Effect of complexation on herbicidal character of Metribuzin with copper(II)

Rajeeva Ranjan, Punam Verma, Rekha Rani, N. C. Bhattacharjee and Shivadhar Sharma*

University Department of Chemistry, Magadh University, Bodh Gaya-823 234, Bihar, India

E-mail: sharma.shivadhar@gmail.com

Abstract: Metribuzin derived from precursor triazine i.e. 4-amino-6-tert.-butyl-3-mercapto-1,2,4-triazine-5-one has been used for complexation with copper(II) with empirical formula [Cu(MBN)_2X_2] where MBN is Metribuzin i.e. 4-amino-6-tert.-butyl-3-methylthio-1,2,4-triazine-5-one and X stands for Cl^-, Br^-, NO_3^-, CH_3COO^- and ClO_4^-.

The newly synthesized complexes have been characterized by microanalysis, IR spectroscopy, molar conductivity, magnetic moment and electronic spectra. The various crystal field parameters like D_q(xy), D(qz), D_s and D_t have been derived from their electronic spectra. The positive values of D_s and D_t are indicative of tetragonal elongation along Z-axis of octahedral symmetry of copper(II) complexes. The herbicidal character of copper(II) complexes has been compared with that of Metribuzin and it has been inferred from the results that herbicidal character of Metribuzin gets enhanced in copper(II) complexes.

Keywords: Herbicidal characters, Metribuzin, tetragonal elongation.

An iron(III)-Schiff base complex as a functional model of phenoxazinone synthase enzyme

Bhaskar Biswas^a and Partha Sarathi Sengupta^b

^aDepartment of Chemistry, Raghunathpur College, Purulia-723 133, West Bengal, India

^bDepartment of Chemistry, Vivekananda Mahavidyalaya, Burdwan-713 104, West Bengal, India

Abstract: A new iron(III) complex, [Fe(L)Cl_2(H_2O)] (1) containing a (N,O,Cl)-donor Schiff base ligand has been synthesized and characterized by different analytical techniques. Room temperature magnetic measurement indicates the existence of high spin iron(III) compound in the solid state. Molar conductance value of the iron compound in methanol medium reveals the existence of 1 : 2 type electrolyte in solution. The structural formulation of the iron-Schiff base complex has been confirmed through optimization with B3LYP density functional theory (DFT) using 6-31g(d) basis set and shows that the proposed structure is in better agreement with the experimental findings. The iron(III) complex has been evaluated to mimic the active site of phenoxazinone synthase enzyme in
methanol medium. The iron(III) complex significantly promotes the catalytic oxidation of 2-aminophenol (AP) to 2-aminophenoxazin-3-one in under aerobic condition with a high turnover number, $k_{\text{cat}} = 4.32 \times 10^3 \text{ h}^{-1}$.

Keywords : Iron(III), Schiff base, phenoxazinone synthase activity.

J. Indian Chem. Soc.,
Vol. 94, June 2017, pp. 579-586

A novel samarium(III) nanocomposite carbon paste electrode based on $N,N'$-bis(8-quinolyl)pyridine-2,6-dicarboxamide as a selectophore

Fateme Pourrezai$^a$, Hassan Ali Zamani$^{a,a}$, Fatemeh Joz-Yarmohammadi$^a$, Soraia Meghdadi$^b$ and Mohammad Reza Abedi$^c$

$^a$Department of Applied Chemistry, Mashhad Branch, Islamic Azad University, Mashhad, Iran
$^b$Department of Chemistry, Isfahan University of Technology, Isfahan 84156-83111, Iran
$^c$Department of Applied Chemistry, Quchan Branch, Islamic Azad University, Quchan, Iran

Abstract : A sufficient amounts of $N,N'$-bis(8-quinolyl)pyridine-2,6-dicarboxamide (QPC) was applied as a new ionophore for fabrication of new nanocomposite carbon paste electrode (CPE) modified with nanosilica/MWCNT. The electrochemical behavior of the new prepared CPE was investigated in the presence of various metal ions. The best composition of ingredients was achieved in optimization stage for QPC : 2%, binder (paraffin oil) : 25%, modifier (MWCNT : 1%, NS : 0.1%), and graphite powder : 71.9%. This new CPE displayed a Nernstian response by the slope of 19.7±0.9 mV decade$^{-1}$ in the linear range of $1.0 \times 10^{-8}$–$1.0 \times 10^{-3}$ mole L$^{-1}$ with a lower detection limit of $9.0 \times 10^{-9}$ mole L$^{-1}$ toward Sm$^{3+}$ ion. The pH range of this new samarium(III) electrode was gained 3.7 to 7.3 with a response time about 13 s. The matched potential method was applied to study the selectivity of Sm$^{3+}$CPE in comparison with many common cations which showed the negligible disturbance of all other cations on the proposed samarium(III) electrode. It was successfully used as an indicator electrode in potentiometric titration of Sm$^{3+}$ ions with EDTA and determination of Sm$^{3+}$ content in several blends of ions.

Keywords : Nanocomposite, carbon paste electrode, samarium(III), ion selective electrode, $N,N'$-bis(8-quinolyl)pyridine-2,6-dicarboxamide, potentiometry, sensor.

J. Indian Chem. Soc.,
Vol. 94, June 2017, pp. 587-591

Gamma radiation effect on structure and photoluminescence properties of RE$^{3+}$ (Tb$^{3+}$/Ce$^{3+}$) activated GdPO$_4$ phosphor

Sudheer Gurugubelli$^a$, Vemareddy Bheeram$^a$, Anima S. Dadhich$^a$, Abhijit Saha$^b$ and Saratchandra Babu Mukkamala$^{a,a}$
Abstract: RE$^{3+}$ (Tb$^{3+}$/Ce$^{3+}$) activated GdPO$_4$ phosphor has been synthesized by hydrothermal route at 150 °C using citric acid as chelating agent. The synthesized phosphor has been characterized by TEM, TG/DTA, Powder X-ray diffraction and photoluminescence spectra. GdPO$_4$ displayed green emission after doping with Tb$^{3+}$. The influence of γ-radiation on structural and photoluminescence properties of GdPO$_4$: Tb$^{3+}$,Ce$^{3+}$ was also examined at 5 and 300 kGy. Quenching of PL intensity was observed in GdPO$_4$: Tb$^{3+}$,Ce$^{3+}$ after exposure to γ-radiation. Moreover, this phosphors exhibited high structural stability upon γ-radiation exposure.

Keywords: Gadolinium phosphate, hydrothermal synthesis, photoluminescence, γ-radiation.

J. Indian Chem. Soc., Vol. 94, June 2017, pp. 593-598

Synthesis, crystal structures and magnetic properties of two cyanide-bridged one-dimensional single chain M$^{II}$-Mn$^{II}$ (M = Ni, Pd) complexes

Chongchong Xue, Jingwen Shi and Daopeng Zhang*

College of Chemical Engineering, Shandong University of Technology, Zibo 255049, China

E-mail: dpzhang73@126.com

Manuscript received online 01 February 2017, accepted 23 February 2017

Abstract: Two cyanide-bridged heterobimetallic M$^{II}$-Mn$^{II}$ (M = Ni, Pd) complexes have been prepared by assembling the mononuclear seven-coordinated closed macrocycle manganese($^{II}$) compound and the tetra-cyanometallic building blocks. Single X-ray diffraction analysis show that these two complexes [Mn(L$^1$)]$^{2+}$[M(CN)$_4$]$^{2–}$ (M = Ni (1), Pd (2); L$^1$ = 3,6-diazaoctane-1,8-diamine) present predictable one-dimensional single chain structures. The molecular structures of the one-dimensional complexes consists of alternating units of [Mn(L$^1$)]$^{2+}$ and [M(CN)$_4$]$^{2–}$, forming a cyanide-bridged neutral polymeric chain. The coordination geometry of manganese($^{II}$) ion in the two complexes is a slightly distorted pentagonal-bipyrididal with two cyanide nitrogen atoms at the trans positions and N$_5$ coordinating mode at the equatorial plane from the macrocyclic ligand. The magnetic properties for these two complexes were investigated and the results showed the very weak antiferromagnetic coupling between neighboring Mn$^{II}$ ions connected by the diamagnetic tetra-cyanometallic building block. A best-fit to the magnetic susceptibility leads to the magnetic coupling constants $J = −0.09$ and $−0.12$ cm$^{-1}$ for complexes 1 and 2, respectively.

Keywords: Cyanide-bridged, 1D complex, crystal structure, magnetic property.
Mn\textsuperscript{II} catalyzed oxidation of \( p \)-phenetidine by periodate ion – A kinetic and mechanistic study

R. D. Kaushik\textsuperscript{*a}, Jaspal Singh\textsuperscript{a}, Priyanka Tyagi\textsuperscript{a} and Ekata Kumari\textsuperscript{b}

\textsuperscript{a}Department of Chemistry, Gurukul Kangri University, Haridwar-249 404, Uttarakhand, India
\textsuperscript{b}Uttaranchal College of Science and Technology, Dehradun-248 001, Uttarakhand, India

\textit{E-mail} : rduttkaushik@yahoo.co.in

Abstract : The kinetics of the periodate oxidation of \( p \)-phenetidine (PEA) in acetone-water medium has been followed by monitoring the increase in the absorbance of reaction intermediate, \( \text{C}_4 \), and the main reaction product is 4-ethoxy-1,2-benzoquinone. Results under pseudo-first order conditions, \([\text{IO}_4^-] >> [\text{PEA}]\), are in agreement with the rate law:

\[
d[C]/dt = kK_3K_4K_w[\text{Mn}^{\text{II}}][\text{PEA}][\text{IO}_4^-][\text{H}^+]/(K_2K_w + K_6[\text{H}^+]) + K_b[\text{H}^+]^2
\]

where \( kK_3K_4 \) is the empirical composite rate constant, \( K_w \) is ionic product of water, \( K_2 \) is acid dissociation constant of \( \text{H}_4\text{IO}_6^- \) and \( K_b \) is base dissociation constant of PEA. In agreement with the rate law the \( 1/k_{\text{cat}} \) versus \([\text{H}^+]\) profile passes through the minimum. Free radical scavengers do not affect the reaction rate. The values of thermodynamic parameters are : \( \Delta E = 17.94 \text{ kJ mol}^{-1} \), \( A = 5.5 \times 10^{10} \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} \); \( \Delta S^\theta = -156.58 \text{ J mol}^{-1} \text{ K}^{-1} \), \( \Delta G^\theta = 66.55 \text{ kJ mol}^{-1} \) and \( \Delta H^\theta = 15.36 \text{ kJ mol}^{-1} \).

Keywords : Kinetics, Mn\textsuperscript{II} catalysed, periodate oxidation, \( p \)-phenetidine, 4-ethoxy-1,2-benzoquinone.

Stopped flow kinetics of Mn\textsuperscript{II} catalysed periodate oxidation of 3,5-dimethyl-aniline – Evaluation of stability constant of the ternary intermediate complex

R. D. Kaushik\textsuperscript{*a}, Jaspal Singh\textsuperscript{a}, Richa Agarwal\textsuperscript{a} and Ekata Kumari\textsuperscript{b}

\textsuperscript{a}Department of Chemistry, Gurukul Kangri University, Haridwar-249 404, Uttarakhand, India
\textsuperscript{b}Uttaranchal College of Science and Technology, Dehradun-248 001, Uttarakhand, India

\textit{E-mail} : rduttkaushik@yahoo.co.in

Abstract : The formation of ternary intermediate unstable complex during the oxidation of aromatic amines by periodate ion catalysed by Mn\textsuperscript{II} has been proposed in case of some anilines. This paper is the first report on kinetic study and evaluation of stability constant of ternary complex forming in the Mn\textsuperscript{II}-catalysed periodate oxidation of 3,5-dimethylaniline (D) in acetone-water medium. Stop-flow spectrophotometric method was used to study the ternary complex formation and to determine its stability constant. The stop-flow trace shows the reaction to occur in two steps. The first step,
which is presumably the formation of ternary complex, is relatively fast while the second stage is relatively quite slow. The stability constant evaluated for D-Mn\textsuperscript{II}-IO\textsubscript{4}-ternary complex by determining equilibrium absorbance is \((4.5\pm0.1)\times10^5\). Kinetics of ternary complex formation was defined by the rate law (A) under pseudo-first order conditions.

\[
\ln\left(\frac{[C_2]_{eq}}{[C_2]_{eq} - [C_2]}\right) = k_{\text{obs}}t
\]

(A)

where, \(k_{\text{obs}}\) is the pseudo-first order rate constant, \([C_2]\) is concentration of ternary complex at given time \(t\), and \([C_2]_{eq}\) is the equilibrium concentration of ternary complex.

Keywords : Stopped flow kinetics, stability constant, ternary complex, Mn\textsuperscript{II} catalysed, periodate oxidation, 3,5-dimethylaniline.

---

**Cyclic voltammetric reduction of amino acid ketimine and its Co(II) complex**

Preeti Choudhary, Anurag Sharma, A. K. Varshney and S. Varshney*

Department of Chemistry, University of Rajasthan, Jaipur-302 004, Rajasthan, India

_E-mail_ : saritavarshney@rediffmail.com

*Manuscript received 28 February 2017, accepted 22 March 2017*

Abstract : The electrochemical behavior of amino acid ketimine synthesized by the condensation of 4-methyl-acetophenone and glycine (1 : 1 molar ratio) was further treated with cobalt(II) acetate (2 : 1 molar ratio) to form Co\textsuperscript{II}-ketimine complex has been studied in two different medium (DMF and CH\textsubscript{3}OH) on glassy carbon electrode (GCE) using cyclic voltammetric technique. The kinetic parameters like cathodic peak potential \(E_{pc}\), cathodic peak current \(I_{pc}\), charge-transfer coefficient \(\alpha_n\), diffusion coefficient \(D_0^{1/2}\) and rate constant \(K_{t,h}^{0}\) have been calculated. The electrode process was shown to be diffusion controlled and irreversible. The effect of sweep rate, pH, concentration and change in buffer was evaluated.

Keywords : Amino acids, ketimine, cyclic voltammetry, charge transfer coefficient \((\alpha_n)\), diffusion coefficient \((D_0^{1/2})\), rate constant \((K_{t,h}^{0})\).

---

**Photocatalytic removal of antacid histamine H2-receptor antagonist Ranitidine**

Rajeev Jain*, Swati Goyal and Satyendra Kadam

Department of Chemistry, Jiwaji University, Gwalior-474 011, Madhya Pradesh, India

_E-mail_ : rajeevjain54@yahoo.co.in

*Manuscript received online 13 February 2017, accepted 20 February 2017*
Abstract: In the present study photocatalytic degradation of an antacid histamine H2-receptor antagonist Ranitidine with TiO₂ as photocatalyst under UV irradiation in aqueous solution has been investigated. The efficiency of degradation was optimized by several parameters such as effect of initial concentration, catalyst loading, pH, temperature, irradiation time and addition of H₂O₂ as a co-oxidant. On optimization of various parameters it was found that almost complete degradation of Ranitidine by TiO₂ could be achieved within 70 min for an initial concentration of 0.20 mg/mL of the drug and at a catalyst loading of 0.06 g/L. Study on the effect of electron acceptors reveals that both decolourisation and degradation increase in the presence of the electron acceptor. The maximum degradation efficiency of Ranitidine was achieved with the combination of UV + H₂O₂ + TiO₂ and the optimum concentration of the H₂O₂ is 0.003 mM. The decolourisation and degradation kinetics was found to follow first-order kinetics according to the Langmuir-Hinshelwood (L-H) model. The activated energy for the photocatalytic degradation of Ranitidine is 21.28 kJ/mol. Over all photocatalytic degradation of Ranitidine by TiO₂ is an effective, economic and faster mode of removing Ranitidine from aqueous solution.

Keywords: Photocatalytic degradation, Ranitidine, kinetic study, TiO₂, UV, H₂O₂.

A greener approach for the one-pot synthesis of substituted thiazolidinones by using an efficient and recyclable ionic liquid

Upender S. Sisodiaᵃ, Sumit Srivastavaᵇ and Seema Kothariᵃ⁺ᵃ

ᵃDepartment of Chemistry, Pacific University, Udaipur-313 001, Rajasthan, India
ᵇDepartment of Chemistry, University of Rajasthan, Jaipur-302 004, Rajasthan, India

E-mail: seemavkothari@rediffmail.com

Abstract: A convenient protocol for the synthesis of 2,3-diarylthiazolidin-4-one have been achieved by one-pot condensation of aryl or heteroaryl amine, aryl aldehyde and 2-mercaptopropionic acid in 3-butyl-1-methyl-1H-imidazol-3-ium trifluoroacetate as ionic liquid [BMIM][TFA] is described. Reported ionic liquid easy to make, recycle and reuse up to three times in good to excellent yields. Synthesized compounds were fully characterized by their spectroscopic data.

Keywords: Heterocycles, thiazolidone, ionic liquid, green chemistry, one-pot synthesis.

Phytochemical studies of marine green algae Boodlea composita from Ukha, west coast of India

P. J. Praveenᵃ⁺ᵇ, Keisham S. Singhᵃ⁺ᵃ, B. G. Naikᶜ and P. S. Parameswaranᵇ

ᵃBioorganic Chemistry Laboratory, ⁣ᵇAcademy of Scientific and Industrial Research,
Abstract: Phytochemical investigation of marine green algae *Boodlea compositae* collected from the Ukha, west coast of India led to the isolation and identification of 22 constituents: β-sitosterol, loliolide and 13^2^-hydroxy-(13^2^-S)-phaeophytin-a being isolated by column chromatography whereas six fatty acids and 13 additional sterols were identified by GC-MS analysis. Characterization of β-sitosterol, loliolide and 13^2^-hydroxy-(13^2^-S)-phaeophytin-a was achieved by NMR spectroscopic data and comparison with those reported in literatures.

**Keywords:** β-Sitosterol, loliolide, pheophytin-a, green algae, GC-mass, spectroscopic data.

---

**Carbon electrodes for bio-electricity generation in microbial fuel cells**

Praveena Mishra, Shraddha Sharma and Rajeev Jain*

School of Studies in Chemistry, Jiwaji University, Gwalior-474 011, Madhya Pradesh, India

*E-mail*: rajeevjain54@yahoo.co.in, praveena.mica2011@gmail.com

*Manuscript received online 10 March 2017, accepted 11 March 2017*

Abstract: Experiments carried out to find out optimum experimental conditions and electrode materials have been compiled with conventional carbon materials i.e. CC, GrR, CP and WC by taking in a microbial fuel cell setup as anode to select the best electrodes material among these. Dual chamber MFC filled with sewage wastewater as substrate was used for the comparative study of current and power production using different anode materials. The electrochemical properties of the electrodes have been investigated by cyclic voltammetry. During power production, stability of anodes along with COD, BOD removal efficiencies were also calculated. The SEM images taken after 45 days of the experiment confirm biocompatibility of anodes. The comparative study suggest better results with CC anode as compared to other anode materials.

**Keywords:** Microbial fuel cells, mixed sewage culture, carbon electrode, chemical oxygen demand (COD).

---

**Composition and antibacterial activities of volatile oil of *Millingtonia hortensis* flowers from Sultanate of Oman**

Jamal Nasser Al Sabahi^a^, Nallusamy Sivakumar^b^ and Ethirajan Sukumar^c^*

^a^Central Instrumentation Laboratory, College of Agricultural and Marine Sciences, Sultan Qaboos University, P.O. Box 34, P.C. 123, Muscat, Sultanate of Oman
**Abstract:** *Millingtonia hortensis* commonly known as Tree Jasmine or Indian Cork Tree, is indigenous to Burma and the Malay Archipelago and cultivated as an ornamental plant in some countries. The flowers, root and bark are used medicinally. In this study, the volatile oil (VO) obtained by the hydro-distillation of the flowers of the plant grown in Sultanate of Oman, has been analyzed by GC-MS. A total of 32 compounds have been identified that formed major part (97.7%) of the volatile oil. The main components of VO were L-linalool (29.16%), α-farnesene (11.80%), nerolidol (11.34%), pentacosane (9.69%), 1-octen-3-ol (7.62%), (e)-isoeugenol (4.87%), α-terpineol (3.82%), linalool oxide (3.68%), heptacosane (3.03%) and tricosane (2.63%). The volatile oil has been tested for its antimicrobial activity against eleven bacteria wherein it exhibited significant inhibition against seven, moderate against two and no response against two strains. The minimum inhibitory concentration (MIC) has also been determined for the volatile oil.

**Keywords:** *Millingtonia hortensis* flowers, volatile oil, composition, antibacterial activity.

---

**J. Indian Chem. Soc.,**
**Vol. 94, June 2017, pp. 653-656**

**Accidental fire due to spray of pesticide in a household**

Gargi Bhattacharjee\textsuperscript{a}, Susmita Neogi\textsuperscript{b} and Sudip Kumar Das\textsuperscript{a}

\textsuperscript{a}Chemical Engineering Department, \textsuperscript{b}Department of Home Science,
University of Calcutta, 92, Acharya Prafulla Chandra Road, Kolkata-700 009, India

\textit{E-mail}: drsudipkdas@vsnl.net

\textit{Manuscript received} 22 February 2017, \textit{accepted} 15 March 2017

**Abstract:** On 13th May 2011 in Pune, India an aerosol insect repellents can exploded in kitchen of a house. The lady processing foods in a gas stove in her kitchen and found some cockroaches near the sink and grabbed a can of insect repellent and sprayed it near the burning gas stove. The flammable aerosol compound propellant came in contact with the flame of the burning stove and it made the explosion. This paper deals the probable causes of the case study and finally some useful general recommendations are discussed.

**Keywords:** Aerosol, pesticides, flammable, LPG, propellant.