

Computational study on imidazole-2-carboxaldehyde-glycylglycine and indole-3-carboxaldehyde-glycylglycine Schiff base ligands and equilibrium studies on their metal complexes

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Abstract : Semiempirical (AM1) calculations were carried out for the Schiff bases, imidazole-2-carboxaldehyde-glycylglycine (imal-glygly) and indole-3-carboxaldehyde-glycylglycine (indal-glygly). Five conformers of imal-glygly and indal-glygly suitable for complex formation were studied. The stable conformers were chosen for further studies. The geometrical parameters are in good agreement with the experimental values. The Schiff bases are planar with C_1 symmetry. The denticity reduction energy for imal-glygly and indal-glygly are respectively 21.04 kcal/mol and 18.24 kcal/mol. imal-glygly is a potentially tetradentate ligand capable of binding through N_4 , N_7 , N_{11}/O_{10} and O_{15} and indal-glygly is tridentate using N_{11} , N_{15}/O_{14} and O_{19} atoms. The basicity of the hetero atoms were studied by calculating the protonation constant. The higher dipole moment values indicate that they are highly soluble in polar solvents. The ionization potential is 11.70 eV and 8.59 eV respectively for imal-glygly and indal-glygly. The chemical hardness has also been studied. Equilibrium studies were carried out for Co^{II} , Ni^{II} , Cu^{II} and Zn^{II} -imal-glygly/indal-glygly systems. $M(AB)$ and $M(AB)_2$ types of complexes were formed for Co^{II} , Ni^{II} and Zn^{II} systems, while Cu^{II} forms only $M(AB)$. The stability of the metal ions follows Irving-Williams order.

Keywords : Computation, equilibrium, Schiff base, imidazole-2-carboxaldehyde, indole-3-carboxaldehyde, potentiometry.

Solvent and structural effects on the photo-reduction of cobalt(III) complexes in aquo-organic solvent media possessing different H-bonding properties

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Abstract : The photo-reduction of a series of cobalt(III) complexes of the type *cis*- β -[Co(ampy)₂(4-R-Py)Cl]Cl₂ where ampy = 2-aminomethylpyridine and R = H, Me, Et, *t*-Bu, COMe, and CN has been studied in propan-2-ol/water and 1,4-dioxane/water medium. The photo-reduction quantum yield ($\Phi_{Co(II)}$) data were correlated with solvent and structural parameters with an aim to shed some light on the mechanism of these reactions. Increase in the percentage of organic co-solvent in both the medium increased the photo-reduction quantum yield. Correlation of $\Phi_{Co(II)}$ with macroscopic solvent parameters viz. relative permittivity indicated that the reactivity is influenced by both specific and non-specific solute-solvent interactions. Kamlet-Taft solvatochromic comparison method was used to separate and quantify these effects. H-bonding property of the mixture was found to dominate the solvation and consequently the magnitude of the quantum yield.

Keywords : Cobalt(III) complexes, photo-reduction, solvent effect, Hammett equation.

2-(2-Hydroxy)phenylazo derivatives of some 1,3-dicarbonyl compounds and their metal complexes

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Abstract : 2-Hydroxyphenylazo derivatives of three 1,3-dicarbonyl compounds (acetylacetone, methylacetoacetate and acetoacetanilide) have been synthesized and characterised. Analytical, IR, ¹H NMR and mass spectral data indicate that the compounds exist in the intramolecularly hydrogen bonded keto-hydrazone form. Dibasic tridentate coordination of these compounds in their [M₂L₂] complexes (M = Ni^{II}, Cu^{II} and Zn^{II}) has been established on the basis of analytical and spectral data.

Keywords : 2-Hydroxyphenylazo derivatives, phenyl hydrazones, keto-hydrazone, metal complexes.

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Sorptive interactions of Cu on soil, clay and humic acid

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Abstract : Sorption and desorption of Cu on soils from four different locations of West Bengal have been studied. Sorption on humic acid and clays of the soils has also been measured. Measurements have been made at a pH of 6.0 without any back ground electrolyte. Comparison of sorption behavior of the soils have been made on the basis of the Langmuir parameters. One of the soils is very rich in organic matter and others are progressively poorer in it though richer in clay content. This enables us to make some guess on the role of each of the constituents on overall adsorption. Humic acids and clays isolated from each soil have also been tested for adsorption efficiency. Adsorption maxima for all these constituents fall far below their individual CEC. Experiments have been done on soil residues after removal of mobile organic matter by alkali extraction. A drop in adsorption maxima has been observed although the decrease will not up to the theoretically calculated amount betraying a more complicated combined existence of humus and clay in native soil. Desorption experiments have been carried out in solutions of NaCl, KCl, MgCl₂ and CaCl₂. The desorbing efficiency of the ions was found to be in the decreasing order of Ca²⁺ > Mg²⁺ >> K⁺ > Na⁺. This result suggests predominantly an ion-exchange reaction.

Keywords : Sorption, desorption, Cu, soils.

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Ultrasonic velocity and related acoustical parameters of 2-(2,4-dinitrophenoxy)-1-[2-(2,4-dinitrophenoxy)naphthalene-1-yl]naphthalene solutions at 35 °C

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Abstract : The density (ρ), viscosity (η) and ultrasonic velocity (U) (2 MHz) of chloroform, THF and 2-(2,4-dinitrophenoxy)-1-[2-(2,4-dinitrophenoxy)naphthalene-1-yl]naphthalene (DBNN) solutions have been determined at 35 °C. Various acoustical parameters namely specific acoustical impedance (Z), isentropic compressibility (κ_s), Van der Waals constant (b), intermolecular path length (L_f), internal pressure (π), free volume (V_f), Rao's molar sound function (R), relaxation time (τ) and classical absorption coefficient ($(\alpha/f^2)_{cl}$) and solvation number (S_n) have been derived from ρ , η and U data and correlated with concentration (C). A fairly good to excellent correlation has been observed between a particular parameter and C . Linear increase of Z , R , b , V_f (except chloroform), $(\alpha/f^2)_{cl}$ and τ ; and linear decrease of κ_s , π and L_f with C supported presence of strong molecular interactions in the solutions, which are further supported by nonlinear increase of S_n with C . A fairly constant Gibb's free energy of activation has been observed in both the systems.

Keywords : Ultrasonic velocity, acoustical parameters, solvation number, Gibb's free energy of activation.

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Power generation in photogalvanic cell composed of Toluidine Blue – Arabinose – NaLS system

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Abstract : In the present paper, the performance and conversion efficiency of the photogalvanic cell composed of Toluidine Blue – Arabinose in presence of anionic surfactant (NaLS) has been studied. It was observed that the cell generate power 48.78 μ W in short time and storage capacity has been obtained 123 min in dark. The effects of various factors like pH, concentration of dye, concentration of surfactant, diffusion length and electrode area on cell's power generation were also observed. A tentative mechanism has also been proposed.

Keywords : Photogalvanic cell, Toluidine Blue, Arabinose, storage capacity.

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Different aspects of hormesis and radiation hormesis[†]

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Abstract : Hormesis is adopted by seeds, plants, micro-organisms, mice, guineapigs and human beings. It is induced by chemicals, pharmaceuticals, heavy metals and toxicological compounds of varied types. Physical inducing agents are temperature and different types of ionizing radiations.

Hormesis follows biphasic time-response and dose-response relationships which can be quantitated. The hormetic response is controlled by summation of informations, effectors and sensors. It has been reported in erythropoetic tissue, lymphokine cascade in antibody formation and thymidine reuse in mammals etc.

Radiation hormesis is connected with radiation dose, LET, dose rate, size and mass of cells, types of radiation, probability of interaction of radiation with target, time lag between dose and response etc.

At its preliminary stage the concept of hormesis was dismissed but later a large number of authors have supported this concept.

Mechanistically radiation hormesis can be attributed to different causes namely : (i) cellular damage of DNA and its repair, (ii) mutagenesis and its repair, (iii) micronuclei formation and its

repair, (iv) different types of chromosomal aberrations and their repair etc. These repairs are done by antioxidants, different types of enzymes and immune responses and cell cycle control etc.

Low dose hormesis has been reported under various conditions namely : (i) environmental and epistemological problems, (ii) background radiation dose estimation, (iii) dose estimation in nuclear installations, (iv) estimation of dose for atomic survivors, (v) accidental dose estimation in Chernobyl etc. In the above cases hormesis depends on internal factors like – lighting condition, intensity and duration of radiation, measurement time of exposure etc.

Societal aspects of hormesis e.g. application in biogerontology, radiation protection aspect, increase in life span for cancer – induced patients applying hormetic principles, environmental and toxicological aspects have been mentioned.

Future prospects of hormesis (both theoretical and practical) are given below :

Theoretical : (i) Low level effects, (ii) linear extrapolation from high level exposure, (iii) shape of dose-response curve and mechanism of radiation effects at low dose, (iv) molecular and cellular studies on mechanism of hormesis, (v) pharmacological hormesis mechanism, (vi) role of hormesis in environmental risk and hazard assessment methods and their evaluation, (vii) role of hormesis in the improvement of harmonization of cancer and non-cancer cases.

Practical : (i) Predictive assay of clinical and therapeutic measures using hormetic principles, (ii) toxicological, agricultural, behavioral, societal, biogerontological and economic aspects of hormesis.

Keywords : Hormesis, radiation hormesis, physical and chemical inducing agents, factors that influence radiation hormesis, detection of hormetic dose by tissue-equivalent dosimeters, maximum limit of exposure, mechanism of radiation hormesis, theoretical and practical aspects of hormesis, future recommendations.

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Bismuth trichloride – A clean, green catalyst for the synthesis of Hantzsch 1,4-dihydropyridines (DHPs)

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Abstract : Hantzsch 1,4-dihydropyridines (DHPs) are synthesized in good to excellent yields from aldehydes, 1,3-dicarbonyl compounds and ammonium acetate using bismuth trichloride which acts as mild Lewis acid promoter and 10 mol% is enough for this protocol under solvent free conditions.

Keywords : Hantzsch 1,4-dihydropyridines, bismuth trichloride, aldehydes, 1,3-dicarbonyl compound, ammonium acetate, solvent-free.

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An efficient synthesis of *E*-2-amino-4-aryl-8-(arylmethylene)-5,6,7,8-tetrahydrobenzo[*d*]pyrimidines and their lower analogues

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Abstract : Base-catalysed cyclocondensation of α,α' -bis(arylmethylene)cyclohexanones with guanidine hydrochloride has been found to generate *E*-2-amino-4-aryl-8-(arylmethylene)-5,6,7,8-tetrahydrobenzo[*d*]pyrimidines in high yield, the structures of which have been established from their

analytical and spectral data. The corresponding lower analogues, α, α' -bis(arylmethylene)cyclopentanones also were found to produce similar products viz. *E*-2-amino-4-aryl-7-(arylmethylene)-cyclopenteno[1,2-*d*]pyrimidines in comparable yield under the same reaction condition.

Keywords : α, α' -Bis(arylmethylene)cycloalkanones, guanidine hydrochloride, *E*-2-amino-4-aryl-8-(arylmethylene)-5,6,7,8-tetrahydrobenzo[*d*]pyrimidines, *E*-2-amino-4-aryl-7-(arylmethylene)cyclopenteno[1,2-*d*]pyrimidines.

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Induced mutation and selection of High Yielding Strain of *Micrococcus glutamicus* for glutamic acid production

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Abstract : The objective of this investigation was to develop a new auxotrophic mutant from a regulatory mutant and to examine its potency for L-glutamic acid production. A high L-glutamic acid yielding strain *Micrococcus glutamicus* AB₁₀₀ was developed from a regulatory mutant *Micrococcus glutamicus* AB₁ by subsequent mutagenic treatments with ethyleneimine solution and UV rays respectively. *Micrococcus glutamicus* AB₁ was treated with ethyleneimine solution, the auxotrophic mutants isolated show varied pattern of extracellular amino acids. Seventy auxotrophic strains were obtained, out of which only twenty seven excreted 0.5–3.0 mg, L-glutamic acid per ml and all auxotrophs require biotin for growth and production of amino acid. Sixteen auxotrophs produced 1.0–2.5 mg, L-glutamic acid per ml and these auxotrophs required amino acids for their growth. Other auxotrophs lost their excretion capacity in subsequent fermentation trials. Further mutation of the biotin requiring auxotroph *Micrococcus glutamicus* AB₁₀ with UV rays resulted in the isolation of seventy seven auxotrophic strains out of which only thirty excreted L-glutamic acid (up to 6.25 mg/ml) higher than the parent auxotroph.

Keywords : Auxotrophic mutant, regulatory mutant, *Micrococcus glutamicus*, mutagenic, ethyleneimine, UV rays, amino acids, L-glutamic acid.

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Study of base line environmental data of fluorspar mining with special reference to Kadipani mine (Gujarat)

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Abstract : Any mining activity is likely to affect the quality of surrounding environment during its operation. The nature and magnitude of impacts on different components of the environment, viz. air, noise, water, land, biological and socio-economic vary depending on the nature and size of the mining project and therefore it is essential to find out the base line environmental data before preparing the environmental management plan. Environment management plan gives the account of measures necessary to prevent the impacts on the baseline environmental situations. Once the base line status of environmental parameters is known the decision regarding corrective and preventive measures becomes more scientific and technologically and financially viable. In present study efforts are made to establish the base line air and water quality of Kadipani District, Vadodara, Gujarat. Therefore this study is useful for making the decisions regarding the environmental measures required by the mining activity.

Keywords : Ground water, surface water, soil, air impacts, ambient air quality, environmental management plan.

Molecular modeling and potentiometric study of some metal complexes of *o*-vanilineglutamate Schiff base

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Abstract : The complexing behaviour of *o*-vanilineglutamate Schiff base ligand with Co^{II}, Ni^{II}, Cu^{II} and Zn^{II} were investigated by semiempirical (AM1), molecular mechanics (MM+) and potentiometric methods. The results demonstrate that the Schiff base ligand is tertridentate in the MAB complexes. Both the molecular modeling and potentiometric studies indicate that the ligand is tridentate in the M(AB)₂ complexes.

Keywords : Semiempirical, molecular mechanics, potentiometry, Schiff base, computation.

Acid-catalyzed hydrolysis of *N*-phenylbenzohydroxamic acid

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Abstract : The kinetics of hydrolysis of *N*-phenylbenzohydroxamic acid have been studied from 0.9 to 10.8 mol dm⁻³ H₂SO₄ in 10/90 (v/v) *n*-propanol-water medium at 55 °C. The rate of reaction increases initially with increasing acidity, reaches a maximum and then decreases. After that at high acidities there is steep increase in reaction rate. The effect of temperature on the rate of hydrolysis has been studied. Activation parameters have been calculated. Bimolecular nature has been supported by Hammett, Zucker-Hammett, Bunnett, Bunnett-Olsen and Arrhenius activation parameters etc.

Keywords : Kinetics, temperature effect, molecularity, *N*-phenylbenzohydroxamic acid.

KHSO₄ assisted Michael addition-elimination reactions of formylated acetophenones in water : A facile general green synthetic route to 3-(alkyl/aralkyl/aryl)amino-1-arylprop-2-en-1-ones

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Abstract : A facile general green synthetic route to 3-(alkyl/aralkyl/aryl)amino-1-arylprop-2-en-1-ones in excellent yields has been developed by reacting formylated acetophenones with primary amines assisted by KHSO₄ in water.

Keywords : Michael addition, formylation, enamines, elimination, acetophenones.

Synthesis and antimicrobial activities of novel 5-substituted pyrimidin-2,4,6-triones

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Abstract : 5-Benzylpyrimidin-2,4,6-triones (3a-c), 5-((furan-2-yl)methyl)pyrimidin-2,4,6-trione (3g) and 5-((3-aryl-1-phenyl-1H-pyrazol-4-yl)methyl)pyrimidin-2,4,6-triones (3h-j) were obtained in two steps. Reaction of barbituric acid (1) with various substituted aromatic aldehydes, furfuraldehyde and 3-aryl-1-phenyl-1H-pyrazole-4-carbaldehydes in methanol yielded the corresponding chalcones 2a-m in 48–85% yield. These chalcones on reduction with sodium borohydride in isopropyl alcohol furnished desired novel compounds 3a-c and 3g-j in 55–85% yield. The structure of all the synthesized compounds have been established by various spectral studies and elemental analysis. All the synthesized compounds have been screened for antimicrobial activity.

Keywords : Chalcones, 5-benzylpyrimidin-2,4,6-triones, antimicrobial activity.

Chemical examination of juice of *Citrus sinensis* variety Jaffa

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Abstract : Phytochemical examination of *Citrus sinensis* juice var. Jaffa resulted in the isolation of 5,7-dihydroxy-3',4'-dimethoxyflavanone 7-O-rhamnosyl(1→2)glucoside which is a hitherto unreported compound.

Keywords : *Citrus sinensis*, Rutaceae, 5,7-Dihydroxy-3',4'-dimethoxyflavanone 7-O-rhamnosyl(1→2)glucoside.

Accumulation of lead, cadmium, nickel and copper in hair of people living near heavy traffic area

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Abstract : Accumulation of Pb, Cd, Ni and Cu in the hair of 462 males living near heavy traffic area and less traffic area in various parts of Rajasthan (India) was studied. Out of 462, 231 lived near heavy traffic area and remaining lived near less traffic area. Head hair samples from nape were obtained from subject under study alongwith filling up of a questionnaire recommended by World Health Organisation. Hair samples were washed, digested to get a colourless and clear solution and then analysed by AAS for Pb, Cd, Ni and Cu concentration. Subjects were grouped into four age groups of 21 to 30 years, 31 to 40 years, 41 to 50 years, 51 to 60 years. While significant concentration of Pb was found in all age groups of people living near heavy traffic area as compared

to people living near less traffic area, that of Ni was not significant. Difference in Cd and Cu concentration of hair of people living near heavy traffic area and less traffic area was not found significant in all age groups.

Keywords : Hair, heavy traffic area, less traffic area, lead, cadmium, nickel, copper, Atomic Absorption Spectrometry.

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Remediation of cadmium from soil by surfactant Triton X-100

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Abstract : This study focuses on batch experiments conducted to evaluate the potential of surfactant Triton X-100 to remove heavy metals from artificially contaminated silt soil. Sorption experiments were carried out by varying concentration of cadmium and pH on soil samples. The soil samples selected for decontamination study were artificially contaminated with 500 mg L⁻¹ cadmium solutions at pH 4 and 7. Non-ionic surfactant Triton X-100 was used to decontaminate the soil at different time intervals. In sorption experiments variation of cadmium remaining with different time intervals was non-linear. It was found that maximum sorption of cadmium occurs at pH 7. Sorption continues till day 10. In desorption of 500 mg L⁻¹ cadmium contaminated soil, maximum desorption occurs at pH 4. The decontamination efficiency range of surfactant for soil contaminated with 500 mg L⁻¹ of cadmium was found to vary from 63.7% to 75.5% depending on pH.

Keywords : Surfactant, heavy metals, cadmium, contamination, sorption, desorption.

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Mechanical pulping for manufacture of hand made paper from Date-Palm leaves (*Phoenix dactylifera* – L)

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Abstract : The present paper highlights the production of pulp from agro-residues by mechanical pulping for the benefit of Indian paper industry. Date-Palm leaf (DPL), a renewable agro-residue is an excellent raw material for making pulp and paper of different grades due to high alpha cellulose (50–58%) and hemi cellulose contents (26–32%). These constituents play a stellar role in mechanical pulping i.e. in beating operation without using any chemical. Ultimate fibre length (1.25 mm to 2.50 mm) is also higher than fibres of other agro-residues, recycled cotton rag and paper. Yield and mechanical properties of the pulp of 100% DPL fibre obtained by mechanical pulping process attained higher values as compared to its blends with recycled cotton rag. Chemo-mechanical process is costly and not environment friendly. Moreover, yield and mechanical properties of the paper obtained in this process are poor. Hemi cellulose (more than 25%) and non-cellulosic polysaccharide which exist in cell wall of fibres contribute to efficient beating operation and fibre bonding. Hemi cellulose also contributes largely towards higher burst index, tensile index and folding endurance to the pulp sheet specially produced without using any chemical in the entire process.

Keywords : Date-Palm leaf, hand made paper, mechanical pulping, properties.