. All the synthesized compounds are characterized by their elemental analysis, IR, 1H-NMR and Mass spectral studies.**(81)**

It has been reported by Kui Cheng, Qing-Zhong Zheng, Yong Qian, et.al that A series of peptide and Schiff bases (PSB) were synthesized by reacting salicylic acid, primary diamines with salicylaldehyde or its derivatives, and 40 of which were newly reported. The inhibitory activities against Escherichia coli b-ketoacyl-acyl carrier protein synthase III (ecKAS III) were investigated in vitro and molecular docking simulation also surveyed. Top 10 PSB compounds which posses both good inhibitory activity and well binding affinities were picked out, and their antibacterial activities against Gramnegative and Gram-positive bacterial strains were tested, expecting to exploit potent antibacterial agent with broad-spectrum antibiotics activity. The results demonstrate compound N-(3-(5-bromo-2-hydroxybenzylideneamino) propyl)-2-hydroxybenzamide (2d) can be as a potential antibiotics agent, displaying minimal inhibitory concentration values in the range of 0.39–3.13 lg/mL against various bacteria.**(82)**

These have been reported by Shanmugavel Sujarania, Thangamuthu Anitha Sironmani and Andy Ramu that Diphenylethylamine is one of the morphine like drugs. A new series of biocompatible compounds have been prepared by Schiff base condensation reaction using 2,2- diphenylethylamine with 4-OH / 4-OMe substituted salicylaldehydes. The solid derivatives have been isolated and characterized by using IR, NMR and UV-Visible spectral techniques. Silver nano particles were synthesized by using starch as reducing and capping agent. The functionalized silver nanomaterials with Schiff base ligand anchored with fluorescent marker Rhodamine B was characterized using UV-Visible, IR, Fluorescent and AFM. Toxicity studies carried out in vivo (mice) and in vitro showed silver nano particles anchored 2-((2,2-dipenylethylimino)methyl)phenols to be biocompatible without any apparent toxicity. A salicylaldehyde group on a definite position of an analgetically active molecule frequently causes an increase in the activity and an enhancement of binding to the opiate receptor. 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.**(83)**

Pavan Kumar Kunda1, J Venkateswara Rao et.al reported that Purpose: To synthesize Schiff bases of 2-aminothiophenes and evaluate their anticonvulsant activity and in silco properties Methods: 2-Amino-N-o-tolyl-5,6-dihydro-4H-cylcopenta[b]thiophene-3-carboxamide was synthesized using 1,1,3,3-tetramethylguanidine lactate as a basic catalyst and by microwave irradiation. 2-substitued-o-tolyl-5,6-dihyro-4H-cylcopenta[b]thiophene-3-carboxamide was prepared by reacting with different substituted aromatic aldehydes. The synthesized compounds were characterized by Fourier transform infrared spectroscopy (FTIR), nuclear magnetic resonance spectroscopy (1H NMR) and mass spectrometry (MS) while their anticonvulsant activity was screened against maximum electroshockinduced seizure (MES), and pentylenetetrazole-induced seizure (PTZ) against phenytoin and diazepam as reference standards. Molecular docking (in silico) studies were performed using 4-aminobutyrateaminotransferase in order to predict possible protein-ligand interactions.Results: Among the 21 synthesized compounds, 2b, 2d, 2f, 2k, 2m, 2n and 2o showed good to moderate activity against MES and PTZ-induced convulsions. Compounds 2b, 2d, 2f, 2k and 2m exhibited lower activity against PTZ than against MES model while compounds 2n and 2o afforded greater protection against PTZ than against MES model. In silico results also revealed maximum binding affinity to GABA-AT protein which was higher than other compounds Conclusion: The synthesized compounds showed potent anticonvulsant activity. Molecular docking results should give an insight into how further modification of lead compound can be carried out for higher inhibitory activity.**(84)**

Adeola Ayodeji Nejo reported that Sixteen symmetrical and four unsymmetrical tetradentate Schiff bases with the N2O2 chromophore were isolated in pure form and fully characterized by elemental analyses, melting point, IR and 1H NMR. The appearance of two different peaks for each of the azomethine protons and phenolic protons confirm the asymmetry nature of the unsymmetrical Schiff bases. All the Schiff bases were successfully coordinated to oxovanadium (IV) ion to form the corresponding complexes. The unsymmetrical Schiff bases were also successfully coordinated to cobalt(II), nickel(II) and copper(II) ions to form their corresponding complexes. In all thirty-two metal(II) Schiff bases complexes were isolated. These complexes were characterized by elemental analyses, melting point, IR, EPR, cyclic voltammetry, magnetic susceptibility measurements, differential scanning calorimetry and electronic spectra. The isolation of the unsymmetrical tetradentate Schiff bases and their complexes as well as some of the symmetrical tetradentate Schiff bases and their complexes are considered to be novel. The purity and composition of both the Schiff bases and the metal(II) complexes were established by elemental analyses.The comparison of the IR spectra of the Schiff-bases and their metal complexes indicated that the Schiff bases acted as tetradentate ligands. The observed shifts in the stretching frequencies of (C=N) and (C¯O) are indicative of the formation of these complexes. Further conclusive evidence of the coordination of these Schiff-bases with the metal ions was shown by the appearance of new bands due to (M¯N) and (M¯O) in the metal complexes. Most of the oxovanadium(IV) complexes exhibit a strong band in the range 959−989 cm−1, which have been assigned to (V=O) in a monomeric square pyramidal coordination environment. The ii oxovanadium(IV) complexes with trimethylene bridge, in which their (V=O) appeared at 848−860 cm.1, have been assigned polymeric structure with [V=O····V=O] interactions, which afforded distorted octahedral coordination geometry. The electronic spectral and magnetic susceptibility measurements were used for assigning the stereochemistry of each metal complex. Electronic spectra indicate a square-planar geometry for all the cobalt(II), nickel(II) and copper(II) complexes. This was also corroborated by the effective magnetic moment of the complexes. The electronic spectra of the oxovanadium(IV) complexes suggest a diversity of geometries. The electronic spectra indicate a square-pyramidal geometry for the fivecoordinate species and distorted octahedral geometry for the six-coordinate species. The room temperature magnetic moments of 1.6.1.8 BM are normal for V(IV) d1 configuration. The solution EPR spectra of the oxovanadium(IV) are consistent with square pyramidal geometry. The cyclic voltammetry of the oxovanadium(IV) complexes revealed only one quasi-reversible wave for each complex and they all showed redox couples with peak- to peak separation values (Ep) ranging from 74 to 83 mV, indicating a single step one electron transfer process. In vitro glucose uptake was carried out on all the oxovanadium(IV) complexes using C_2C1_2 cell line. All the complexes tested increased glucose utilization in C_2C1_2 cells over basal values except two of the complexes whose percentage glucose uptake was lower than the basal glucose uptake (DMSO). Eighteen of the complexes significantly increased glucose uptake when compared to the basal glucose uptake of the solvent vehicle (DMSO). Cytotoxic test carried out on all the complexes using MTT assay showed that the complexes were not toxic to the cells iii at both low and high concentrations. Two of the complexes showed activities comparable or greater than that of insulin. Four unsymmetrical and five symmetrical Schiff base complexes of oxovanadium(IV) have been tested in vivo for their insulin mimetic activities. An acute oral administration of the four unsymmetrical Schiff base complexes of oxovanadium(IV) elicited a progressive reduction in plasma glucose over 6 h in STZ rats. Two of the unsymmetrical Schiff base complexes of oxovanadium(IV) induced a significant reduction in plasma glucose over a 6 h period. Oral administration of the five symmetrical complexes also elicited a progressive reduction in plasma glucose over 6hrs. Two of these complexes induced a significant reduction in plasma glucose during the 6 hour period.**(85)**

Nura Suleiman Gwaram, Hapipah Mohd Ali, and Mahmood Ameen Abdulla et.al reported that Alzheimer’s disease (AD) is the most common form of dementia among older people and the pathogenesis of this disease is associated with oxidative stress. Acetylcholinesterase inhibitors with antioxidant activities are considered potential treatments for AD. Some novel ketone derivatives of gallic hydrazide-derived Schiff bases were synthesized and examined for their antioxidant activities and in vitro and in silico acetyl cholinesterase inhibition. The compounds were characterized using spectroscopy and X-ray crystallography. The ferric reducing antioxidant power (FRAP) and 2,2-diphenyl-1-picrylhydrazyl (DPPH) assays revealed that all the compounds have strong antioxidant activities. N-(1-(5-bromo-2-hydroxyphenyl)-ethylidene)-3,4,5-

trihydroxybenzohydrazide (**2**) was the most potent inhibitor of human acetyl cholinesterase, giving an inhibition rate of 77% at 100 μM. Molecular docking simulation of the ligand-enzyme complex suggested that the ligand may be positioned in the enzyme's active-site gorge, interacting with residues in the peripheral anionic subsite (PAS) and acyl binding pocket (ABP). The current work warrants further preclinical studies to assess the potential for these novel compounds for the treatment of AD.**(86)**

These have been reported by Rodrigo Arancibia, A. Hugo Klahn, Gonzalo E. Buono-Core et.al. that In the search for new therapeutic tools for the treatment of American trypanosomiasis, a series of novel ferrocene and cyrhetrene imine compounds, derived from 5-nitro-heterocycles, were designed, synthesized and characterized. The 1H and 13C NMR spectra indicated that these compounds adopted an anti-(E) conformation in solution, and this was confirmed by X-ray crystallography for one of the complexes (NT2). To study the relationship between the physicalechemical properties of N-iminyl substituents of nitrofurfuryl and nitrothienyl groups and their antitrypanosomal activity, we have carried out cyclic voltammetry and electron spin resonance studies of a series of organometallic imine compounds. The results demonstrated that the electronic properties of the side chain of the 5-nitroheterocyclic compound could be correlated to its trypanocidal effect.**(87)**

It has been reported by E. Canpolat that $Co(L)_2$, $Ni(L)_2$, $Cu(L)_2$ and $Zn(L)_2$ were synthesized from p-aminoacetophenoneoxime and 5-chlorosalicylaldehyde and $Co(AcO)_2\_4H_2O$ or $Ni(AcO)_2\_4H_2O$ or $Cu(AcO)_2\_H_2O$ or $Zn(AcO)_2\_2H_2O$ in 1:2 molar ratio, employing a template approach. Based on elemental analyses, molar conductivity and magnetic susceptibility data, IR, 1H- and 13C-NMR and UV spectra, as well as thermal analyses (TG), a tetrahedral geometry for the complexes was determined. The data show that the ligand coordinates to the metal ion via -C=N- and -C-O- groups. All complexes are soluble in common organic solvents such as DMF and DMSO.**(88)**

E. Szlyk, I. Szymañska and R. Szczêsny reported that Me_3SiCH_2COOAg, $[Ag(Me_3SiCH_2COO)(PPh_3)]$ and $[Ag(Me_3SiCH_2CH_2COO)(PPh_3)]$ were prepared and characterized in solution by 1H, 13C, 29Si, 31P and 29Si, 31P CPMAS NMR. Spectral analysis suggests bidentate bridging carboxylates and monodentately bonded PPh3 in solution and in the solid state. Two crystallographically inequivalent molecules of PPh3 appeared in the solid state, what is evident from 31P CPMAS NMR. Thermal studies of both complexes demonstrate two stage decomposition process (exothermic followed by endothermic) with formation of metallic silver in the range 483–548 K. TGA/IR and MS studies of Me_3SiCH_2COOAg and $[Ag(Me_3SiCH_2COO)(PPh_3)]$ revealed volatile products of decomposition (CO_2, Me_3 Si-) and recombination reactions such as $(Me_3SiCHCO)_2O$, $(Me_3Si)_2O$. The mechanism of complexes thermal decomposition is proposed.**(89)**

Those were reported by R. Pastorek, J. Kameníèek, Z. Trávníèek, et.al. that Ni(II) ithiocarbamates with AsI3 or SbI3 as ligands of the composition $[Ni(hmidtc)_2(AsI_3)]$ (1), $[Ni(bzbutdtc)_2(AsI_3)]$ (2), $[Ni(bzbutdtc)_2(SbI_3)]\_2CHCl_3$ (3), $[Ni(bz_2dtc)_2(AsI_3)]$ (4), $[Ni(bz_2dtc)_2(SbI_3)]\_CS_2$ (5), $[Ni(hmidtc)_2(AsI_3)_2]\_CHCl_3$ (6), $[Ni(hmidtc)_2(SbI_3)_2]$ (7) and $[Ni(cetdtc)_2(AsI_3)_2]$ (8), (hmidtc = hexamethyleneiminedithiocarbamate, bzbutdtc =benzylbutyldithiocarbamate, bz_2dtc = dibenzyldithiocarbamate, cetdtc = cyclohexylethyldithiocarbamate, dtc = S_2CN–) have been synthesized. The complexes have been characterized by elemental analyses, thermal analysis, IR and V/VIS spectroscopies, magnetochemical and conductivity measurements as square-pyramidal (1–5) and octahedral(6–8) complexes. X-ray analysis of $[Ni(bz_2dtc)_2(AsI_3)]$ and $[Ni(bz_2dtc)_2(SbI_3)]\_CS_2$ confirmed square-pyramidal arrangement around nickel in both complexes with the NiS_4As and NiS_4Sb chromophore, respectively.**(90)**

A. Zwoliñska and B. Ptaszyñski reported that Zinc(II) complexes with the commercial auxin herbicides 2,4-dichlorophenoxyacetic acid (2,4D; $C_8H_6O_3Cl_2$) and 2-(2,4-dichlorophenoxy)-propionic acid (2,4DP; $C_9H_8O_3Cl_2$) were prepared and characterized. The formulae of the solid complexes $Zn_2(C_8H_5O_3Cl_2)_3\_5H_2O$ (Zn-2,4D) and $Zn(C_9H_7O_3Cl_2)_2\_1.5H_2O$ (Zn-2,4DP) were established on the basis of the results of elemental analysis and Zn(II) determination.Water solubility of synthesized complexes at room temperature was examined. X-ray powder analysis was carried out. The discussion of IR spectra and conductivity data is presented. Thermal decomposition of these complexes in air was studied by TG, DTG, DTA and TG/MS methods with simultaneous analysis of the solid and gaseous products. The formation of complexes Zn-herbicide in the water solution by potentiometric pH titration was also investigated. The dissociation constants (pK) of 2,4D and 2,4DP were determined at 25°C and I = 0.1 (KNO3).**(91)**

It has been reported by L. Zhang1, Q.-H. Liu1, F. Peng1 and M. Du that A novel cobalt complex, [Co(bdpm)(OBz)](ClO4) (bdpm = bis(3,5-dimethyl-1-pyrazolyl) methane, OBz = benzoate), was synthesized and characterized by elemental analysis, UV–Vis, IR spectroscopy and X-ray diffraction. The complex crystallizes in the trigonal system, space group P3121 with a = 19.2583(9), b = 19.2583(9), c = 25.5269(17) Å and _ = 120_. The complex can catalyze the selective oxidation of alkanes to corresponding alcohols and ketones, and a presumptive mechanism was proposed.**(92)**

Fouzia Rafat, K.S. Siddiqi and M.Y. Siddiqi reported that Complexes of Mn(II), Fe(III), Co(II), Ni(II), Cu(II) and Zn(II) with Schiff bases derived from isatin and ethylenediamine (L1) or diethylenetriamine (L2) have been synthesized and characterized by microanalysis, IR, UV-Vis, 1H NMR, EPR and conductance measurements.

Electrical conductance of the Fe(III) chelates indicated them to be 1:1 electrolyte whilst those of divalent metal ions are non-electrolytes in DMSO. On the basis of magnetic moment and spectral data a pseudooctahedral geometry has been suggested for all of the complexes. The EPR spectrum of [Cu(L1)Cl2] complex indicates a considerable exchange interaction in the solid state.**(93)**

A. Manohar, K. Ramalingam, G. Bocelli and A. Cantoni Mixed ligand complexes of the general type [Cd2(dtc)4(4,4_-bipy)] (dtc = diethyldithiocarbamate or piperidinedithiocarbamate anions; 4,4_-bipy = 4,4_-bipyridine) have been synthesized and characterized. IR spectra of the complexes show that the thioureide _(C–N) bands are observed at lower frequency than the values obtained for the parent dithiocarbamates. Charge transfer transitions are observed in the region 310–340 nm. Thermogravimetric studies show that the 4,4_-bipyridine adducts are more stable than the 2,2_-analogues. Also, the crystal structure of the benzene solvate of [Cd(pipdtc)2]2 (pipdtc = piperidinedithiocarbamate anion) is reported. The coordination geometry can be described as a distorted trigonal bipyramid around each cadmium.**(94)**

These have been reported by G. Vuèkoviæ, M. Antonijeviæ-Nikoliæ, M. Korabik, that Three complexes: $[Cu_2(C_6H_5COO)tpmc](ClO_4)_3$_$CH_3OH$, (A), (tpmc = N,N_,N__,N___- tetrakis(2-pyridilmethyl)-1,4,8,11-tetraazacyclotetradecane), $[Cu_2(Hpht)tpmc](ClO_4)_3$_$3H_2O$ (H_2pht = phtalic acid) (B) and $[Cu_4(ipht)(tpmc)_2](ClO_4)_6$_$NaClO_4$_$2CH_3CN$ (H_2ipht = isophtalic acid) (C) previously described were investigated by magnetic measurements, cyclic voltammetry (CV) and were tested towards some strains of microorganisms. It is found that all three complexes were electrochemically stable in the investigated ranges. The least stable was _-iphtcomplex (**C**) due to the reaction of central ion, which is seen from weak peaks in its cyclic voltammogram. Complexes were characterized by variable temperature magnetic measurements (4.2–300 K) and the observed data were successfully simulated by the equation based on the spin Hamiltonian operator, H_ −2JS_ S_ 1 2, giving the ferromagnetic exchange parameters J = 0.92 cm–1 for A, J = 0.55 cm–1 for B and J= 0.65 cm–1for C. For the complex **C** model of molecular magnet with two magnetically isolated dimeric subunits was used. These results indicate the presence of weak ferromagnetic spin exchange interaction between the CuII magnetic centers within each molecule.**(95)**

E.D. Raczyñska, K. Duczmal and M. Darowska reported that Extended quantum-chemicalcalculations {HF, MP2, DFT(B3LYP) in vacuo} were performed for neutral pyruvic acid and its enol forms. Among various tautomers-rotamers considered, three keto (Tce, Tte and Cte) and six enol structures (E1–E6) are found to be thermodynamically stable. The stability order for the keto and enol isomers: Tce > Tte > Cte > E1 > E2 > E3, E4, E5 > E6 is the same at each level of computations. The keto Tce structure has the lowest Gibbs free energy (G). The G value of the most stable enol E1 structure is larger than those of the three keto structures by a few kcal mol^{-1}.**(96)**

It has been reported by B. Lêska, G. Schroeder and B. Gierczyk that The new P-podands (P3.1, P3.2, OP3.1 and OPH2.1) have been used as complexation agents in reactions with copper cations and the complexes btained have been studied by NMR and kinetic methods. Two types of reactions, one between P-ligands and Cu(I) and the other between OP-podands and Cu(II), have been observed for the ligands studied.**(97)**

These have been reported by W. Nawrocka, B. Sztuba, H. Liszkiewicz, et.al that A series of 2-methylpyrimido[1,2-a]benzimidazole derivatives has been synthesized in the reactions of 2-aminobenzimidazole (1) with selected halogeno _-diketones: 1,1,1-trifluoro- 2, 1-chloro-1,1-difluoro- 3, 3-chloro-2,4-pentadione- 4 and with 4-fluorobenzoylacetone 5. 2-Aminobenzimidazole (1) in the reactions with _-chloro- and _-bromocinnamaldehyde gave Schiff bases 10 and 11 which have been subjected to reduction using NaBH4 and 3-benzylideno-1,2-dihydro- (12) and 3-benzylideno-1,2,9,10- tetrahydroimidazo[1,2-a]benzimidazole (13) were obtained. The structures 2–13 were identified by the results of elemental analysis and their IR, 1H NMR and MS spectra. Compounds 2–13 were examined for their antiproliferative activity in vitro against the cells of 3 human cancer cell lines, using SRB (sulphorhodamine B) or MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide) technique. Four out of all tested compounds revealed cytotoxic activity in vitro.**(98)**

B. Gierczyk and G. Schroeder have reported that The influence of ion complexation on the hydrolysis process of Si-podands was studied. On the basis of kinetic measurements a mechanism of the hydrolysis as well as a mechanism of the ion complexation effect were proposed.**(99)**

It has been reported by Z. Pianowski1 and K. Staliñski that New N-coordinated dimethyl and di-n-butyl tin hydrides containing the oxazole moiety appeared to be useful in radical cyclizations of acyclic dihalides at the steady state. Both the hydrides were prepared in three steps starting from (–)-(S)-(2-bromophenyl)-4-isopropyl-4, 5-dihydrooxazole. The advantages of the hydrides are at least twofold. First, a resolution of the radical intermediates allows generating higher stereomeric excess than in the case of commercially available hydrides. Second, tin by-products are easily removed.**(100)**

D. Sobolewski, W. Kowalczyk, I. Derdowska, et.al. reported that The present work is a part of our studies aimed at clarifying the influence of sterical constraints in N-terminal part of AVP analogues on the pharmacological activity of the resulting peptides. In this study we described the synthesis of four new analogues of AVP substituted at positions 2 and 3 or 3 and 4 with two diastereoisomers of 4-aminopyroglutamic acid and four peptides in which we combined the above modification with the placement of 3-mercaptopropionic acid at position 1. All new peptides were not active in bioassays for pressor, antidiuretic and uterotonic activity.**(101)**

These have reported by F. S. czewski1 and A. Bu akowska that Aseries of analogues of methotrexate 23–31 in which aminopteridine ring was replaced by 2,4-diamino-1,3,5-triazine moiety were obtained. The syntheses of the analogues were accomplished by alkylation of p-aminobenzoic acids with appropriate 6-bromomethyl-triazines 1–5 followed by conjugation with alkyl glutamate, aspartate or methioninate to give esters 14–22. Saponification of the esters afforded target compounds 23–31 which were evaluated for their in vitro antitumor activity against MCF-7 (breast), DAN-G (pancreas) and LCLC-104 (lung) cancer cell lines.**(102)**

E.D. Raczyñska reported that Variations of the n- electron distribution during the tautomeric interconversion and substituent effects were analysed for simple keto-enol tautomeric systems of general formulae H_3C–C(R)=O H_2C=C(R)–OH and RH_2C–CH=O RHC=CH–OH using the geometry-based HOMA index.**(103)**

V.J. Šukyt_e, R. Ivanauskas and V. Janickis have reported that The process and results of the formation of thin Cu–Te–S films on the polyamide (PA) surface are described. For clarifying the influence of various factors (the concentration of the initial solution of sodium telluropentathionate dihydrate, $Na_2TeS_4O_6$_$2H_2O$, pH, an exposure time and temperature) the kinetics of the sorption-diffusion of tellurium and sulfur into PA from freshly prepared solutions of sodium telluropentathionate was studied. Some structural properties and electrical resistance's values of obtained films have been investigated also. Cu–Te–S polymer composites indicate p-type properties of electrical conductivity and have electrical resistance in the range of 1.5_103–4.0_103 k/_to 3–5 k/_ after to 2–3 h of an exposure and 1.0–1.5 k/_ after 24–72 h of exposure in 0.01–0.1 mol dm–3 solutions of $Na_2TeS_4O_6$.**(104)**

It has been reported by K. H C-Wydro, P. Wydro and P. Dynarowicz-Latka Tri-n-octylphosphine oxide (TOPO) was found to be capable of Langmuir monolayer formation at the air/water interface. Surface pressure-area (π-A) isotherms obtained at different experimental conditions (barrier speed, number of deposited molecules, temperature and presence of metal ions in the aqueous subphase), compression modulus (C_s^{-1}) values andBAMimages have been analyzed. The stability of TOPO monolayers has also been thoroughly examined. The obtained results indicate a liquid state of TOPO monolayers independently of subphase temperature or ionic strength. Such experimental conditions as the barrier speed or the number of deposited molecules were found to have no influence on the shape and position of the isotherms. Moreover, the performed experiments proved a high stability of monolayers from TOPO at the air/water interface.**(105)**

B. Baranowski and L. Dêbowska have reported that the penetration depths of hydrides formed in 6.8 kbar of gaseous hydrogen in cylindrical samples was investigated at 25°C in Pd-Ni alloys of 80, 120, 150, 200 and 250 _mdiameters. The exposition time was about 4 months, thus, sufficient for the stationarity in respect to equilibration of the sample composition. In all alloys the penetration depth was limited, exhibiting a linear increase with radii of the wires applied with the slope of about 0.6 _m per 1 _m of the wire radius. These results are interpreted in terms of the coherent character of the hydride formation, supporting the thermodynamic reason for the limited penetration depth of metallic hydrides.**(106)**

II. Conclusion

The Survey in the field shows that though a lot of work has been done so far in spectral studies of organic compounds but simulation of spectra is a new dimension which may prove to be useful in research and teaching.

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