

## Schiff bases of 3-(2-thiazolylazo)-2,4-pentanedione with phenylenediamines and their metal complexes

K. Krishnankutty<sup>a</sup>, Muhammed Basheer Ummathur<sup>b\*</sup> and P. Sayudevi<sup>c</sup>

<sup>a</sup>Department of Chemistry, University of Calicut, Calicut -673 635, Kerala, India

<sup>b</sup>Department of Chemistry, Unity Women's College, Manjeri-676 122, Kerala, India

E-mail : mbummathur@rediffmail.com

<sup>c</sup>Department of Chemistry, NSS College, Manjeri-676 122, Kerala, India

Manuscript received 11 June 2008, revised 31 December 2008, accepted 2 January 2009

---

**Abstract :** Reaction of phenylenediamines with 3-(2-thiazolylazo)-2,4-pentanedione yielded a new series of polydentate Schiff base ligands. Spectral and analytical data revealed the condensation of *o*- and *m*-phenylenediamines in the 2 : 1 ratio and *p*-phenylenediamine in the 1 : 2 ratio. Analytical, IR, <sup>1</sup>H NMR and mass spectral data suggest neutral tetradentate N<sub>4</sub> coordination for the Schiff bases of *o*- and *m*-phenylenediamines with Ni<sup>II</sup>, Cu<sup>II</sup> and Zn<sup>II</sup> ions. In the metal complexes of the Schiff base of *p*-phenylenediamine, the intramolecularly hydrogen bonded hydrazone protons are replaced by the metal ions.

**Keywords :** 3-(2-Thiazolylazo)-2,4-pentanedione, Schiff base, phenylenediamine, IR spectra, <sup>1</sup>H NMR spectra, mass spectra.

## C<sub>16</sub>TAB catalyzed oxidative decolorisation of methylene blue by acidic *N*-chloro-*p*-toluenesulfonamide

Mona Pipada, Brijesh Pare<sup>a\*</sup>, V. W. Bhagwat and Manisha Ayachit<sup>a</sup>

School of Studies in Chemistry, Vikram University, Ujjain-450 010, Madhya Pradesh, India

<sup>a</sup>Department of Chemistry, Madhav Science College (Vikram University), Ujjain-456 010, Madhya Pradesh, India

E-mail : brijesh\_pare@hotmail.com

Manuscript received 11 April 2007, revised 30 September 2008, accepted 19 December 2008

---

**Abstract :** Kinetics and mechanism of uncatalyzed and C<sub>16</sub>TAB catalyzed oxidation of methylene blue (phenothiazin-5-inum, 3,7-(dimethyl amino)-chloride) [MB<sup>+</sup>] by *N*-chloro-*p*-toluenesulfonamide in acidic media has been studied spectrophotometrically. With excess concentrations of other reactants, the reaction rate follows pseudo-first order kinetics with respect to methylene blue. The uncatalyzed reaction has fractional order dependence on chloramine-T and zero order dependence on H<sup>+</sup> concentration (in the range 1.0 × 10<sup>-2</sup> M to 9.0 × 10<sup>-2</sup> M). Cationic surfactant cetyl trimethyl ammonium bromide catalyzes the reaction even before its CMC. A bathochromic shift is the evidence of dye-surfactant interaction. The pre-micellar kinetics has been rationalized in the light of Piskiewicz positive co-operativity. Positive co-operativity index (*n* = 1.27) has been computed. Variations of ionic strength have no influence on the reaction rate. The basic stoichiometry equation is as follows :



where, P<sub>2</sub><sup>+</sup> = 4*aH*-phenothiazine-3,7-diamine 5-oxide. On the basis of product analysis a pertinent mechanism is proposed.

**Keywords :** Chloramine-T, methylene blue, C<sub>16</sub>TAB, Piskiewicz, pre-micellar.

# Modeling of lipophilicity of some organic compounds using structural and topological indices

Vijay K. Agrawal<sup>a\*</sup>, Vinay K. Dubey<sup>a</sup>, Basheerulla Shaik<sup>a</sup>, Jyoti Singh<sup>a</sup>, Kamana Singh<sup>a</sup> and Padmakar V. Khadikar<sup>b</sup>

<sup>a</sup>QSAR and Computer Chemical Laboratories, A. P. S. University, Rewa-486 003, Madhya Pradesh, India

*E-mail* : jyoti\_singh07@rediffmail.com, vijay-agrawal@lycos.com

<sup>b</sup>Research Division, Laxmi Fumigation and Pest Control Pvt. Ltd., 3, Khatipura, Indore-452 007,

Madhya Pradesh, India

*E-mail* : pvkhadikar@rediffmail.com

*Manuscript received 22 April 2008, accepted 19 December 2008*

---

**Abstract** : In the present work we have considered miscellaneous set of 48 compounds and modeled their log *P* using classical as well as topological descriptors. The results indicate that the estimation (modeling) of log *P* is very much effective when the structural and topological descriptors are used together. The most appropriate model for the estimation (modeling) of log *P* indicated that by using the combination of structural and topological descriptors the results account for 93% variation in log *P*.

**Keywords** : Lipophilicity, log *P*, topological descriptors, QSAR.

J. Indian Chem. Soc.,  
Vol. 86, April 2009, pp. 346-351

# Studies on interaction of molybdenum(VI) with modified lignocellulosics using a novel spectrophotometric method

M. K. Sreedhar<sup>a\*</sup>, T. S. Anirudhan<sup>b</sup>, T. J. John<sup>a</sup> and R. Remya<sup>a</sup>

<sup>a</sup>Department of Chemistry, University College, Thiruvananthapuram -695 034, Kerala, India

*E-mail* : drmkdsdharuc@hotmail.com

<sup>b</sup>Department of Chemistry, University of Kerala, Thiruvananthapuram-695 581, Kerala, India

*Manuscript received 23 April 2008, revised 16 December 2008, accepted 19 December 2008*

---

**Abstract** : A new adsorbent (PGPEP-COOH) bearing carboxylate functional group was prepared through graft co-polymerization of acrylic acid onto pulverized *Phyllanthus emblica* planks using ferrous sulphate/H<sub>2</sub>O<sub>2</sub> redox initiator system. The adsorbent obtained was tested for the uptake of molybdenum(VI) from aqueous solutions. The efficiency of the PGPEP-COOH to remove Mo<sup>VI</sup> ions at different time of contact, initial adsorbate concentration, adsorbent dose, pH, ionic strength and temperature was studied by batch experiments. The amount of molybdenum(VI) in aqueous system was determined using a very simple and sensitive method of estimation using potassium hexacyanoferrate(II). Reddish brown solution of the molybdenum complex at pH 3.2 shows absorption maximum at 390 nm. To establish the most appropriate correlation for adsorption equilibrium, isotherm studies were performed using Langmuir, Freundlich and Redlich-Peterson models. The suitability of isotherm models was compared using linear least square fitting. Experimental kinetic data were described using a diffusion controlled first order reversible model and diffusion coefficient was evaluated at different temperatures. Applying Eyring equation thermodynamic parameters were calculated. PGPEP-COOH adsorbed 99.2% Mo<sup>VI</sup> from a solution of 10 mmol dm<sup>-3</sup> concentration at 303 K. Desorption and regeneration studies of the adsorbent under different conditions were also studied.

**Keywords** : Spectrophotometric determination, adsorption, molybdenum, isotherm, lignocellulose.

## Complexation behaviour of (3,4-dihydroxyphenyl)alanine in some mixed coordinated systems : Equilibrium studies

Neerja Dwivedi (Upadhyaya)<sup>a\*</sup>, K. Dwivedi<sup>a</sup> and R. Nair (Ahuja)<sup>b</sup>

<sup>a</sup>School of Studies in Chemistry, Jiwaji University, Gwalior-474 011, Madhya Pradesh, India

*E-mail* : nd\_chem@sify.com

<sup>b</sup>Vijaya Raje Govt. Girl's P.G. College, Morar, Gwalior-474 006, Madhya Pradesh, India

*Manuscript received 12 June 2008, accepted 19 December 2008*

---

**Abstract** : Thermodynamic stability of complexes of Ni<sup>II</sup> and Co<sup>II</sup> with (3,4-dihydroxyphenyl)alanine (DOPA) and L-alanine, L-phenylalanine, L-aspartic acid and L-glutamic acid were investigated. Thermodynamic formation constants of these complexes were determined at three different ionic strengths at 20 ± 1°C and 30 ± 1 °C in aqueous medium under equimolar condition by subjecting experimental data to the computation applying SCOGS computer program.

Thermodynamic parameters for mixed coordinated systems were calculated by using van't Hoff isotherm, van't Hoff isochore and Gibb's Helmholtz equation. Species distribution is obtained for all ternary (biligand) systems. Complexation behaviour of ligands is discussed.  
**Keywords** : Thermodynamic stability, mixed coordinated system.

## Spectrophotometric determination of Buclizine as hydrochloride (BUCZ) using I<sub>2</sub>/PMAP-SAc, AM/PTC and PMA/cobalt(II)/EDTA

V. Annapurna<sup>a</sup>, G. Jyothi<sup>a</sup>, V. Nagalakshmi<sup>a</sup> and B. B. V. Sailaja<sup>b\*</sup>

<sup>a</sup>Department of Chemistry, St. Theresa's College for Women, Eluru-534 003, Andhra Pradesh, India

<sup>b</sup> Department of Inorganic & Analytical Chemistry, Andhra University, Visakhapatnam-530 003, Andhra Pradesh, India

*E-mail* : sailaja\_bbv@yahoo.co.in

*Manuscript received 14 July 2008, accepted 24 December 2008*

---

**Abstract** : Simple, accurate and reproducible UV spectrophotometric methods were established for the assay of BUCZ based on the formation of precipitation, charge transfer and redox products. Precipitation/charge transfer complex formation of the BUCZ with I<sub>2</sub>/p-N-methyl amino phenol sulphate (PMAP)-sulphanilic acid (SAc) by Method A, the precipitation/complex formation with ammonium molybdate (AM)/potassium thiocyanate (PTC) by Method B and precipitation/redox reaction of BUCZ with phosphomolybdic acid (PMA)/Co<sup>II</sup>/EDTA by Method C were proposed. Determination of BUCZ in bulk form and in pharmaceutical formulations were also incorporated.  
**Keywords** : Estimation, Buclizine, precipitating agent, charge transfer complex.

## Kinetics, mechanism and thermodynamic studies of rhodium(III) catalysed oxidation of alanine by alkaline hexacyanoferrate(III)

P. K. Chourasia\*, N. C. Bhattacharjee and T. K. Singh

---

**Abstract :** The kinetics and mechanism of rhodium(III) catalysed oxidation of alanine in alkaline solution of hexacyanoferrate(III) have been studied. The kinetic data shows zero order dependence on each hexacyanoferrate(III) and sodium hydroxide whereas first order dependence each on alanine and  $Rh^{III}$ . Negligible effect of ionic strength of the medium has been reported. A suitable mechanism consistent with the observed kinetics has been suggested.

**Keywords :** Rhodium(III), mechanism, hexacyanoferrate(III), alanine.

J. Indian Chem. Soc.,  
Vol. 86, April 2009, pp. 367-376

## **Kinetics of potassium adsorption and desorption in some soils of West Bengal**

**Debjani Ghosh, Abhijit Deb Nath\* and Saroj Kumar Sanyal**

Department of Agricultural Chemistry and Soil Science, Bidhan Chandra Krishi  
Viswavidyalaya,  
Mohanpur-741 252, Nadia, West Bengal, India

*E-mail :* debjani\_pg17@yahoo.co.in, adebnathbckv@yahoo.com, sarojsanyal@yahoo.co.in

*Manuscript received 4 November 2008, accepted 23 December 2008*

---

**Abstract :** Kinetics of potassium (K) adsorption and desorption were studied in eight soils of widely varying physicochemical properties with a view to identifying the major rate-limiting steps. The study was described by using first-order, Elovich, parabolic-diffusion, power function and zero-order equations. From the overall studies of kinetic equations, it was found that the parabolic-diffusion equation as well as the first-order equation was equally good to describe the adsorption and desorption of K in soils which suggests that the given adsorption and desorption processes tended to be diffusion controlled. The rate constants were closely related to the clay mineralogical make-up of the given soils. In general, the soils dominated by kaolinite, exhibited lower adsorption rate coefficient ( $k_a$ ) than the other soils studied, while showing much higher desorption rate coefficient ( $k_d$ ). This was attributed to the absence of specific sites for K in the clay fraction of these soils. From the Gibbs standard free energy change ( $DG^\circ$ ) values, the Gayeshpur, Memari, Goaltore and Kalimpong soils were found to favour Ca-K exchange.

**Keywords :** Kinetics, potassium, adsorption, desorption, first-order, Elovich, parabolic-diffusion, power function, zero-order.

J. Indian Chem. Soc.,  
Vol. 86, April 2009, pp. 377-382

## **Solid phase extraction of $Hg^{II}$ ions with cross-linked poly(acrylic acid), coated on silanized silica gel**

**Pranesh Chowdhury\*, Susanta K. Pandit and Bhabatosh Mandal\***

Analytical Laboratory, Department of Chemistry, Visva-Bharati, Santiniketan-731 235, West Bengal, India

*E-mail :* pranesh\_02@yahoo.co.in

*Manuscript received 15 December 2008, accepted 24 December 2008*

---

**Abstract :** A selective and reliable method has been developed for the extraction and separation of  $Hg^{II}$  with high molecular mass cross-linked poly(acrylic acid) coated on silanized silica gel. The coated material acts as stationary phase for the extraction. Ion exchange and break-through capacity of the exchanger have been measured. The optimum pH range for the quantitative extraction of  $Hg^{II}$  was found to be 5.0–6.0. The elution behaviors of  $Hg^{II}$  have been investigated. A plausible mechanism

for Hg<sup>II</sup> extraction and elution has been suggested. Hg<sup>II</sup> has been isolated quantitatively from various synthetic mixtures containing heavy metal ions (Pb<sup>2+</sup>, Cd<sup>2+</sup>, Zn<sup>2+</sup>, Co<sup>2+</sup>, Ni<sup>2+</sup> and Cu<sup>2+</sup>).  
Keywords : Cross-linked poly(acrylic acid), silanized silica gel, ion exchange, solid-phase extraction.

J. Indian Chem. Soc.,  
Vol. 86, April 2009, pp. 383-387

## Oxidation reactions catalysed by polymer anchored transition metal complexes

J. Dhavamani and V. R. Parameswaran\*

Department of Chemistry, Annamalai University, Annamalaiagar-608 002, Tamilnadu, India

E-mail : vrpchem@mail.com

Manuscript received 11 August 2008, accepted 30 December 2008

---

**Abstract :** Polymer-anchored transition metal complexes were synthesized by supporting cobalt, iron and copper on cation exchange resin (polystyrene). The catalysts were characterized by CHN analysis, SEM, IR spectroscopy, ESR and thermal studies. The catalysts were found to be active for oxidation of some alcohols under mild conditions of temperature and pressure. The influence of polarity of solvent on the rate of reaction was studied. The rate of oxidation was influenced by the concentration of catalyst and substrate as well. The catalysts retain the same efficiency for 5-6 runs.  
**Keywords :** Polymer-anchored catalysts, oxidation, molecular oxygen, recycling efficiency.

J. Indian Chem. Soc.,  
Vol. 86, April 2009, pp. 388-392

## Synthesis of spirocyclic compounds: A photochemical approach

Ramesh C. Kamboj\*, Mandeep Thakur, Rita Arora, Surinder Berar, Urmila Berar and Satish C. Gupta

Department of Chemistry, Kurukshetra University, Kurukshetra-136 119, Haryana, India

E-mail : rckamboj@rediffmail.com Fax : 91-1744-238277

Manuscript received 18 August 2008, accepted 12 November 2008

---

**Abstract :** The phototransformations of 2-thienyl-3-cycloalkenyloxy benzopyrans in benzene lead to fused spirocyclic compounds bearing thiophene ring system.  
**Keywords :** Spiropyran, photoirradiation, type-II reaction, cycloalkenyloxychromone.

J. Indian Chem. Soc.,  
Vol. 86, April 2009, pp. 393-396

## Studies on the Biginelli reaction : Synthesis of 3,4-dihydropyrimidin-2(1H)-thiones via aryliidene intermediate and one pot reaction

Nainesh Kansagara, Jagdish Godhasra, Mahesh Patel and Viral Shah\*

Department of Chemistry, Kamani Science College, Amreli-365 601, Gujarat, India

E-mail : naineshkansagara@yahoo.co.in

Manuscript received 30 August 2007, revised 5 August 2008, accepted 23 December 2008

---

**Abstract :** The series of 4-aryl-6-isopropyl-5-[N-(3-nitrophenyl)aminocarbonyl]-3,4-dihydropyrimidin-2(1H)-thiones 2a-l were prepared via aryliidene (route-1) intermediates by condensing 2-aryliidene-4-methyl-N-(3-nitrophenyl)-3-oxopentanamide and thiourea in the presence of potassium bicarbonate. Then 2a-l were prepared by single step (route-2) in the presence of conc. HCl

catalyst, with better yield in short time compare to route-1. Some of these compounds showed potential antimicrobial activity.

Keywords : Biginelli reaction, arylidene, one pot reaction, antimicrobial activity.

J. Indian Chem. Soc.,  
Vol. 86, April 2009, pp. 397-401

## Synthesis of phthalimido or succinimido[2-aryl-4-oxo-3-{2-phenyl-4(3H)-quinazolinon-3-yl}-1,3-thiazolidin-5-yl]ethanoate

Shweta Sharma, Chirag Sharma, Bhawana Thadhaney and G. L. Talesara\*

Synthetic Organic Chemistry Laboratory, Department of Chemistry, M. L. Sukhadia University,  
Udaipur-313 001, Rajasthan, India

E-mail : gtalesara@yahoo.com

Manuscript received 11 June 2008, revised 5 November 2008, accepted 23 December 2008

**Abstract :** Treatment of benzoxazine 1 with hydrazine hydrate in ethanol furnished 3-amino-2-phenylquinazolin-4-(3H)-one 2, which upon condensation with aldehydes 3a-d yielded the corresponding 3-arylideneamino derivatives 4a-d. Cyclization of these derivatives using mercaptosuccinic acid afforded 1,3-thiazolidin-4-one ethanoic acids 5a-d, which after esterification with *N*-hydroxyphthalimide or *N*-hydroxysuccinimide via acid chlorides produced the respective ethanoic esters 7a-e.

Keywords : *N*-Hydroxyphthalimide, *N*-hydroxysuccinimide, benzoxazine, quinazolinone, thiazolidin.

J. Indian Chem. Soc.,  
Vol. 86, April 2009, pp. 402-405

## Base-catalysed cyclocondensation of $\alpha,\alpha\zeta$ -bis(arylmethylene)cyclohexanones with thiourea : Formation of *E*-8-(arylmethylene)-4-aryl-1,2,3,4,5,6,7,8-octahydrobenzo[d]pyrimidine-2-thiones

Rammohan Pal, Tapas K. Mandal and Asok K. Mallik\*

Department of Chemistry, Jadavpur University, Kolkata-700 032, India

E-mail : mallikak52@yahoo.co.in

Manuscript received 11 November 2008, accepted 23 December 2008

**Abstract :** Base-catalysed cyclocondensation of  $\alpha,\alpha\zeta$ -bis(arylmethylene)cyclohexanones with thiourea has been found to generate *E*-8-(arylmethylene)-4-aryl-1,2,3,4,5,6,7,8-octahydrobenzo[d]pyrimidine-2-thiones in high yield, the structures of which have been established from their spectral data. However, corresponding cyclopentanones were found to be unreactive under similar reaction condition.

Keywords :  $\alpha,\alpha\zeta$ -Bis(arylmethylene)cycloalkanones, thiourea, *E*-8-(arylmethylene)-4-aryl-1,2,3,4,5,6,7,8-octa-hydrobenzo[d]pyrimidine-2-thiones.

J. Indian Chem. Soc.,  
Vol. 86, April 2009, pp. 406-409

## Development and validation of a liquid chromatographic method for the determination of clopidogrel from pharmaceutical dosage form

N. Sultana<sup>a</sup>, M. S. Arayne<sup>b\*</sup>, M. Nawaz<sup>b</sup> and Kiran Amir Ali<sup>a</sup>

<sup>a</sup>Research Institute of Pharmaceutical Sciences, Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Karachi, Karachi-75270, Pakistan

<sup>b</sup>Department of Chemistry, University of Karachi, Karachi-75270, Pakistan

E-mail : msarayne@gmail.com

Manuscript received 18 July 2007, revised 15 July 2008, accepted 19 December 2008

**Abstract :** A rapid, specific, precise and sensitive reversed-phase high-performance liquid chromatographic method was developed and validated for the determination of clopidogrel from pharmaceutical dosage form in the presence of flurbiprofen as internal standard. Clopidogrel and internal standard were analyzed on Purospher start C18, 5 mm column having 250 × 4.6 mm i.d., with mobile phase containing methanol : water (80 : 20; pH 3.4) was used. The flow rate was 1.0 mL min<sup>-1</sup> and detector response was monitored at 235 nm. The retention time of clopidogrel and internal standard was 4.2 min and 6.4 min respectively. Calibration curve was linear in concentration range of 0.25–50.0 mg mL<sup>-1</sup> with coefficient of determination (*r*<sup>2</sup>) of 0.9994. Detection (LOD) and quantitation limits (LOQ) were 0.09 and 0.28 mg mL<sup>-1</sup>, respectively. The intra-day accuracy ranged from 96.0–103.6% with a precision of 2.30–2.86%. Similarly, the inter-day accuracy was between 98.18 and 99.99% with a precision of 1.18–10.59%.

**Keywords :** Clopidogrel, liquid chromatography, HPLC-UV detection.

J. Indian Chem. Soc.,

Vol. 86, April 2009, pp. 410-415

## Extraction chromatographic studies of copper(II) and bismuth(III) with Aliquat-336

Malay Datta and Uday Sankar Roy\*

Department of Chemistry, Visva-Bharati, Santiniketan-731 235, West Bengal, India

Manuscript received 21 August 2007, revised 16 December 2008, accepted 19 December 2008

**Abstract :** A selective method has been developed for extraction chromatographic studies of Cu<sup>II</sup> and Bi<sup>III</sup> with Aliquat-336 (liquid anion exchanger) coated on silica gel as a stationary phase. Quantitative extraction of Cu<sup>II</sup> has been achieved at 4.0–6.0 M HCl and quantitative extraction of Bi<sup>III</sup> has been achieved at 0.1–4.0 M HCl, 0.1–6.0 M HNO<sub>3</sub> and 1.0–3.0 M H<sub>2</sub>SO<sub>4</sub>. The effects of different acids, stripping agents, flow rate on extraction and elution have been investigated. Cu<sup>II</sup> and Bi<sup>III</sup> have been separated from several metal ions. In order to assess the possible analytical application, both the metal ions have been separated from several multicomponent mixtures containing metal ions commonly associated with it. Attempts have been made to extract Cu<sup>II</sup> from standard alloy and ore samples. The proposed method is simple, rapid and selective.

**Keywords :** Extraction chromatography, Aliquat-336, multicomponent separation, exchange capacity.

J. Indian Chem. Soc.,

Vol. 86, April 2009, pp. 416-418

## Electrochemical reactions at sacrificial electrodes. Part-XXI<sup>†</sup> : Synthesis of unique antimony(III) alkoxides

J. S. Banait\*, Baljit Singh and Sarbjit Rala

Department of Chemistry, Punjabi University, Patiala-147 002, Punjab, India

E-mail : js\_banait@yahoo.com

Manuscript received 11 June 2008, revised 15 December 2008, accepted 23 December 2008

**Abstract :** Electrochemical reactions of acetylacetone, cyanoacetamide, ethylcyanoacetate, ethylacetoacetate and diethylmalonate (RH<sub>2</sub>) have been carried out in acetonitrile at sacrificial antimony anode using tetrabutylammonium chloride as supporting electrolyte. The products isolated from the anode compartment have been identified by elemental analysis and infrared spectral studies and are found to be unique antimony(III) alkoxides. Coordination compounds of all these products

with 1,10-phenanthroline and 2,2'-bipyridyl have also been synthesized electrochemically and characterized by various physical methods. All these reactions proceed with high current efficiencies.  
Keywords : Antimony(III) alkoxide, electrochemical reactions, electrodes, synthesis.

J. Indian Chem. Soc.,  
Vol. 86, April 2009, pp. 419-424

## Density and viscosity study of binary mixtures of eucalyptol with methanol, ethanol, 1-propanol, 1-butanol and 2-methylpropan-1-ol at 303.15, 308.15 and 313.15 K

Sangita Sharma\*, Pragnesh B. Patel, Rignesh S. Patel and J. J. Vora

Department of Chemistry, Hemchandracharya North Gujarat University, Patan-384 265, Gujarat, India

E-mail : smridhee2000@yahoo.co.in

Manuscript received 19 April 2007, revised 19 December 2008, accepted 19 December 2008

---

**Abstract :** Density and viscosity of the binary liquid mixtures of eucalyptol with methanol, ethanol, 1-propanol, 1-butanol and 2-methylpropan-1-ol have been measured at 303.15, 308.15 and 313.15 K. From density and viscosity data, the values of excess molar volume ( $V_m^E$ ), the excess viscosity ( $\eta^E$ ) and the excess Gibb's free energy of activation of flow ( $\Delta G^{\#E}$ ) have been determined. The computed results have been fitted to Redlich-Kister polynomial equation. Further, the density and viscosity data have been theoretically analysed for the validity of several viscosity models. The main thrust of the study is to correlate the excess properties and the relevant interaction parameters with the nature of molecular interactions between the mixing components. Deviations from ideal behavior are discussed from the point of view of molecular interactions present between the unlike molecules. The strength of interaction is related to alkyl chain length of alcohols. The results are discussed in terms of the interaction parameters obtained from Grunberg-Nissan, Tamura-Kurata and Hind viscosity models and excess properties.

Keywords : Eucalyptol, viscosity, binary mixture, density.

J. Indian Chem. Soc.,  
Vol. 86, April 2009, pp. 425-428

## Use of valence delta, $d^v$ in the molecular connectivity calculations and correlation with molar refraction

A. R. Saksena, Sunanda Das and Arti Gupta\*

Department of Chemistry, C.M.P. Degree College (University of Allahabad), Allahabad-211 002,

Uttar Pradesh, India

E-mail : guptarti@yahoo.co.in

Manuscript received 4 February 2008, revised 18 August 2008, accepted 19 December 2008

---

**Abstract :** Molecular connectivity calculations have been carried out for highly anisotropic bidentate ligands ( $C_{2v}$  symmetry), organometallic substrates of the formulae,  $R_2MX_2$  (where R is an alkyl group and X is a halogen atom) and organometallic chelates of the formulae,  $R_2ML_x$  (where L is a bidentate ligand). Multiple Chi,  ${}^mC_t^v$  with reference to valence delta,  $d^v$  have been calculated for the hydrogen suppressed graphs (skeletal structures) for each molecule and have been correlated with molar refractions. These correlations will play a vital role in the SAR studies of biologically active molecules.

Keywords : Molecular connectivity, organometallics, ligands, molar refraction, chelates, conformational analysis.

## A one-pot route to the synthesis of functionalized butan-1-one analogues

A. R. Naresh Raj and C. A. M. A. Huq\*

P.G. and Research Department of Chemistry, The New College (Affiliated to the University of Madras), Chennai-600 014, India

*E-mail* : drmdabdulhuq@yahoo.com

*Manuscript received 22 July 2008, accepted 19 December 2008*

---

**Abstract** : We report the first instance where the treatment of 1-*N*-phenyl-2-pyrrolidinone with RMgX gave acyclic nitrogen based compounds i.e. 1-aryl-4-(arylamino)butan-1-one derivatives instead of fused nitrogen heterocycles. The formation of 1-aryl-4-(arylamino)butan-1-one derivatives involves unusual ring opening.

**Keywords** : 1-*N*-Phenyl-2-pyrrolidinone, ring opening reaction, Grignard reaction.