Invited Lectures
Among asymmetric synthesis, the catalytic version of this process has received a great attention in the last few years due to the possibility of preparing chiral molecules from prochiral starting materials by using a chiral catalyst [1]. In general the catalyst belongs to one of the following series: (a) metal-containing catalyst, (b) organocatalyst, and (a) biocatalyst (enzymes or microorganisms). Considering the first group, usually the active species consists in a metal component and a chiral ligand, which gives the anisotropic information necessary in order to get the corresponding induction. Concerning different methodologies involving carbon-carbon bond formation [2], one of the most studied has been the enantioselective addition of an organometallic reagent to a prochiral carbonyl compound [3]. However, this process is especially difficult when ketones are used as the electrophilic component [4], this reaction being of great interest because it could be a way to generate chiral compounds bearing quaternary stereocenters [5]. In this presentation, the last findings in the enantioselective addition of dialkylzinc reagents to proquiral ketones using not only first generation (1), but also second (2) an third generation (3) ligands will be shown (Chart 1) [6]. Especially in the case of the last ligands 3, they are interesting from a practical point of view due the possibility of recovering and reusing them many times.
The fight against AIDS: new avenues for inhibiting Reverse Transcriptase (RT), an old target

Maurizio Botta

Dipartimento Farmaco Chimico Tecnologico, Università degli Studi di Siena, Via Alcide de Gasperi 2, I-53100, Siena, Italy, botta@unisi.it

The Acquired Immunodeficiency Syndrome (AIDS) related to HIV-1 infection is one of the most serious threats to human health and it has been estimated that more than 25 million people were killed since it was first recognized. In the fight against AIDS, first and second generation non-nucleoside reverse transcriptase inhibitors (NNRTIs) are now established as part of highly active antiretroviral therapy (HAART) for treating HIV infection. However, the efficacy of currently available NNRTIs, e.g. nevirapine (NVP, Viramune®), delavirdine (DLV, Rescriptor®) and efavirenz (EFV, Sustiva®, Stocrin®), is impaired by rapid emergence of drug resistance. On the other hand, as patients live longer on HAART therapy and the pool of NNRTI-resistant viruses increases, so does the need for the development of new NNRTIs with antiviral activity against clinically relevant mutant strains. Our research group has been recently involved in a multi-target approach to defeat the HIV-virus, focusing on the inhibition of HIV-1 Reverse Transcriptase according to both classical and non-classical approaches.

Here it will be reported an efficient methodology for the parallel solution-phase synthesis of a series of thiouracils, in turn selectively $S$-benzylated under microwave irradiation to give new $S$-DABOs. $S$-DABO derivatives, endowed with subnanomolar anti-HIV-1 activity, were subjected to docking and molecular dynamic studies, with the aim to rationalize their activity both within the wt:RT and K103N:RT non-nucleoside binding pocket (NNBP).

A combinatorial approach, lead instead to the identification of a new class of compounds (namely 6-vinylpyrimidines) endowed with an unprecedent mechanism of action: these compounds resulted in fact to be the first non-nucleoside RT inhibitors (NNRTIs) competing with the nucleotide substrate. An enzymological and computational study has been conducted to elucidate their unique mechanism of action.

Acknowledgment: Fabrizio Manetti, Lucilla Angelì, Luca Bellucci, Marco Radi, Maddalena Alongi, Claudia Mognaini, Federico Corelli, Silvio Massa, Giovanni Maga, José A. Esté.
DISCOVERING NEW ASYMMETRIC CATALYSES: ENANTIOSELECTIVE SYNTHESIS OF CHIRAL TERTIARY ALCOHOLS

Miguel Yus

Instituto de Síntesis Orgánica and Departamento de Química Orgánica, Facultad de Ciencias, Universidad de Alicante, Apdo. 99, 03080 Alicante, Spain
yus@ua.es

Among asymmetric synthesis, the catalytic version of this process has received a great attention in the last few years due to the possibility of preparing chiral molecules from prochiral starting materials by using a chiral catalyst [1]. In general the catalyst belongs to one of the following series: (a) metal-containing catalyst, (b) organocatalyst, and (a) biocatalyst (enzymes or microorganisms). Considering the first group, usually the active species consists in a metal component and a chiral ligand, which gives the anisotropic information necessary in order to get the corresponding induction. Concerning different methodologies involving carbon-carbon bond formation [2], one of the most studied has been the enantioselective addition of an organometallic reagent to a prochiral carbonyl compound [3]. However, this process is especially difficult when ketones are used as the electrophilic component [4], this reaction being of great interest because it could be a way to generate chiral compounds bearing quaternary stereocenters [5]. In this presentation, the last findings in the enantioselective addition of dialkylzinc reagents to proquiral ketones using not only first generation (1), but also second (2) an third generation (3) ligands will be shown (Chart 1) [6]. Especially in the case of the last ligands 3, they are interesting from a practical point of view due the possibility of recovering and reusing them many times.

References
ASYMMETRIC 1,3-DIPOLAR CYCLOADDITION REACTIONS OF
AZOMETHINE YLIDES AND ALKENES: SYNTHESIS OF PROLINE
DERIVATIVES

Carmen Nájera, M. Gracia Retamosa, José M. Sansano

Departamento de Química Organica, Facultad de Ciencias, and Instituto de Síntesis
Organica, Universidad de Alicante, 03080 Alicante, Spain, cnajera@ua.es

The asymmetric 1,3-dipolar cycloaddition of azomethine ylides and alkenes provides a
direct access to the synthesis of enantioenriched highly substituted pyrrolidine or proline
derivatives in a high diastereo- and enantioselective form [1]. The most direct way for the
preparation of the corresponding dipoles is to generate in situ a metallo-azomethine ylide
from α-imino esters derived from amino acids. There are three main strategies for the
asymmetric 1,3-dipolar cycloaddition of azomethine ylides: a) by attaching a chiral auxiliary
to the imino group or to the ester in the dipole, b) by attaching the chiral auxiliary group to
the dipolarophile, and c) by using a chiral catalyst. We will present our work in this field
using the last two strategies.

\[
\begin{align*}
R^1 & \overset{R^2}{\underset{\text{EWG}}{\overset{\text{Ag(I) salt}}{\underset{\text{base}}{\overset{H}{\underset{\text{CO}_2R^3}{\overset{\text{R}^4}{\underset{\text{EWG}}{\overset{\text{R}^2}{\underset{\text{R}^1}{\text{N}}} \text{CO}_2R^3}}}}}}}}
\end{align*}
\]

We have found that the use of chiral acrylates 1 derived from methyl (R)- and (S)-
lactate as dipolarophiles with imino esters in the presence of AgOAc as catalyst and KOH as
base at room temperature afforded the corresponding cycloadducts with high regio-,
diastereo- and enantioselectivity [2]. This methodology has been applied to the synthesis of
substituted prolines, which are hepatitis C virus RNA polymerase inhibitors 2 [3]. For the
enantioselective version Ag(I) complexes with phosphorus ligand such as phosphines and
phosphoramidites have been used as chiral catalysts. The employment of binap-AgClO₄
complex has allowed to recover, just by simple filtration, and to reuse this catalyst during 5
runs [4]. Different phosphoramidites derived from binol have also been used as the first
monodentate chiral ligands in this type of enantioselective 1,3-dipolar cycloaddition of
azomethine ylides and alkenes.

\[
\begin{align*}
\text{(S)-1} & \quad \text{HO}_2\text{C} \quad \text{(R)-1} \\
\text{[(R)-binap]AgClO}_4 & \quad \text{[(R)-binap]AgClO}_4
\end{align*}
\]

Acknowledgments: This research has been supported by the DGES of the Spanish Ministerio de Educación y
Ciencia (Consolider INGENIO 2010 CSD2007-00006, CTQ2007-62771/BQU, and CTQ2004-00808/BQU), the
Generalitat Valenciana (GV05/144), and the University of Alicante.

References
From Environmental Awareness to Sustainable Development:

Views of a Chemist

Jalal Hawari, Diane Fournier, Annamaria Halasz, Fanny Monteil-Rivera, Abdessalem Yezza, Jian-Shen Zhao

Biotechnology Research Institute, Montreal, Canada

Until recently petroleum was considered the principal source of most chemical industrial products, including polymers and plastics. Nearly $24 billion (US) worth of hydrocarbon feedstocks are used annually by the chemical industry. Environmental damage caused by excessive use of fossil fuels combined with limited future availability, have encouraged various industries and government agencies to search for renewable feedstocks as alternative sources for chemicals and energy. Such renewable feedstocks should be available locally in large supply, high biomass yield at low cost, and above all with no impact on the food supply chain or the environment. The present study will therefore be structured to address two of our main research activities; 1) remediation of contaminated sites and 2) development of green processes in the manufacture of biomaterials and fine chemicals from agricultural feedstocks (biorefinery). In the case of environmental remediation I will present several case studies, including monitoring and remediation of contaminated sites in the Arctic and in coastal waterways in harbors adjacent to the Pacific and Atlantic Oceans. As for the use of agricultural feedstock residues, e.g. lignocellulosic materials as a clean source of fine chemicals, I will present two research examples: In the first case, I will describe the use of a microwave based-technology to successfully extract phenolics compounds such as ferulic acid from triticale / wheat straw. Ferulic acid is one of the two top aromatic acids identified by the US DOE as a versatile commodity chemical. In the second example, I will describe the use of maple sap, a landmark forestry product in Canada that is rich in sucrose (10-20 g/L) as an ideal medium for biomanufacturing of fine chemicals. When the bacterium Alcaligenes latus was allowed to grow on maple sap we obtained poly-3-hydroxybutyrate (PHB). PHB is a biodegradable polymer with thermoplastic and elastomeric properties that competes well with plastics derived from polyethylene. When valeric acid was added to the sap a copolymer composed of valerate and butyrate was produced. Finally, we used maple sap, for the production of lactic acid, a versatile chemical with potential industrial applications, e.g. synthesis of polylactate-based bioplastic.
Fifty Years (or More) Playing at Opening and Closing Heterocycles: From the Cusmano-Ruccia Reaction to the Discovery of Calcium Channel Modulators by a Multidisciplinar Approach

Domenico Spinelli

Department of Organic Chemistry “A. Mangini”, University of Bologna, Via San Giacomo 11, Bologna 40126, Italia
e-mail: domenico.spinelli@unibo.it

In the lecture, starting from the Cusmano-Ruccia reaction (1), a ring-opening/ring-closing sequence whereby 4(5)nitr oso-5(4)-phenylimidazoles afford 3-benzoyl-1,2,4-oxadiazoles by the treatment with hydrochloric acid, a series of new reactions involving nitrosoimidazoles condensed with five- and six-membered rings (2,3) will be described. Thus 6-aryl-5-nitrosoimidazo[2,1-b][1,3]thiazoles, by treatment with hydrochloric acid provided 8-aryl-8-hydroxy-8H-[1,4]thiazino[3,4-c][1,2,4]oxadiazol-3-ones, a new class of compounds showing a very interesting biological profile. As a matter of fact, while only moderately inhibiting the cell growth of some tumor-derived cell lines (colon cancer, melanoma and breast cancer) (2c), such heterocycles showed a significant activity as L-type Ca\(^{2+}\) channels blockers (LTCCBs), some times being more potent (2-10 times) than diltiazem (4a).

The characterization of the pharmacological profile has been extended to a large series of acetals with different structures at C-8 evaluating the role of acetal chain (4b). From selective biological assays on the most active derivatives, 5b elicited a potent negative inotropic potency in myocardium due to its calcium antagonism (EC\(_{50}\) 0.04 M, about 20 times more potent than diltiazem, EC\(_{50}\) 0.79 M), having been excluded both the muscarinic and the adenosin mechanism.

A 3D QSAR model was obtained and validated with homologous literature data, and a virtual receptor scheme was derived for the unknown binding site. The following pharmacophoric features favourably affect the potency: one positively charged centre, three lipophilic groups, and two hydrogen-bonding acceptor groups.

Starting from the above 3D QSAR model and after the determination of the absolute configuration of 5b, the stereospecificity of the ligand-channel interaction has been assigned (4c). Thereafter, a virtual screening procedure was performed with the aim of identifying novel chemotypes for LTCCBs, starting from a database of purchasable compounds. Thus,
340,000 molecules were screened in silico in order to prioritize structures of interest for bioscreening. As a result, 20 compounds were tested by means of functional and binding assays which revealed several hits with promising behaviour as LTCCBs.

Finally, by further examining the chemical reactivity of 8-aryl-8-hydroxy-8H-[1,4]thiazino[3,4c][1,2,4]oxadiazol-3-ones new interesting molecules with higher and higher activity as LTCCBs have been identified.

References
Recent Progress in the Synthesis of Heterocycles from 1,2-Diaza-1,3-butadienes

Orazio A. Attanasi

Istituto di Chimica Organica, Università di Urbino “Carlo Bo”, Via Sasso 75, 61029 Urbino, Italy (e-mail: attanasi@uniurb.it)

Pyrroles, pyrazoles, imidazoles, thiazoles, selenazoles, 1,2,3-thiadiazoles, 1,2,3-selenodiazoles, 1,2,3-diazaphospholes, pyridazines, pyrazines, 1,2,4-triazines, and mixed heterocyclic systems have been obtained from 1,2-diaza-1,3-butadienes.

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EFFICIENT APPROACHES TO FUSED PYRIMIDINES

Stanislaw Ostrowski\textsuperscript{a,b}

\textsuperscript{a) Institute of Chemistry, University of Podlasie, ul. 3 Maja 54, 08-110 Siedlce, Poland
\textsuperscript{b) Institute of Organic Chemistry, Polish Academy of Sciences, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland

\textit{e-mail: stan@ap.siedlce.pl}}

The pyrimidine nucleus is embedded in a large number of alkaloids, drugs, antibiotics, agrochemicals, and antimicrobial agents.\textsuperscript{1} Thus, many fused pyrimidine derivatives are of significant importance due to potential application of these compounds in chemistry, biology, medicine, etc.. Their synthesis is well recognized in the literature and it was thoroughly reviewed in many articles and monographs.\textsuperscript{2} Often the limiting factor for the above approaches is the difficulty encountered in obtaining the key intermediates or their precursors.

Recently, this problem was successfully solved in several ways by the use of vicarious nucleophilic substitution of hydrogen (VNS).\textsuperscript{3} As a result, many quinazolines and new bicyclic and tricyclic heteroaromatic compounds and their mono-\textit{N}-oxides were obtained, when starting from aromatic nitro compounds.\textsuperscript{3}

These approaches were also successfully applied to the synthesis of purines with the use of 4-nitroimidazole derivatives.\textsuperscript{5}

References:

EFFICIENT SYNTHESIS OF FUNCTIONALIZED THIAZOLES

Issa Yavari

Chemistry Department, Tarbiat Modares University, P.O. Box 14115-175, Tehran, Iran
e-mail: yavarisa@modares.ac.ir

Thiazoles occupy a prominent position among heterocycles. In nature, the thiazolium ring is the chemically active center in the coenzyme derived from vitamin B$_1$ (thiamin). A large number of thiazoles obtained from microbial and marine origins exhibit important biological effects such as antitumor, antifungal, antibiotic, and antiviral activities [1]. Synthetic thiazoles have also been shown to exhibit a wide variety of biological activity, while others have found application as liquid crystals and cosmetic sunscreens. The classical method for the synthesis of thiazoles is the Hantzsch process, in which an -haloketone is condensed with a thioamide. This method gives excellent yields for simple thiazoles. This method gives excellent yields for simple thiazoles; however, for some substituted examples low yields have been reported as a result of dehalogenation of the -haloketone during the reaction.

As part of our current studies on the development of new routes in heterocyclic synthesis [2], we report an efficient synthetic route to functionalized thiazoles. The reaction of ammonium thiocyanate 1, acid chlorides 2 and ethyl bromopyruvate 3 in the presence of tetramethyl thiourea 4 produced ethyl 5-[(methylamino)carbothioyl]-2-(dimethylamino)-1,3-thiazole-4-carboxylates 5 (7 examples) in 76-90% yields (Scheme).

\[
\begin{align*}
\text{NH}_4\text{SCN} + \text{RCl} + \text{CO}_2\text{Et} \xrightarrow{\text{acetone, r.t.}} \text{Me} \quad \text{Me} \\
\text{NH}_4\text{SCN} + \text{RBr} + \text{CO}_2\text{Et} \xrightarrow{\text{acetone, r.t.}} \text{Me} \quad \text{Me} \\
\text{NH}_4\text{SCN} + \text{RCl} + \text{CO}_2\text{Et} \xrightarrow{\text{acetone, r.t.}} \text{Me} \quad \text{Me} \\
\text{NH}_4\text{SCN} + \text{RBr} + \text{CO}_2\text{Et} \xrightarrow{\text{acetone, r.t.}} \text{Me} \quad \text{Me} \\
\text{NH}_4\text{SCN} + \text{RCl} + \text{CO}_2\text{Et} \xrightarrow{\text{acetone, r.t.}} \text{Me} \quad \text{Me} \\
\text{NH}_4\text{SCN} + \text{RBr} + \text{CO}_2\text{Et} \xrightarrow{\text{acetone, r.t.}} \text{Me} \quad \text{Me} \\
\end{align*}
\]

The structures of compounds 5 were apparent from their mass spectra, which displayed in each case, the molecular ion peak at the appropriate m/z values. The $^1$H and $^{13}$C NMR spectroscopic data, as well as IR spectra, are in agreement with the proposed structures.

References

Oral Lectures
Synthesis and Properties of Novel Hydroxylamino-Substituted 1,2,4–Oxadiazoles and 1,2,4–Triazole

Detlef Geffken and Nabih Lolak

Institut of Pharmacy, Division of Pharmaceutical Chemistry, University of Hamburg, Bundesstrasse 45, 20146 Hamburg (Germany)

Aminosubstituted 1,2,4-triazoles and 1,2,4-oxadiazoles play an important role as pharmacophores/toxophores in drug chemistry and agricultural chemistry [1-4]. As part of our research directed to novel bioactive heterocyclic compounds, we became interested in the title compounds and report here on a straightforward synthetic route to the desired heterocycles 3, 4 and 5, starting from easily available $N^1$-aralkoxy-(alkoxy)-$N^3$-cyano-$O$-phenylisoureas (2).

![Chemical structures](image)

References

Synthesis and Reactions of Heterocyclic Compounds Containing Thienopyridines

Adel Mohamed Kamal El-Dean

Chemistry Department, Faculty of Science, Assiut University, Assiut 71516, Egypt
e-mail: a.eldean@acc.aun.edu.eg

In continuation of our work [1,2] of thienopyridines, herein we report synthesis of some new heterocyclic compounds containing thienopyridines.

3-Amino-4,6-dimethyl-thieno[2,3-b]pyridine-2-carbaldehyde (1) was synthesized and reacted with different reagents namely, ethyl acetoacetate, malononitrile, ethyl cyanoacetate, diethyl malonate, and cyclohexanone to afford compounds 2a-f. Hydrazinolysis of compound 2a using hydrazine hydrate affords the corresponding carbohydrazide 3, which is converted into carboazide 4 using nitrous acid. Upon heating carboazide 4 in inert solvent, it underwent Curtius rearrangement followed by cyclization to give pyrrolopyridothienopyridine 5. Also carboazide was reacted with alcohols to give the corresponding carbamate 6. When carbohydrazide 3 was allowed to react with carbon disulfide in pyridine, it afforded oxadiazolyl derivative 7, while its reaction with phenyl isothiocyanate followed by treatment with sodium hydroxide gave triazolyl derivative 8.

![Chemical structures](image)

References

Muhammad Ashram
Chemistry Dept., Mutah University, Mutah Al Karak, Jordan.

The first synthesis of the C3-symmetrical p-tert-butylhexahomotrithiacalix[3]arene 7d via one-pot procedure by the reaction of 2,6-bis(chloromethyl)-p-tert-butylphenol 8d with sodium sulfide nanohydrate under high-dilution conditions is reported. Also, hexahomotrithiacalix[3]arenes 7d-f (where d-f designate the type of the substituents R at the p-positions of the phenolic rings: d, R = t-Bu; e, R = CH3; f, R = Cl) were synthesized via a convergent approach in good yield by the [2+1] cyclization reaction of 2,6-bis(chloromethyl)phenol monomers 8d-f and bis(chloromethyl)phenol dimers 15d-f in presence of sodium sulfide nanohydrate under high-dilution conditions. The structures of 7d-f were determined by $^1$H, $^{13}$C-NMR, MS and elemental analysis. A preliminary study of the binding properties of 7d with alkali and heavy metal cations using biphasic picrate extraction method showed only weak abilities to bind the cations examined.
Synthesis of Some New Schiff Base Crown Ethers from 2-Hydroxynaphthaldehyde

Shehadeh Mizyed and Rana Kiwan
Chemistry Department, Yarmouk University, Irbid, Jordan

This study has been carried out on the synthesis of some Schiff base crown ethers. Crown ethers 1, 2, 3a, b and 4a, b are synthesized in a good yield by the reaction of o-2-bromoethoxynaphthaldehyde with different diamines such as 4,5-dimethyl-o-phenylenediamine, 1,2-phenylenediamine, 4-methyl phenylenediamine and 4-chlorophenylenediamine in the presence of potassium carbonate in acetonitrile under inert atmosphere and reflux conditions. The products were characterized by $^1$H-NMR, $^{13}$C-NMR, IR, and mass spectrometry. The synthetic routes of these compounds will be presented.
Effect of UV-Vis Light On Stabilility of Plasticized Substituted Polystyrene in Solid Films

Khalid E. Al-Ani and M. Hawi
Chemistry Department, Faculty of Science, Hashemite University, P O Box 150459, Zarka, JORDAN
Email: khalid7@hu.edu.jo

The effect of added plasticizer, of dibutyl phthalate, dioctyl phthalate, dimethyl terephthalate, diethyl terephthalate, and dioctyl terephthalate plasticizers on poly (para-methoxystyrene), poly (para-methylstyrene), poly (para-α-methylstyrene), poly (para-tert-butylstyrene) photodegradation and photo oxidative degradation was investigated by UV-vis, fluorescence and LC-MS spectroscopy. The samples were exposed to 265 nm radiation and the fluorescence spectra were recorded before and after plasticization. It was found that plasticization of para-substituted polystyrene solid films caused a quenching to the polymer fluorescence intensity, and the formation of exciplex emission at higher wavelength. The decrease in the excimer fluorescence upon the increase in the time of exposure to UV-radiation provides an evidence for the photodegradation of polymeric chains through chain scission processes. Besides, phthalate plasticizers revealed a higher efficiency of fluorescence quenching than terephthalate, indicating that terephthalate plasticizers showed a higher stability towards photo irradiation than that for phthalate plasticizers. The photodegradation of the polymer increased with the increase in the bulkiness of the plasticizer molecule.
Kinetic and Mechanistic Studies on W and Mo Oxides Catalyzing Oxidations with Peroxides

Ahmad M. Al-Ajlouni

Department of Applied Chemical Sciences, Jordan University of Science and Technology, Irbid 22110, Jordan, E-mail: aajlouni@just.edu.jo

Kinetic studies on the catalytic activity of phenylphosphopolyperoxotungstate complexes \([C_{21}H_{37}N_2][(PhPO_3){WO(O_2)_2}{WO(O_2)_2H_2O}]\) (A) and \([C_{21}H_{37}N_2][(\rho-NO_2Ph(O)PO_3){WO(O_2)_2}{WO(O_2)_2H_2O}]\) (B) and organometallic Mo oxides in the epoxidation of olefins and in the oxidation of organic sulfides with hydrogen peroxide and t-butylhydroperoxide as oxidizing agents were carried out under homogeneous and biphasic conditions. The activity of the catalyst increases with its acidity. On the other hand, the rate of the reaction increases with the substrate nucleophilicity. The oxidation rate constants are correlated with \(\sigma\) (or \(\sigma^+\)) according to the Hammett equation and produce positive reaction constants (\(\rho \sim -1.0\)). The electronic effect and the reaction stereoselectivity suggest a mechanism, which involves an external nucleophilic attack of the nucleophilic substrate onto the electropositive oxygen of the M-peroxo group. Catalytic cycles involving formation of the active M-peroxo species followed by the oxygen-transfer step (rate-determining) are proposed.

References
The Effect of Sequence Distribution and Nature of Monomers on the Electrical Conductivity of Some Unsaturated Amide-Ester Copolymers

Asaad F.Khattab, Sa’ad F. Mahmood and Yousif A. Shahab
Department of Chemistry, College of Science, University of Mosul, Mosul, Iraq

Amide copolymer was prepared via the condensation of terephthaloyl dichloride, isophthaloyl dichloride, maleic anhydride and maleoyl dichloride as diacids with different diols. The synthesis with different sequence distribution was achieved in order to attain three types of copolymers; random, block and alternate. The prepared copolymers have the structure below:


The electrical conductivity of the copolymers are determined in the pure and doped states. The results show that two factors are important in determining the conductivity levels\(^{1,2}\); the flexibility of the copolymer chains\(^{3}\) and the efficiency of conjugation along the chains. The latter factor originates from the decrease in the electronic energy gap between HOMO and LUMO\(^{4}\). Thus, the acidic units that give rise to coiled chains structure (isophthalic) and hence flexible segments yield high conductivity compared with acid units that give rise to extended structure and rigid segments like terephthalic acid. The introduction of saturated units that interrupts the chains conjugation decreases the electrical conductivity of the polymers. Also the results showed that the conductivity decreased as going from the alternate to the random to the block copolymers with the same monomer constitution.

References
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Using electron beam evaporation, Pd thin films of 300 nm (12 µin.) thickness have been deposited on 301-stainless steel for high temperature electrical contact studies. The structure and composition of the films were studied in detail using x-ray diffraction (XRD), scanning electron microscopy (SEM), electron probe microanalysis (EPMA), and x-ray photoelectron spectroscopy (XPS) with sputter depth profiling. The contact properties, such as contact resistance, fretting wear resistance, and thermal stability have been measured. The contact resistance remains low after heat-aging in air for 168 h at 150 and 200°C, but increases significantly after heat-aging at 340°C. This increase in contact resistance is caused by the formation of about a 27 µm (1 in.) thick PdO. In contrast, the thickness of the PdO is too thin to cause measurable contact resistance increases after heat-aging at 150 and 200°C. The fretting wear resistance of Pd coated 301 stainless steel is better than that of electroplated Sn of several thousand nm thickness. Thus, vapor deposited Pd coatings on 301 stainless steel may replace electroplated Sn for electrical contact applications at elevated temperatures.
Towards The Total Synthesis of a Cardiotoxin-Batrachotoxin

Abdul Rauf Raza*\textsuperscript{a} & Philip J. Parsons\textsuperscript{b}

\textsuperscript{a} Department of Chemistry, University of Sargodha, Sargodha-40100, Pakistan  
roofichemist@hotmail.com, Fax: +92 48 3222 121  
\textsuperscript{b} Department of Chemistry, School of Life Sciences, University of Sussex  
Falmer, Brighton, BN1 9QJ, England

Batrachotoxin 1 ranks amongst the most toxic substances known to man. It contains some unique features that other toxins lack. These include the ketal-linkage between C-3 and C-9 of steroidal nucleus and oxazepine ring at the CD ring junction.

The Pd-mediated coupling of chloro-intermediate 2 under the conditions reported by Hartwig \textit{et al}, failed to couple with cyclopent-2-enone. In contrast, the Pd-mediated coupling of 3 with cyclopent-2-enone, in the presence of a catalytic amount of (Ph\textsubscript{3}P)\textsubscript{4}Pd \textit{in situ} without any solvent, afforded 4 and 5 in 5:1 ratio. All other conditions examined for coupling reactions were unsuccessful for the desired transformation (Scheme 1).

The radical based transformation of 3 and its bromo-derivative with \textsuperscript{4}Bu\textsubscript{3}SnH, using AIBN as radical initiator under thermolysis or photolysis conditions, were unsuccessful. However, some interesting products were produced by radical-mediated cascade cyclization under different conditions. Such findings will also be presented.
Synthesis and Characterization of Some Pyrazolo[3,4-\textit{b}]pyrazinones

Feda' S. Al-Masri, Kayed A. Abu-Safieh and Mikdad T. Ayoub

Chemistry Department, Faculty of Science, Hashemite University, Zarqa-Jordan

A new series of 1,3-dimethyl-6-substituted-1,4-dihydro-5\textit{H}-pyrazolo[3,4-\textit{b}]pyrazin-5-ones (101a-f) have been synthesized. The strategy of this synthesis involves the preparation of different \textit{N}-(1,3-dimethyl-4-nitro-1\textit{H}-pyrazol-5-yl)-\textit{\alpha}-amino acids (100a-f) from the commercially available 5-chloro-1,3-dimethyl-4-nitro-1\textit{H}-pyrazole (38) and different \textit{\alpha}-amino acids, followed by intramolecular reductive cyclization using (H\textsubscript{2}-5\% Pd/C) to obtain the target pyrazinones (101a-f), which were characterized using IR; MS; elemental analysis and NMR spectral data.

\[
\begin{align*}
\text{Compd. No.} & \quad a \quad b \quad c \quad d \quad e \\
100, 101 & \quad \text{H} \quad \text{CH}_3 \quad \text{CH}(\text{CH}_3)_2 \quad \text{CH}_2\text{CH}(\text{CH}_3)_2 \quad \text{CH}_2\text{C}_6\text{H}_5
\end{align*}
\]
Carboxylate Ligand Executes Fluxional Behavior in Dimeric Tetraorganodicarboxylato Stannoxanes

Muhammad Danish\textsuperscript{a} and Saqib Ali\textsuperscript{b}

\textsuperscript{a} Department of Chemistry, University of Sargodha, 40100-Sargodha, Pakistan
\textsuperscript{b} Department of Chemistry, Quaid-e-Azam University, 45320-Islamabad, Pakistan

Dimeric tetraorganodicarboxylatostannoxanes comprise one of the most interesting class of organotin compounds as they show different sets of $^1$H and $^{13}$C-NMR signals for R-groups attached to Sn(IV) and only one set of signals for carboxylate ligand. A similar dichotomy is observed in $^{119}$Sn-NMR spectra\textsuperscript{1,2}. Two types of signals are only possible if there are two environments for the R-groups and Sn(IV) atoms. When two type of signals are observed for R-groups and tin atoms then, why only one for carboxylate ligand. It is suggested that one set of signals for carboxylate ligand is possible only if it executes fluxional behavior in the molecule. This process is too fast to be observed on NMR time scale even at -100\textdegree C. It is proposed that the ease of fluxional process depends upon the nature of R-groups as well as the carboxylate ligands. It is recommended that fluxional process can be stopped if there is another donor group in the ligand in close vicinity of the tin atom. The attachment of this donor group to tin centre may stop the fluxionating ability of the carboxylate ligand.

\textbf{References}
A Technique for Purifying Wastewater with Polymeric Flocculants Produced from Polystyrene Wastes

Moyad N. Khalaf, Raed K. Al-Tamimi and A. Taoubi

Chemistry Department, College of Science, University of Basra, Basra-Iraq
Email: moayad_khalaf@yahoo.com

One of the most important treatment processes in surface water treatment is coagulation. Surface waters such as rivers and lakes contain suspended particles and turbidity. With the aid of coagulants and by flocculation process followed by sedimentation and filtration, these impurities can be removed from raw waters. Besides, conventional chemicals such as alum and ferric chloride, polymers such as polystyrene sulfonate (SPS) are getting common. In this study, we are interested in waste plastics. Different wastes polystyrene such as cheese cup, expanded polystyrene, and body pen were converted into a polymeric flocculants by chemical modification. Specifically, waste polystyrene consisting of white coffee cups was sulfonated to produce a water-soluble polymer. The sulfonation was characterized by FTIR technique and the degree of sulfonation was determined by titration.

The polymer provides high purification of the supernatant after flocculating a kaolin suspension. Moreover, the material provides a pure supernatant in the treatment of actual wastewater comparable to conventional polymeric flocculants. A new reclamation technology to convert waste plastic into a functional polymer is reported.
Synthesis and Reactivity of Cyclopentadienyl Ruthenium Complexes Containing 5-Membered N-Heterocyclic Thiolates

Mohammad El-Khateeb\textsuperscript{a}, Sahar Mohammad\textsuperscript{a} and Deeb Taher\textsuperscript{b}

\textsuperscript{a} Chemistry Department, Jordan University of Science and Technology, Irbid 22110, Jordan.
\textsuperscript{b} Department of Chemistry, Tafila Technical University, Tafila, Jordan.

Mononuclear ruthenium-thiolate complexes of structural type CpRu(PPh\textsubscript{3})\textsubscript{2}SR (R= 2-mercaptoimidazolyl, 2-mercaptop-1-methylimidazolyl, 2-mercaptop-5-methyl-1,3,5-thiadiazolyl and 3-mercaptop-5-methyl-1,3,5-thiadiazolyl) were accessible by the reaction of CpRu(PPh\textsubscript{3})\textsubscript{2}Cl with LiSR. The one-pot reactions of CpRu(PPh\textsubscript{3})\textsubscript{2}Cl with LiSR and the bisphospine ligands (P-P) afforded CpRu(P-P)SR (P-P = Ph\textsubscript{2}P-CH\textsubscript{2}PPh\textsubscript{2}: dppm, Ph\textsubscript{2}P(\textit{CH}\textsubscript{2}\textsubscript{2})PPh\textsubscript{2}: dppe). If CO gas was bubbled through a THF solution of CpRu(PPh\textsubscript{3})\textsubscript{2}S(C\textsubscript{4}N\textsubscript{2}H\textsubscript{5}), the complex CpRu(PPh\textsubscript{3})(CO)S(C\textsubscript{4}N\textsubscript{2}H\textsubscript{5}) was produced. The new ruthenium-thiolate complexes have been characterized by elemental analysis and spectroscopic methods (IR, \textsuperscript{1}H, \textsuperscript{31}P\textsuperscript{1}\textsuperscript{H} NMR and MS). The solid state structures of CpRu(dppe)S(C\textsubscript{3}N\textsubscript{2}H\textsubscript{3}), CpRu(dppe)S(C\textsubscript{4}N\textsubscript{2}H\textsubscript{5}) and CpRu(PPh\textsubscript{3})(CO)S(C\textsubscript{4}N\textsubscript{2}H\textsubscript{5}) were determined by single crystal X-ray structure analysis.
Heterogeneous Composites of Pellicular Zirconium Phosphate Membranes of Different Crystallinity and Fibrous Cerium Phosphate Membrane

S.K. Shakshooki and S. R. El-Tarhuni

Department of Chemistry, Faculty of Science El-Fateh University, P.O.Box 13203, Tripoli, Libyan Arab Jamahirya
E-mail: shakshooki2002@yahoo.com

Inorganic solid–solid composite materials are well established [1]. However, to date, there are no reports about heterogeneous composites of pellicular zirconium phosphate–fibrous cerium phosphate membranes [2].

Flexible thin films, with different degree of crystallinity of pellicular zirconium phosphate membranes, \( \text{Zr(HP\text{O}_4)_2} \cdot 1.28\text{H}_2\text{O}, \text{Zr(HP\text{O}_4)_2} \cdot 0.75\text{H}_2\text{O}, \) and \( \text{Zr(HP\text{O}_4)_2} \cdot 1.0\text{H}_2\text{O}, \) were prepared by refluxing 26g wet gel zirconium phosphate in 90ml of 3, 5 and 6M \( \text{H}_3\text{PO}_4 \) solutions, respectively, for 50 hrs. The resulting pellicular membranes were designated as \( \text{ZrPM}_3, \text{ZrPM}_5 \) and \( \text{ZrPM}_6, \) respectively [3]. Their \( d_{001} \) values were found to be \( \sim 7.6 \text{Å}. \)

Fibrous cerium phosphate membrane, \( \text{Ce(HP\text{O}_4)_2} \cdot 2.78\text{H}_2\text{O}, \) was prepared from the reaction of 0.05M \( \text{CeSO}_4 \cdot 4\text{H}_2\text{O} \) in 0.5M \( \text{H}_2\text{SO}_4 \) with 6M \( \text{H}_3\text{PO}_4 \) at \( \sim 90^\circ\text{C} \) for 5 hrs [2]. The product was designated as \( \text{CePf}, \) its \( d_{001} \) found to be 10.863Å.

Heterogeneous composites of pellicular Zr- and fibrous Ce phosphate membranes \( ([\text{Zr(HP\text{O}_4)_2}]_{0.51}[\text{Ce(HP\text{O}_4)_2}]_{0.49} \cdot 1.87\text{H}_2\text{O}, \) \( [\text{Zr(HP\text{O}_4)_2}]_{0.54}[\text{Ce(HP\text{O}_4)_2}]_{0.46} \cdot 2.8\text{H}_2\text{O} \) and \( [\text{Zr(HP\text{O}_4)_2}]_{0.77}[\text{Ce(HP\text{O}_4)_2}]_{0.23} \cdot 3.45\text{H}_2\text{O} \) were obtained by mixing wt/wt% ratio of \( \text{ZrPM}_3, \) \( \text{ZrPM}_5 \) and \( \text{ZrPM}_6 \) with \( \text{CePf} \) membrane (50:50%, 55:45% and 75:25%, \( \text{ZrPM}_3-6: \text{CePf}, \) respectively) with stirring at room temperature for 48 hrs and at 45°C for 2 hrs.

All resulting composite membranes were characterized by chemical x-ray, thermal analysis and by IR spectra. X-ray diffractogram of composite materials consists of \( d \)-values at \( \sim 11.0 \text{Å} \) and \( \sim 7.6 \text{Å}, \) characteristic of the resulting composite materials of pellicular Zr-fibrous Ce phosphate membranes. These composite materials can be considered as new inorganic ion exchange materials and as new solid acid catalysts.

References
Phosphite Ozonides are unstable species prepared by the reaction of phosphite and ozone at -78 °C according to the scheme below. These compounds decompose by increasing the temperature to yield phosphoric ester and singlet oxygen. The kinetics of decomposition reaction of phosphite ozonides have been the object of many investigations. Gibbs energy of activation has been determined experimentally for different phosphite ozonides. Recently, attention is focused on ab initio calculations using DFT calculations at the Becke3PW91/6-31+G(d) level of theory. Single point calculations provided the activation energy for the decomposition of phosphite ozonides with different environment around phosphorus atom. The compounds considered in this work are: tri(tetrahydro-furan-2-yl)methyl phosphite ozonide 1 and a newly prepared bicyclic phosphite ozonide 2 obtained from the ozonation of 2,7,8-trioxa-1-phosphabicyclo[3,2,1]octane. The calculated values of activation energy were 59.4 and 117.1 kJ/mol for compound 1 and 2 respectively; these values are in good agreement with the experimental values of Gibbs energy of activation for the decomposition of compound 1 and 2 which are 57.3 and 90.5 kJ/mol, respectively.

References
Determination of Traces of Cd, Pb and Cu in Beverages by Differential Pulse Anodic Stripping Voltammetry and Atomic Absorption Spectrometry

Mahmoud A. Ghandour, Azza M. M. Ali and Mohammed Abdel Aal
Chemistry Department, Faculty of Science, Assiut University, 71516-Assiut, Egypt
ghanpour10@hotmail.com Email:

Differential pulse anodic stripping voltammetry DPASV at a hanging mercury drop electrode has been used for the determination of trace amounts of the toxic heavy metals cadmium, lead and the essential trace element copper in different beverages commonly consumed in Egypt, i.e. tea (black and green), coffee, cinnamon, anise, fenugreek, hibiscus(karkade) and cocoa. The infusions of the samples have been prepared by boiling in bidistilled water. The optimal conditions for the detection of traces of the metal ions in beverages i.e. deposition potential, supporting electrolyte composition, effect of pH and deposition time have been studied. The concentration of each metal ion in the samples is determined by using standard addition method. The performance of the DPASV technique was compared with the atomic absorption spectrometry. The precision of the method is satisfactory with relative standard deviation 1.2%-2.8% (n=5). The average concentration of trace metal ions Cd, Pb and Cu in the samples are varied from 0.002-0.087, 0.026-0.603 and 0.002-2.003 μg/g, respectively.
Synthesis of Some Imidazopyrazolopyrimidines, Pyrazolopyrimidopyrimidines and Pyrazolopyrimidothiazines

A. M. Elkhawaga, A. M. Kamal El-Dean, Sh. M. Radwan and M. M. Ahmed
Chemistry Department, Faculty of Science, Assiut University, Assiut 71516, Egypt

Chloroacylation of 3-amino-2-phenylpyrazole-4-carboxamide (1) using chloroacetyl chloride or using b-chloropropionyl chloride affording 6-chloromethyl(ethyl)-1-phenylpyrazolo[3,4-d]pyrimidin-4[5H]-one (2a,b). Pyrazolopyrimidine 2 underwent nucleophilic substitution reaction of chlorine with primary or secondary amines in refluxed ethanol to give 6-Alkyl(aryl)aminomethyl-1-phenylpyrazolo[3,4-d]pyrimidin-4[5H]-one (3a-g). When arylaminomethyl(ethyl)pyrazolopyrimidine was treated with formaline (30%) solution in ethanol at 30-40 °C, underwent Mannich reaction to afford imidazopyrazolopyrimidines (5a-e) or pyrazolopyrimidopyrimidine (6a-e). Chloroethylpyrimidine derivative 2a was converted into corresponding mercaptomethylpyrazolopyrimidine 7. Which cyclized using bromomalononitrile or o-bromo-acetophenone into pyrazolopyrimidothiazine 8, 9.
Improving the Selectivity of Non-Polar Alkanes, Alkenes, and Aromatic Hydrocarbon Compounds by Application of Acetonitrile as a CI Reagent

Fadel Wedian

Department of Applied Chemistry, Tafila Technical University, Tafila, Jordan

Selectivity enhancement of membrane introduction mass spectrometry of non-polar alkanes, alkenes, and aromatic hydrocarbon compounds by application of Acetonitrile chemical ionization was investigated. Acetonitrile CI is able to produce unique fragment ions for many test compounds that can be used to identify and quantify the parent neutrals. Detection limits of the test compounds were relatively high, however, the method could potentially be useful for analytical applications such as detection of non-polar hydrocarbons for environmental studies if CH₃CN CI/MIMS is coupled with a preconcentration method.
Utility of Dimedone in Organic Syntheses: Synthesis of some New Fused Quinolines

Mahmoud F. Farhat\textsuperscript{a}, Ahmed M. El-Saghier\textsuperscript{b}, Osama S. Moustafa\textsuperscript{c}, Mansour A. Makhlouf\textsuperscript{a} and Mufida A.M. Abdalla\textsuperscript{c}

\textsuperscript{a} Chemistry Department, Faculty of Science, Al-Fateh University, Tripoli, Libya
E-mail: mf_farhat@yahoo.com.
\textsuperscript{b} Chemistry Department, Faculty of Science, Sohag University, Sohag, Egypt
E-mail: el_saghier@yahoo.com.
\textsuperscript{c} Chemistry Department, Faculty Art and Science, Tarhona, Al-Mergeb University, Libya

7,7-Dimethyl-5-oxo-4-phenyl-2-thioxo-1,2,5,6,7,8-hexahydro-quinoline-3-carbonitrile (2) was prepared via reaction of dimedone, benzaldehyde and cyanothioacetamide. Compound (2) was allowed to react with a variety of ethyl chloroacetate, chloroacetonitrile or chloroacetamide to afford the S-alkylated derivatives (4), (6) or (8) respectively. Cyclization of compounds (4), (6) or (8) in presence of an excess amount of fused sodium acetate afforded 5,6,7,8-tetrahydro-thieno[2,3-b]quinoline derivatives (5), (7) or (9) respectively. Also, compounds (5), (7) or (9) were easily prepared via reaction of compound (2) with the corresponding halo compound in presence of sodium ethoxide in one-pot reaction. 2-(alkylthio)-quinoline-3-carbonitriles (10a,b) were prepared by reacting of compound (2) with methyl iodide or ethyl iodide respectively. Compound (10a) or (10b) was allowed to react with hydrazine hydrate to afford the corresponding pyrazolo[3,4-b]quinolin-5-one (11). Reaction of compound (7) with formic acid or ethylenediamine in presence of CS\textsubscript{2} afforded the corresponding quinolin[3',2':4,5]thieno[2,3-d]pyrimidin-4(3H)-one (12) or thieno[2,3-b]quinoline-2-carbothioamide (13) respectively.
Synthesis and Mesomorphic Behavior of some Novel Compounds Containing 1,3,4-Oxadiazole and 1,2,4-Triazole Rings

Jumbed H. Tomma\textsuperscript{a}, Ivan H. Rou’ilb\textsuperscript{b} and \textbf{Amar H. Al-Dujailia}

\textsuperscript{a} Department of Chemistry, College of Education, Ibn Al-Haitham, University of Baghdad, Baghdad, Iraq
\textsuperscript{b} Department of Chemistry, College of Science, University of Al-Mustanseryia, Baghdad, Iraq

Email: ahdujaili@yahoo.com

Two new series namely, 1,4-bis\{3-[2-(4-alkoxybenzlideneamino)-1,3,4-thiadiazole-5-methylenethio]-1,2,4-triazole-5-yl\}phenyl\textsuperscript{I}n and 5-(4-methoxyphenyl)-3-[2-(4-n-alkoxybenzlideneamino)-1,3,4-thiadiazole-5-methylenethio]-1,2,4-triazole\textsuperscript{II}n were prepared by many step procedures. The synthesized compounds were characterized by FTIR, \textsuperscript{1}HNMR, \textsuperscript{13}CNMR, and mass spectroscopy. Their mesomorphic behavior was verified using differential scanning calorimetry (DSC) and hot-stage optical polarizing microscopy (OPM). All new compounds of series \textsuperscript{I}n exhibited enantiotropic nematic mesophase except compound with n=3 did not show any liquid crystalline properties. The compound of series \textsuperscript{II}n with n=1 exhibited enantiotropic nematic mesophase, and that with n=3 shows enantiotropic nematic phase on heating and monotropic smectic A phase on cooling, while \textsuperscript{X}2 did not show any liquid crystalline properties.
Syntheses, Crystallography and Spectroelectrochemical Studies of Ruthenium Azomethine Complexes

Mousa Al-Noaimi, Haytham Saadeh, Salim F. Haddad, Musa I. El-Barghouthi, Mohammad El-Khateeb and Robert J. Crutchley

Three novel families of azomethine ligands L of the type $C_6H_5N=NC(OCH_3)=N(4-Y.C_6H_4)$ (1), $C_6H_5N=NC(\text{CO}_2\text{CH}_3)=N(4-Y.C_6H_4)$ (2) and $4-\text{Cl}.C_6H_5N=NC(\text{CO}_2\text{CH}_3)=N(4-Y.C_6H_4)$ (3), Y = H (a), CH$_3$ (b), Cl (c), Br (d), C$_{10}$H$_7$ (e), OCH$_3$ (f), NO$_2$ (g) have been synthesized and reacted consecutively with RuCl$_3$, 2,2$'$-bipyridine (bpy) and lithium chloride in ethanol under refluxing conditions to produce three novel families of trans-[Ru$^{II}$(bpy)LCl$_2$] complexes. These complexes were characterized by elemental analysis, IR, $^1$H-NMR, UV-visible spectroscopy and cyclic voltammetry. Crystallographic studies of two ruthenium (II) azomethine complexes show that the Ru(II) ion occupies a distorted octahedral coordination sphere in which the chloride ligands are trans to each other and the azomethine and bipyridine nitrogen donor atoms are equatorially coordinated. Crystallographic, electrochemical, electronic spectral data and time-dependent DFT calculations are all consistent with azomethine ligands possessing strong π-acceptor properties. These π-acceptor properties can be “tuned” by a judicious choice of substituents on the azomethine ligand.

References
Chemical Effects of Irrigation Water Quality on Two Types of Ammonium Fertilizers and Its Effect on Growth and Yield of Wheat

H. M. Shukri\textsuperscript{a} and A. K. A. Jarallah\textsuperscript{b}

\textsuperscript{a} Biotechnology Research Center, AL-Nahrain University, Iraq
\textsuperscript{b} Soil science department, College of Agriculture, University of Babel, Iraq

A pot culture experiment was conducted to evaluate the two fertilizers use efficiency of mono ammonium phosphate (MAP) and diammonium phosphate (DAP) on wheat productivity with saline water irrigation. Six salinity level of drainage water and river water (1 dSm\textsuperscript{-1}) was used as control using factorial experiment randomized complete block design (RCBD).

Results showed that biological yield and other characteristics, i.e, total dry weight, grain yield, weight of 100 seeds, protein content and N and P absorption significantly decreased as salinity of irrigation water increased from 4 to 12 dSm\textsuperscript{-1}. Also the results revealed that using the MAP fertilizer increased all plant parameters as compared with DAP fertilizer.

A negative linear significant relation between plant parameters and irrigation water salinity was found. It was concluded that water with salinity 4 dSm\textsuperscript{-1} and leaching fraction to 20% can be safely used for irrigation of wheat cultivated in fine soil textured (silty clay) with efficient drainage system under suitable agriculture practices. Ammonium phosphates are efficient fertilizers for plants, and MAP was in this study found to be superior and a more efficient fertilizer as compared with DAP.
Aspartame, discovered in 1965, is a low-calorie sweetener that is used worldwide in more than 5,000 products, including tabletop sweeteners, various foods and carbonated beverages. Because aspartame is up to 200 times sweeter than sugar, very little aspartame is needed for the desired sweetness. Aspartame is made of two amino acids, aspartic acid and phenylalanine, which are building blocks of proteins that are found in all protein-containing foods, including meats, grains, and dairy products. Aspartame is made when these two amino acids are joined and a methyl group is added. This methyl group breaks down during digestion and forms methanol. The body metabolizes the amino acids in aspartame in the same way as those from other protein-containing foods. Aspartame is an endocrine disrupting drug, it stimulates prolactin and causes infertility in the woman. A recent study in Japan wrote of infertility in the man. If a woman gets off aspartame and gets pregnant, aspartame - an abortifacient and also a teratogen- causes birth defects and mental retardation. Aspartame depletes serotonin from which victims suffer manic depression, hallucinations, paranoia, rage, suicidal tendencies, anxiety and panic.

Diabetic specialist Roberts says aspartame can precipitate diabetes, simulates and aggravates diabetic retinopathy and neuropathy, and destroys the optic nerve. It keeps blood sugar out of control and can cause diabetics to go into convulsions. It also interacts with insulin.

The reason aspartame causes joint pain is it hardens the synovial fluids. This was proven on studies in South America by Searle. The studies also showed aspartame destroys the brain and central nervous system. The Trocho study shows that formaldehyde converted from the methanol accumulates in the cells and damages the DNA with most toxicity in the liver but substantial amounts in the brain, retina, adipose tissue (fat cells) and kidneys. when you damage DNA you are talking about survival of the human race.

Tinnitus or ringing in the ears is another big time symptom of aspartame. The components of aspartame and their multiple breakdown products are potentially toxic to the brain and inner ear. These organs are highly vulnerable to metabolic disturbances and neurotoxins because of their unique metabolic requirements. Methanol converts to formaldehyde and formic acid in the retina and destroys the optic nerve. Methanol is classified as a narcotic, so chronic methanol toxicity that affects the dopamine system of the brain can cause addiction. Dr. Morgan ophthalmologist and specialist in methanol toxicity said that if vision is in the wet stage, it will improve when get off this toxin. Depression and suicidal tendencies are triggered by depletion in serotonin. Aspartame triggers this big time & memory loss. Aspartame also reduces IQ and triggers such things. A study in Norway a few years ago showed that aspartame destroys the brain, especially in the area of learning. The aspartic acid in aspartame is an excitotoxin, product that stimulates the neurons of the brain to death causing brain damage. It is also a chemical hypersensitization agent, has an additive and synergistic effect with MSG, and it interacts with fluoride, vaccines & other toxins.
Theoretical study of the effect of selenium as antioxidant on some of amino acid

Suher Al-Saaty \textsuperscript{a} and Hathem Al-Wahab \textsuperscript{b}

\textsuperscript{a} Department of Environmental Science College of Environmental Science and Technology
Mosul University

\textsuperscript{b} Department of Chemistry College of Science Mosul University

Due to the fact that selenium is similar to sulfur, a theoretical study of the effect of selenium as antioxidant on some of amino acid and biochemical compounds which contain sulfur in their chemical construction was performed using Semi empirical Molecular Orbital Package (MOPAC) Program in (CS Chem Office) to calculate some of the physical properties by using minimization energy methods.
Thermodynamics of Solution of Non-Mesomorphic Solutes in the \( n \)-Hexyl-
\( n' \)-Cyanobiphenyl (6CB) Liquid Crystal Solvent

Oweimreen, Ghassan A.

Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, ghassan@kfupm.edu.sa 31261, Saudi Arabia, Email:

From specific retention volume measurements for 30 solutes (normal alkanes, branched alkanes, alkenes, hexadienes and benzene) at four temperatures in each of the nematic and isotropic phases of \( n \)-hexyl-\( n' \)-cyanobiphenyl (6CB), infinite dilution solute activity coefficients (\( \gamma^\infty_2 \)), solute partial molar excess enthalpies (\( \Delta H^e \)) and entropies (\( \Delta S^e \)) and partial molar enthalpies (\( \Delta H^\delta \)) and entropies (\( \Delta S^\delta \)) of solution were obtained \[1\] and analyzed in the light of an infinite dilution statistical model \[2\] to interpret the observed trends. In this study these results were further analyzed to express \( \gamma^\infty_2 \) as a function of the Flory-Huggins size effect correction (\( \gamma^\infty_{FH} \)) and an interaction parameter (\( \kappa \)); the sum of the thermal (\( \gamma^\infty_T \)) and athermal (\( \gamma^\infty_{T-S} \)) contributions to \( \gamma^\infty_2 \). From regular solution theory solute (\( \delta_2 \)) and solvent (\( \delta_1 \)) solubility parameters were obtained at different temperatures for all the solutes in the nematic and isotropic solution phases.

Plots of \( \Delta H^\delta \) versus \( \Delta S^\delta \) were reasonably linear. Such \( \Delta H^\delta - \Delta S^\delta \) compensation reflects similar solute solubility in the nematic and isotropic phases. Also an average \( \ln \gamma^\infty_{2,N} / \ln \gamma^\infty_{2,I} \) value of 1.077 ± 0.003 where \( N \) and \( I \) refer, respectively, to the nematic and isotropic phases, indicates lesser solute compatibilities with the nematic phase.

For all the solutes studied plots of \( \delta_1 \) versus temperature (\( t \)) showed a drastic and sharp change in \( \delta_1 \) at the nematic-to-isotropic transition (29.0°C) which is reminiscent of enthalpy and density changes in first order transitions. The extent of the discontinuity in \( \delta_1 \) may thus be used as a measure of the strength of the transition while a continuous variation of \( \delta_1 \) across the phase transition would be associated with a second order transition. This finding can help in identifying second order transitions in liquid crystals or polymers. Currently results for \( n \)-octyl-\( n' \)-cyanobiphenyl (8CB) are being analyzed to test the nature of the much debated \[3,4\] smectic A-to-nematic transition of 8CB.

References

Net-analyte signal calibration method was proposed and successfully applied for simultaneous determination of three common food dyes, Allura Red, Sunset Yellow and Tartrazine. The sensitivity vector ($s^*$) for each dye was determined over the spectral range (300-650 nm) and used for prediction of dye concentration in future samples. Initially, the three dyes were simultaneously determined in their standard mixtures using net-analyte signal calibration procedure without the need from any chromatographic separation. The obtained recoveries with R.S.D. were 99.8 (2.8), 102(3.3), and 100 (4.5) for Allura Red, Sunset Yellow and Tartrazine, respectively. The optimized net-analyte signal calibration method was applied for analysis of food dyes in powdered soft drinks. The food samples were dissolved in water, heated and centrifuged prior spectral measurement and chemometric analysis. Satisfactory results were obtained for dyes quantification in commercial drinks (like TANG and SQUEEZE). The proposed chemometric method was validated against a standard HPLC method. Statistical analyses showed insignificant differences between the results of two methods. The developed multivariate calibration method offers a simple and rapid procedure for analysis of food dyes in powdered soft drinks in comparison with HPLC methodology.
Reactions of Some Hetero Aromatic Aldehyde-Ketone Azines (Alketazines) with DMAD

Ma’un H. Tawara, Abdullah El-Alali*

Department of Chemistry, Mu’tah University, Alkarak- Jordan.
Phone (962-79-5987153), Fax(962-3-2375540), e-Mail(elalali@mutah.edu.jo)

Aldehyde – Ketone azines (Alketazines) are reacted with two moles of dimethyl acetylenedicarboxylate (DMAD). A bicyclic azine is formed, which is, in some cases, depending on the nature of aldehyde or ketone used, a final product. In some cases, this bicyclic form undergoes rearrangement either into an open form (acyclic tetraene azine), if only ketones are used, or into an N-allyl pyrazole, if only aldehydes are used.

\[ \text{If ketones are used} \]
\[ \text{Open-chain tetraene azine} \]

\[ \text{If aldehydes are used} \]
\[ \text{N-allyl pyrazole} \]

\( X= O, S, NH \quad R= \text{H or CH}_3 \quad Ar= \text{Aromatic moiety} \)

References

Structures of six triterpenes isolated from Lagerstroemia indica will be discussed:

The plant Lagerstroemia indica is among the longest blooming trees with flowering periods lasting from 60-120 days. It is in flower from July to September. Originally from Asia, crape myrtle is found throughout the United States as far north as Massachusetts, where it grows as an herbaceous perennial. First introduced to England and the United States in the eighteenth century, crape myrtle is now widely cultivated throughout the world.

The stem bark is febrifuge, stimulant and styptic. The bark, flowers and leaves are considered to be a drastic purgative. A paste of the flowers is applied externally to cuts and wounds. The root is astringent, detoxicant and diuretic. Decoction of the flowers is used in the treatment of colds.

The compounds isolated are:
- $\text{3\beta-hydroxy-lupa-5,20(29)-diene [I]}$
- $\text{3\beta-hydroxyolean-12-ene [II]}$
- $\text{Lageflorin [III]}$
- $\text{3\beta-acetoxy-cycloart-24-one [IV]}$
- $\text{3\beta-acetoxynor-cycloart-24-one [V]}$
- $\text{3\beta-hydroxy-cycloart-24-one [VI]}$
Complexes of group (VIII) (or metal chlorides) & (IB) metals with Diaminothiuramdisulfide

Ihsan A. Mustafa, Afyaa' Moayad
College of Science, Mosul University, Iraq
Email: ihsan_mustafa@yahoo.com

Diaminothiuramdisulfide, \([H_2\text{NNHC(S)S}]_2\), was reacted with group (VIII) metals (or metal chlorides) \([\text{Fe}(0), \text{Co}(0), \text{Ni}(0), \text{NiCl}_2, \text{RhCl}_3, \text{PdCl}_2 & \text{Pt}(0)]\) and group (IB) metals \([\text{Cu}(0), \text{Ag}(0) & \text{Au}(0)]\). The diaminothiuramdisulfide (TDS) was first reduced to aminothiocarbamate anion \([H_2\text{NNHC(S)S}^-]\), \((L)\), and reacted as such with the oxidized metals and metal chlorides to give complexes of the type \([\text{M}(L)_2]\) \([\text{M}=\text{Fe}(II), \text{Co}(II), \text{Cu}(II), \text{Pd}(II), \text{Ag}(II) & \text{Pt}(II)]\), \([\text{M}(L)_2]_2\) \([\text{M}=\text{Fe}(II), \text{Co}(II) & \text{Ni}(II)]\), \([\text{M}(L)_3]\) \([\text{M}=\text{Fe}(III), \text{Cu}(III), \text{Rh}(III) & \text{Au}(III)]\) and \([\text{Ni}(L)_3]_2\).

The oxidative addition reactions were carried out in different solvents, viz., tetrahydrofuran, N,N-dimethylformamide, dry toluene, diethylether and ethanol, and in some cases the product was found to be solvent dependent. The reaction of metallic iron with a mixture of iodine and (TDS) gives the complex \([\text{Fe}(L)_2\text{I}]_2\). Similarly, with mixtures of (TDS) & iodine, cobalt yields \([\text{Co}(L)\text{I}]_2\). The reaction of gold metal with (TDS) in the presence of bidentate donor ligand \((1,10\text{-phenanthroline})\) forms 1:1 adduct, \([\text{Au}(L)_3\text{phen.}]\). The complexes and the adduct were characterized by metal analysis, infrared, UV/Visible spectroscopy, magnetic & conductivity measurements.
The two complexes synthesized by the reaction of Co III and Fe III ions with potassium cyclopentyl xanthate have been characterized by elemental analysis, conductance, magnetic susceptibility, infrared and electronic spectra measurements. A 1:2 complex was formed with Fe III and a 1:3 complex in the case of Co III. The value of magnetic moment provides evidence for the existence of an octahedral high spin xanthate complex in the case of Fe III, whereas the Co III complex was found to be non-magnetic. Molecular Mechanics MM+ and MM2 calculations were performed using the hyper chem. and the ChemOffice molecular modeling program. All calculations confirmed the octahedral arrangement around the Co III and the Fe III.
A simple spectrophotometric method for the determination of paracetamol in aqueous solution is developed. The method is based on the oxidative coupling reaction of paracetamol, with N-(1-naphthyl)ethylene diamine in an acidic medium (pH 3.15) in presence of sodium periodate as oxidizing agent to produce an intense orange coloured, water-soluble and stable dye, which exhibits maximum absorption at 463 nm. Beer’s law is obeyed over the range 10-120 µg of paracetamol in final volume of 25ml (0.4-4.8 ppm) with a molar absorptivity of 104 l.mol⁻¹.cm⁻¹ (0.70 g.cm⁻²) and a relative error of -1.78 to +2.27 µg. Sandell’s sensitivity index of 0.021 % and relative standard deviation of +0.69 to +2.65% depending on the concentration level were found. The method has been successfully applied to the determination of paracetamol in pharmaceutical preparations.
Synthesis and Characterization of New Heterocyclic Compounds Derived from 4-Amino-4H-1,2,4-Triazole-3-Thiol and 4-Amino-5-Methyl-4H-1,2,4-Triazole-3-Thiol

Taleb T. Al-Nahari*
Department of Chemistry, Faculty of Applied Sciences, Thamar University, Yemen. P.O. Box 87246

Starting from the 4-Amino-4H-1,2,4-triazole-3-thiol and 4-Amino-5-methyl-4H-1,2,4-triazole-3-thiol 1a and 1b, respectively, a series of new heterocyclic compounds derivatives (2a,b to 6a,b) was synthesized. The structures of all the newly synthesized compounds have been confirmed by elemental analysis, \(^1\)H-NMR, \(^13\)C-NMR and IR spectroscopy.

Synthetic pathways for the preparation of compounds 2a, 2b to 6a, 6b
Preparation and Study of Some New Complexes of Iron (II), Cobalt (II), Nickel (II) and Copper (II) with N-O Donor Macroyclic Ligand

Mowafak Salman Al-Fadhel

Research Center for Dams and Water Resources, Mosul University, Mosul, Iraq
E-mail: mowfak_alfadhel@yahoo.com

Several new macrocyclic complexes of Iron(II), Cobalt(II), Nickel(II) and Copper(II) formed with N-O donor Schiff base ligand of macroyclic type by the condensations of malonyl-di-hydrazides and benzil \(^1\text{-}^2\).

The complexes having the general formula \([\text{M(LH}_2\text{X}_2] \text{ and [M(L)]}, \text{ (M=Fe, Co, Ni, Cu)}, \text{ LH}_2 \text{ and I are the neutral and dibasic forms of the ligand.}\)

\[
\text{MX}_2\text{nH}_2\text{O} + \text{LH}_2 \rightarrow [\text{M(LH}_2\text{X}_2] \text{ + nH}_2\text{O}
\]

\[
\text{MX}_2\text{nH}_2\text{O} + \text{LH}_2 + 2\text{KOH} \rightarrow [\text{M(L)}] \text{ + 2KX + (2+n) H}_2\text{O}
\]

Characterization of the resulting complexes by elemental analysis, molar conductance measurements and the study of infrared and electronic spectra \(^3\) confirmed, neutral hexacoordinate complexes with octahedral structure for neutral medium complexes where the ligand acts as neutral tetradeinate, while in basic medium neutral tetra coordinate tetrahedral and square planar complexes were obtained for which the ligand acts as dibasic tetradeinate\(^4\).

REFERENCES
Kinetic Modeling of the Heterogeneously Catalyzed Liquid-Phase Hydrogenation of Phenylpropanal and Cinnamyl Alcohol over Ir/Al₂O₃ Catalysts

Ayman Hammoudeh and Sabri Mahmoud

Chemistry Department, Yarmouk University, P.O.Box 566, Irbid, Jordan

In spite of the elegance and environmental superiority of cinnamyl alcohol production through the selective heterogeneously catalyzed hydrogenation of cinnamaldehyde, the conventional production methods via the Meerwein-Ponndorf-Verley reduction or by the reduction with alkali borohydrides of cinnamaldehyde couldn’t be displaced. This is because 100% selectivities toward cinnamyl alcohol formation couldn’t, for thermodynamic and kinetic obstacles, be achieved. Since both phenylpropanal (II) and cinnamyl alcohol (III) are intermediates in the above selective hydrogenation, the kinetic study of their further hydrogenation is, with this respect, highly appreciated. In this work, a systematic study of the hydrogenation reaction of phenylpropanol (II) and cinnamyl alcohol (III) under mild conditions over alumina-supported Ir catalysts is presented. The experimental results were analyzed and where found to conform in both cases with a Langmuir-Hinshelwood surface reaction as the rate determining step. The kinetic models describe successfully the negative effects of the initial concentration and temperature in the case of phenylpropanal hydrogenation and the positive ones in the cinnamyl alcohol hydrogenation. The kinetic models in both cases indicate a relatively weak interaction of hydrogen with the Ir surface.

Ph-CH=CH-CHO (I)  \[ \xrightarrow{\text{k}_1} \text{Ph-CH}_2\text{-CH}_2\text{-CHO (II)} \xrightarrow{\text{k}_3} \text{Ph-CH}_2\text{CH}_2\text{CH}_2\text{OH (IV)} \]  \[ \xrightarrow{\text{k}_2} \text{Ph-CH=CH-CH}_2\text{OH (III)} \xrightarrow{\text{k}_4} \]

References:
New Complex Salts of First Transition Metal Chloride with Diazonium Salt of α-Naphthyl

N. H. Buttrus*1, A. F. Mohammed1 and J. Allias2

1 Chemistry Department, College of Science, Mosul University, Mosul, Iraq
2 Chemistry Department, College of Education, Mosul University, Mosul, Iraq

New complex salts of the type B2[MCl4] and B2[M'Cl6], where M = Mn2+, Co2+, Ni2+, Cu2+ and Zn2+, M' = Cr3+ and Fe3+, were prepared by treatment of diazonium salt of α-naphthyl with metal chloride in (2:1) or (3:1) molar ratio. The new complex salts were characterized by their metal contents, conductance measurements, spectroscopic data (I.R. and UV/Vis) as well as magnetic measurements. The results of electronic spectra and magnetic measurements indicate that the complex salts have tetrahedral geometry for Mn2+, Co2+, Ni2+, Cu2+ and Zn2+, while the complex salts of Cr3+ and Fe3+ have an octahedral environment.
Study of the Volatile Organic Compounds in Sea water by Using HS-SPME-GC-FID

Sami Hussein Al Mabrouk
Faculty of Science, Chemistry Department, Benghazi University, P.O.Box 1308
Benghazi-Libya
Email: samihus2000@yahoo.com

Headspace solid-phase micro-extraction (SPME) is combined with gas chromatography-flame ionization detector for the analysis of volatile organic compounds (VOCS) such as acetone, dichloromethane, butane, benzene, and toluene in sea water. The combined method HS-SPME-GC-FID uses fibers coated with a 100 µm Polydimethylsiloxane. The extraction fiber of the SPME system was exposed for 40 min in the headspace of the vial. The compounds adsorbed on the fiber were desorbed by exposing the fiber in the injection port of GC-FID system. Different SPME parameters (extraction time, extraction temperature, effects of pH and salinity on extraction) were studied. The aims of this investigation have been met. The application of HS-SPME was shown to be a suitable methodology for the mentioned VOCS. Parameters affecting the method performance have been optimized. The extraction time of 40 min working at the comprehensive temperature of 70ºC was optimum for all compounds as mixture. The liner response of ($R^2 > 0.99$, N=3) was obtained in the concentration range 2000 ng/ml to 10000 ng/ml for each compound. The sensitivity of the method was enhanced with the addition of sea salt to the sample solutions. The Overall effect of pH on extracting these compounds from water is difficult to predict because different reactions can occur simultaneously. Internal standards are important to increase the sensitivity when the gas-chromatography-FID combination with HS-SPME is applied for quantitative measurement.
Isolation and Identification of an Anthocyanin Compound from Cherry Fruit (Prunus Avium) and Study of Its Antibacterial Activity

Kamal M. Mahmoud

Salahaddin University – Science College – Chemistry Department – Erbil-Iraq

A certain anthocyanin compound was isolated from Kurdistan cherry fruit (Prunus avium) at room temperature. The chemical and physical properties (purification and identification) of this compound were studied using thin layer chromatography (TLC), preparative thin layer chromatography (PTLC), high performance liquid chromatography (HPLC), column chromatography (CC), infrared (I.R.), ultraviolet (U.V.), $^1$H-NMR, $^{13}$C-NMR, mass spectroscopy (MS).

The antibacterial activity of the extracted anthocyanin compound was determined against types of standard strains of bacteria such as *Staphylococcus aurens* (g –ve) and *Escherichia Coli* (g +ve) by disk diffusion method. The results indicated that the anthocyanin compound has inhibiting *Escherichia Coli*.

References

Aim of this work was to investigate the benefit effect of cobalt chloride for reducing blood glucose in experimental diabetes. Forty male weaning normal albino (Wistar) rats of 8 weeks of age were fed with a basal diet. Twenty rats (n = 20) were then intraperitoneally injected with alloxan to induce diabetes. Then after one week ten rats from each group (n = 20) were given 2 mM of CoCl₂ in the drinking water for further two weeks. Body weight gain and food intake were recorded regularly. On day 21 after an over night fasting, animals were killed and Concentrations of blood glucose, serum cholesterol, serum triglycerides, serum creatinine, serum albumin, serum urea, were estimated. Activities of serum glutamic oxallic transaminase (GOT), serum glutamic pyruvic transaminase (GPT) and serum alkaline phosphatase were also estimated. The diabetic state had an effect on growth rate and food intake. However treatment with CoCl₂ resulted in no change in body weight gain or food consumption. The administration of CoCl₂ significantly reduced blood glucose, serum creatinine, serum albumin, serum urea concentrations and GOT, GPT. Whereas the activity of alkaline phosphatase was increased of diabetic rats compared to their control counterparts. We conclude that these results suggest that cobalt resulted in reduction of blood glycemia, which is mediated, by reduction in the rate of systematic appearance of glucose and hepatic gluconeogenesis.
Biochemical Analysis of Urinary Stones in Nenavah Governorate

Mohamed Fathel Hadad

Technical Institute, Dept. Of Clinical Analysis, Mosul, Iraq

Urinary stones are the third most common affliction of the urinary tract, after infection of prostate, and most of patients will experience one or more recurrence within years. Chemical analysis of 90 stones (59 males, 31 females) was conducted in private clinical laboratories between 1999 and 2007. The incidence of renal stones seems to be highest in females, especially in age group (40-49) years in both sexes. From 90 stones, 41.1% were pure calcium oxalate, 33.3% were pure uric acid and 35.6% phosphate (Ammonium Magnesium phosphate AMP). But cystine stones were not identified in the current study.
Mono, Homo and Hetero Trinuclear Palladium (II) Complexes with bis-
(Substituted Thio) Butane

Nabeel H. Buttrus and Rana A. Kepaa

Dept. Chem, College of science, Mosul University, Mosul- Iraq

Mono, homo and hetero trinuclear complexes of the type [Pd(L)Cl2], [Pd3(L)2Cl4]Cl2, [PdNi2(L)2Cl4]Cl2 [L=bis-(benzylthio)butane (L1), bis(butylthio)butane (L2) (benzylthiobutylthio)butane (L3) and bis-(p-tolythio)butane (L4), have been prepared by the reaction of newly prepared sulphur containing ligands (L1)-(L4) with PdCl2 in 1:1 or PdCl2 and NiCl2.6H2O in 2:3 ligand to metal ratio. The complexes have been characterized on the basis of their metal content, IR and electronic spectra, magnetic and conductivity measurements. Square planar geometry around Pd(II) or Pd(II) and Ni(II) have been deduced on the basis of magnetic and spectral studies.
A series of new organotellurium(IV) of the general formula (cyclo-C₆H₁₁)₂TeX₂ (where X = I(1), Br(2) Cl(3)) and (cyclo-C₆H₁₁)₂Te(R)X (where R = CH₃, X = I(4); R = C₂H₅, X = Br(5); R = C₂H₅, X = I (6); R = C₃H₅, X = Br (7); R = CH₃, BPh₄ (8) ) have been prepared and characterized. Reaction of (cyclo-C₆H₁₁)₂Te with benzyl bromide and 4-bromophenacyl bromide gave unexpectedly dibenzylcyclo-hexyltelluronium bromide (9) and bis(4-bromophenacyl)cyclohexyltelluronium bromide (10), respectively. Reaction of (9) with NaBPh₄ gave the corresponding tetraphenylborate derivatives (11) in high yields. ¹H NMR studies revealed that in DMSO solution, telluronium salts eliminate alkyl halide. Reactions of (cyclo-C₆H₁₁)₂Te with Na₂PtCl₄, Na₂PdCl₄, HgX₂ (X = Cl or Br), CuI and AgNO₃ are also reported. Conductivity measurements, IR, ¹H, ¹³C-NMR and thermal data for the new compounds are presented and discussed.
Study of Charge Transfer Complexes of Salicylideneanilines with Eu(fod)₃ in Cyclohexane by U.V. Spectroscopy

S. T. Sulaiman, L. M. N. Saleem & I. J. AL-Nuri

Chemistry Department, College of Science, Mosul University, Mosul, Iraq

Salicylideneanilines in Cyclohexane (C.H) form 1:1 charge transfer complexes with Eu(fod)₃, indicated by the observation of a new longer wavelength band ( \( \sim 435 \) nm). The colourless solution of Schiff bases were changed to yellow on complexation with shift reagent Eu(fod)₃ in C.H.

Equilibrium constant values (K) for the complexes were obtained by applying Benesi-Hildebrand equation at different temperatures. The factors affecting these values were established computationally, followed by the formulation of multiple linear regression equation using SPSS program. From the equation it is apparent that the charge on nitrogen plays the major role in determining these values.
Posters
Chemical Composition and Antibacterial Activity of Tymus Algeriensis Essential Oil

C. Chelghoum\textsuperscript{1} and T. Dob\textsuperscript{2}

\textsuperscript{1} Laboratoire de Chromatographie, Faculté de Chimie, Usthb, BP 32, ELalia Bab Ez zouar, Alger, Algérie, Email: c.chelghoum@yahoo.fr

\textsuperscript{2} Laboratoire de Molécules Bio-ctives et de la Valorisation de la Biomasse ENS, Kouba, Alger, Algérie

Essential Oil of tymus algeriensis was isolated from fresh vegetative aerial parts of the plants by hydrodistillation using a Clevenger – type apparatus and analyzed by GC / MS and GC / FID. A total yield of 0.98 g of essential oil per 100 g of plant weight was obtained and more than 80 compounds were identified. This oil shows high antibacterial activity.
Kinetics of The Alkaline Hydrolysis of some Aryl Acetates

Taher S. Kassem and Magda F. A. Fathallah
Chemistry Department, Faculty of Science, Alexandria University, Alexandria, Egypt

The kinetics of the alkaline hydrolysis of acetoxybenzene, 1,4-diacetoxybenzene, 1-acetoxynaphthalene, 1,4-diacetoxynaphthalene and 1,5-diacetoxynaphthalene have been studied in 50% (v/v) dioxane-water. Analysis relationship was observed for such substituted acetoxynaphthalene where a good correlation between log k vs $\delta_{ij}$ was observed of the data showed that an increase in the rate was found to be dependent on the position of the acetoxy group. Also the presence of oxo-group caused an inhibition in the rate to a great extent either in the naphthalene or benzene compounds.

The various thermodynamic parameters were deduced. A linear free energy relationship was observed for such substituted acetoxynaphthalene where a good correlation between log k vs $\delta_{ij}$ was observed.

(1) For the benzene esters:

\[
\begin{array}{ccc}
\text{H}_3\text{C} & \text{C}=\text{O} & \text{H}_3\text{C} \\
\text{O} & \text{C}=\text{O} & \text{O} \\
\text{O} & \text{C} & \text{O} \\
\text{O} & \text{C} & \text{O} \\
\end{array}
\]

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<th>0.943</th>
<th>5.480</th>
<th>0.037</th>
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<td>Relative rate.</td>
<td>1.000</td>
<td>5.810</td>
<td>0.007</td>
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(2) For the naphthalene esters:

\[
\begin{array}{ccccc}
\text{OAc} & \text{OAc} & \text{OAc} & \text{OAc} & \text{OAc} \\
\text{OAc} & \text{OAc} & \text{OAc} & \text{OAc} & \text{OAc} \\
\text{OAc} & \text{OAc} & \text{OAc} & \text{OAc} & \text{OAc} \\
\text{OAc} & \text{OAc} & \text{OAc} & \text{OAc} & \text{OAc} \\
\end{array}
\]

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References:
Lead-Sensitive Membrane Electrode Based on Chelating Ion Exchanger

Alasier. A. S. a, Entisar. S. A b and H A. Elbishi b

a Renewable Energies and Water Desalination Research Center, National Bureau of Research and Development, Tripoli-Libya P.O. Box 30878.
E.mail. a_elaseer2007@yahoo.cu.uk

b Advanced Chemical Analysis Laboratory, National Bureau of Research and Development, P. O. Box 13439 Tripoli Libya.
E.mail. AAL@LTTNET.NET

A new selective membrane electrode for measurement of lead activities is proposed. The preparation of active components of the membrane is described. The ready made electrode insert was used in which the PVC membrane was replaced by the prepared membrane [1]. Experimental results document the emf response profile (Figure 1), the selectivity, the detection limit and the effect of the sample media. The prepared electrode was applied for the measurement of the lead concentration in water samples. Activated alumina micro column was used for preconcentration of lead in the analyzed water samples [2]. The obtained results were compared with those determined by atomic absorption spectrometry [3].

Figure (1) shows the experimental emf response, E, vs. the molar concentration of Pb^{2+}.

References

Ab-Initio Molecular Orbital Study of 1,4-Oxathione

M. Khorassani

Department of Chemistry, School of Science, Alzahra University. P.O.Box 1993891176, Tehran, Iran
e-mail: rhekmatus@yahoo.com

The stereochemistry of oxathians ring reveals peculiar features. The chirality of unsubstituted ring\(^1\) is due to a virtual tri-coordinatined chiralcenter \(^2\) and surprisingly close values of many dimensions of oxathianes to those of average values measured for similar dioxanes and dithiones have been observed\(^3\). Ab-initio calculation at HF/6-311+G* levels of theory for geometry optimization and mp2/6-311+G*///HF/6-311+G* and B3Lyp/6-311G*///HF/6-311+G* for a single-point total energy calculation were studied for the chair and twist conformations of 1,4-oxathione 1.

References

High temperature X-ray diffraction study of Tantalum carbides

AREZKI AFIR

USTHB- Faculté de Chimie, BP 32 Elalia–Bab Ezzouar, Alger, Algeria
arezkiafir@yahoo.fr

The oxidation of metallic Tantalum was monitored in an oven for X-rays with a graphite resistance under continuous vacuum or under controlled carbon monoxide pressure. We demonstrate that this brought into play the formation of two varieties of Ta$_2$O$_5$, hemicarbide Ta$_2$C and monocarbide TaC likely to be formed between 293K and 2288 K, in accordance with a reaction mechanism which we found to take place over several stages. We determined the crystalline characteristics at high temperature for all observed solid phases. Particular importance is attached to the study of thermal expansion of carbides phases.
High temperature X-ray diffraction study of Tantalum oxides phases

Houria Chikh-Afir

USTHB- Faculté de Chimie, BP 32 ElAlia– Bab Ezzouar, Alger, Algeria
Email: houriachikh@yahoo.fr

The structures and lattice parameters of the Tantalum and Ta₂O₅ phases were determined by high temperature X-ray diffraction under vacuum and low pressure carbon monoxide between 293 and 2278 K. We show that the metallic phase structure is stabilized by inclusion of oxygen into the metal octahedral hole. We determined the crystalline characteristics at high temperatures for Ta and Ta₂O₅ Phases.
Identification of Adhesive Fingerprint by Pyrolysis Gas Chromatography

Abubaker Sharif a, Andrej Oriňák b, Ibrahim Ammar a

a Sebha University, Faculty of Science, Department of Chemistry, Sebha Libya
b University of P.J.Safarik, Institute of Chemistry, Department of Physical and Analytical Chemistry, Kosice, Slovakia

Gas chromatography (GC) is used for the separation of volatile samples. Different detectors can be used in order to quantify the separated products by the peak area or height.

Analytical pyrolysis, where a pyrolyzer is combined with a gas chromatograph and a mass spectrometer, has been used for a long time for qualitative analysis of non-volatile substances like natural and synthetic polymers. The pyrolyzer thermally degrades the non-volatile substances in an inert atmosphere to more volatile components in order to be able to use the gas chromatograph for the separation and mass spectrometer for qualitative and quantitative identification of the pyrolysis products.

Adhesives are defined as products that can join two solid surfaces together so that they are joined and kept together by a glue joint. It should be noted that some of the types of adhesive could be used for joining wood, paper, carton, textile and plastic surfaces, and other types of material such as metals and glassware. The physical drying types of adhesives harden when solvents or water in the adhesive evaporate. The aqueous adhesives are normally emulsion adhesives except adhesives based on starch and cellulose (paste).

In this study, pyrolysis technique has been described and pyrolysis of commercial adhesive was presented. The sample has been applied directly to pyrolytic injector by two ways, capillary through the pelletizer and by an especial SGE microsyringe. The system was set up using an on/line pyrolytic injector linked to a capillary column DB-5 to characterize the fingerprint of adhesive (white glue water-soluble for gluing wood, paper, cork and textile) that can be purchased in the Slovak retail. Analyses have been done at different pyrolysis temperature. Py-GC seems to be very effective method for this proposes because this allows injection of liqued and solid samples.
Solvent Effect on Electrospinning of Hydrophilic Copolymers Based on 2-Hydroxyethyl Methacrylate with 2-Ethoxyethyl Methacrylate

L. Martinová\textsuperscript{a}, D. Lubasová\textsuperscript{a}, M. Přádný\textsuperscript{b}

\textsuperscript{a} Technical University of Liberec, Department of Nonwovens, Studentská 2, Liberec, 461 17, Czech Republic

\textsuperscript{b} Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic; Prague, Czech Republic

lenka.martinova@tul.cz

The effect of different types of solvents, solvent mixtures and properties of solvents on electro-spinability of prepared solutions of hydrophilic copolymers based on 2-hydroxyethyl methacrylate (HEMA) and 2-ethoxyethyl methacrylate (EOEMA) were investigated. Morphological appearances of electrospun copolymer nanofibers were subsequently analyzed. Though basic solvent for these copolymers is ethanol or its mixture with water, different co-solvents strongly influence not only electrospinning process by Nanospider technology (Jirsak et al., 2005) but also morphology of processed nanofibers.

Biocompatible polymers based on HEMA or its copolymer with EOEMA are attractive candidate materials for tissue engineering. The latter co-monomer reduces the hydrophilicity of poly(HEMA), without significant deterioration of biocompatibility and mechanical properties of the resulting material. Nanofiber sheets from copolymers HEMA/EOEMA with different co-monomer ratio and from pure poly(EOEMA) were successfully tested as scaffolds regarding of this geometric characteristic (pore size, porosity) and physiochemical properties.

In the electrospinning process of polymer solution, solvent is one of the main contributors for solution properties, e.g. conductivity or viscosity. Solvent can influence diameter of nanofibers, porosity, efficiency of process and above all development of electrospinning process.

Thus copolymer HEMA/EOEMA dissolution behavior in different solvents or their mixture plays an important role. Solubility parameters can be determined by direct measurement, correlation with other physical parameters, or indirect calculations. Solubility parameters are of technical importance in the fields of spinning fibers and casting films (Small, 1953).

First of all we tried to use the one-component Hildebrand solubility parameter for prediction of solvent optimal mixture for copolymer HEMA/EOEMA. This parameter is useful for regular solutions, e.g. solutions without molecular polarity or specific interactions. The solubility parameter has been defined as the square root of the cohesion energy density (CED) and describes the attractive strengths between molecules of the material. But our results were not sufficiently predicative. We decided to employ the Hansen’s three-component solubility parameters. Hansen (1967, 1983) proposed a practical extension of Hildebrand parameter method for polar, non-polar and H-bonding systems, primarily for use in polymer-liquid interactions.

The Hansen parameter was calculated firstly for pure poly(HEMA) and poly(EOEMA) polymer. Many solvents and their mixtures in different proportions (ethanol, acetone, chloroform, 1,2-dichloromethane, dichlorehthane) were used for preparation of nanofibers. The aim was to find a solvent, in which Hansen dispersion, polar and H-bonding parameters are
similar as in HEMA/EOEMA (30/70) co-polymer and pure poly(EOEMA). The solubility parameter for each component was estimated using the group contribution method described by van Krevelen (van Krevelen, 1972). As optimal composition of solvent mixture was confirmed a mixture of ethanol/2-isopropanol (50/50 wt). Effect of co-solvent induced different average fiber diameter or porosity of nanofibers.

Nanofiber sheets from HEMA/EOEMA were successfully electrospun using continual electrospinning process Nanospider and sheets were tested for proliferation of hepatocytes and mezenchymal cells.

![SEM micrographs of nanofiber sheets prepared (A) from copolymer HEMA/EOEMA (30/70) dissolved in ethanol with concentration 10 wt%, Mag.1000x, (B) copolymer HEMA/EOEMA (30/70) dissolved in the mixture dichlormethane /methanol (96/4 vol.) with concentration 10 wt %. Mag.10 000x.]

References
Synthesis, Characterization and Antibacterial Activity of Schiff-Base Ligand Incorporating Coumarin Moiety and Its Metal Complexes

Amel F. El Husseiny, Elham S. Aazam, Jemila Al Shehary

Chemistry Department, Faculty of Science, Girls Section, King Abdulaziz University, Jeddah, (SAUDI ARABIA)

Six transition M(II) complexes [where M = Cu(II), Zn(II), Cd(II), Co(II), Ni(II) and Pd(II)] of the organic ligand 4-methyl-7-(salicylidineamino)-coumarin HL have been synthesized and characterized by a variety of physicochemical techniques. An octahedral structure is proposed for the Cd(II) complex, a square planar for Co(II), Ni(II) and Pd (II) complexes while a tetrahedral structure for the Zn(II) complex. The ligand HL and its metal complexes are screened for their antimicrobial activities against A.niger fungi and E. coli bacteria. The studies demonstrated that metallation can increase the antibacterial activity rather than the free ligand. The Cd(II) complex exhibited the maximum bacterial inhibition, however, no significant antifungi activity of the organic ligand HL or its complexes were demonstrated.

References
Spectrophotometric Determination Pipazethate HCl and Dextromethorphan HBr Based on their Oxidation by Potassium Permanganate

Rabee. El-Hlag¹, Ayman. A. Gouda², Zeineb. El Shafey³, Nagda. Hossny³, Rham. M. El-Azzazy³

¹Chemistry Department, Faculty of Science, Al-Azhar University, Cairo, Egypt
²Chemistry Department, Faculty of Science, Zagazig University, Zagazig, Egypt
³Chemistry Department, Faculty of Science (Girls), Al-Azhar University, Cairo, Egypt

Rapid, simple and sensitive validated spectrophotometric methods have been described for the assay of pipazethate HCl (PiCl) and dextromethorphan HBr (DEX) either in pure form or in pharmaceutical formulations. The proposed methods were based on the oxidation of the studied drugs by a known excess of potassium permanganate in acidic medium and estimating the unreacted permanganate with amaranth dye (method A), acid orange II (method B), indigocarmine (method C), and methylene blue (method D), in the same acid medium at a suitable \( \lambda_{\text{max}} = 521, 485, 610 \) and 664 nm, respectively. Beer’s law is obeyed in the concentration range of 2-16 \( \mu \text{g mL}^{-1} \) with correlation coefficient \( (n = 6) \geq 0.9993 \). The molar absorptivity, Sandell sensitivity, detection and quantification limits were also calculated. Different variables affecting the reaction were studied and optimized. The proposed methods were applied successfully to the determination of the examined drugs either in a pure or pharmaceutical dosage forms with good accuracy and precision. No interferences were observed from excipients and the results obtained were in good agreement with those obtained using the official methods.
Synthesis of Thiazolone, Piperazinone and Benzopiperazinone derivatives from N-substituted maleimides

M. Amari\textsuperscript{a}, N. Khier\textsuperscript{a}, Y. Bentarzi\textsuperscript{b}, M. Fodili\textsuperscript{a}, B. Nedjar-Kolli\textsuperscript{b} and P. Hoffmann\textsuperscript{c}

\textsuperscript{a} Laboratoire de Chimie des Substances Naturelles, C. U. Djelfa, Algeria
\textsuperscript{b} Laboratoire de Chimie Organique Appliquée, Faculté de Chimie – USTHB – BP32, El-Alia, 16111 Bab Ezzouar, Algiers, Algeria
\textsuperscript{c} Laboratoire de Synthèse et Physico-Chimie de Molécules d’Intérêt Biologique, UMR 5068, Université Paul Sabatier, 118 route de Narbonne, 31062 Toulouse cedex 4, France

The piperazinone (2-oxopiperazine) and benzopiperazinone (1,2,3,4-tetrahydroquinoxalinone) ring structures possess a number of interesting biologically properties and constitute convenient conformationally constrained peptidomimetics, in which the two peptidic nitrogen atoms are linked in a constrained system by an ethylene bridge that preclude a free rotation of the peptide backbone [1]. A number of synthetic approaches [2-4], such as the condensation of organoboronic acids with 1,2-diamines [5], and solid phase syntheses [6] have been developed to access to piperazinone compounds. As part of our effort to study the reactivity of diamine derivatives in Mannich type reactions, we previously reported the synthesis of a series of benzimidazoles, benzimidazolones and benzodiazepines starting from \textit{o}-phenylenediamines [7]. Here the study is extended to the condensation of a series of 1,2-ethylene-diamines (EDA), \textit{o}-phenylenediamines (OPDA), and thioureas (TU) with \textit{N}-substituted maleimides leading to new piperazinone (2), benzopiperazinone (3) and thiazolone (4) derivatives, respectively.

References
Mass Spectrometry Study of Some Heterocyclic Compounds of Biologic Interest

O. Bouaziz, M. Fodili and M. Amari*

Chemistry Faculty, USTHB. BP 32 El-Alias, 16111 Bab Ezzouar, Algiers, Algeria,
* e-mail : mohadam2001@yahoo.fr

Currently the teaching and the development of the mass spectrometry must follow and must answer the different needs of users in varied domains such as medicine, biology, pharmacology, organic and mineral chemistry, electronics … etc.

The development of new systems heterocyclic, susceptible to present interesting pharmacological properties is a major preoccupation (1-4).

The identification of these molecules requires spectroscopic methods as NMR, IR, UV and mass of Spectroscopy. In this work, we chose to show the behavior of these biological interest molecules by mass of spectroscopy.

* Benzodiazepineses like tranquillizers, anxiolytic and antipsychotic [5].
* Benzimidazoles like anti-nématodose [6].
* Quinoxalines used in the treatment of the cancer [7].
* Piperazines like antihelminthiques [8].

Our survey is based on the teaching of propositions of the mechanisms of fragmentations to identify the structure of these compounds.

References:
Thermal Behaviour and Thermokinetic Studies of Co(II), Ni(II), Cu(II) and Cd(II) 1,2,4-Triazole-3-Thione Schiff Bases Complexes

M.A.El-Gahami, S.A.El-Gyar, A. Abd El-Sameh and S.A.Ibrahim

Chemistry Department, Faculty of Science, Assiut University, Assiut, Egypt. Email: elgahami@yahoo.com

1,2,4-triazole-3-thiones Schiff bases and their complexes have been reported to be biologically versatile compounds having bactericidal properties\(^{(1-3)}\).

Series of complexes of 1,2,4-triazole-3-thione Schiff bases with Co(II) Ni(II), Cu(II) and Cd(II) ions have been prepared according to procedure reported in the literature\(^{(4)}\). The structures of the complexes were determined by means of elemental analysis, molar conductance, magnetic measurements, infrared and electronic spectral data and thermal studies\(^{(4)}\). The thermal decomposition study of Co(II), Ni(II), Cu(II) and Cd(II) complexes was monitored by TG, DTG and DTA analysis in dynamic atmosphere of nitrogen. The thermal degradation takes place in three to five steps depending on the metal ion present. The decomposition course and steps were analyzed and the kinetic parameters: order of the decomposition reaction \((n)\), correlation coefficient \((r)\), activation energy \((E)\) and pre-exponential factor (collision factor) \((Z)\) of the non-isothermal decomposition steps were computed using Coats-Redfern\(^{(5)}\) and Horowitz-Metzger\(^{(6)}\) methods and discussed. Comparison of the two sets of kinetic parameters shows that deviation between them is not so great, considering the approximations involved in the Horowitz-Metzger method. Thermodynamic parameters: entropy \((\Delta S^\#)\), enthalpy \((\Delta H^\#)\) and Gibbs free energy \((\Delta G^\#)\) of activation, were calculated using standard relations\(^{(7)}\) and are discussed. The dehydration stability of the complexes increases in the order (Cu, Ni, Co) which is in accordance with both Irving-Williams order\(^{(8)}\) and the ionic volume of the metal ions\(^{(9)}\). The activation energies of the thermal degradation steps lie in the range 0.7-70.61 kJmol\(^{-1}\).

Fig.1. TG-DTG curves of \([\text{Cu(ABT)}_2 \cdot 2\text{H}_2\text{O}]\text{Cl}_2\) (nitrogen atmosphere)

Fig.2. Relationships between the initial dehydration temperature or activation energy and metal ion type of ABT complexes

Fig3: Horowitz-Metzger plots for the three decomposition steps\([\text{Cu(ABT)}_2 \cdot 2\text{H}_2\text{O}]\text{Cl}_2\)
   a) first step b) second step c) third step.
References


Synthesis of Trisubstituted Imidazoles Using Lewis and Bronsted Acid Catalysts

Rahim Hekmat Shoar, Hajar Jahanbakhshi, Maryam Farzaneh

Department of Chemistry, School of Science, Azzahra University, Vanak, Tehran, Iran

Imidazoles are common scaffolds in many biologically active compounds [1] and have attracted the attention of synthetic chemists for over a century.[2] Multi-substituted imidazoles have received significant attention as a result of their diverse medical uses.[3] Because of this, numerous classical methods for their synthesis have been reported.

In recent years, the use of solid acid catalysts [4] received considerable importance in organic synthesis. Such catalysts offer many advantages including: no need for solvents or the use of less toxic ones (e.g., hydrocarbons), milder reaction conditions, easier separation of the catalyst from the reaction mixture, and its possible regeneration and reuse, reducing the production of waste and thus harm to the environment.

An efficient and one-pot method for the preparation of trisubstituted imidazoles by condensation of benzil, different aldehydes and ammonium acetate in the presence of a catalytic amount of NiSO₄·7H₂O or H₃BO₃ under different conditions is reported.

References:
Electrochemical Synthesis of Copper Sulfide Nanoparticles

Lida Fotouhi and Maral Rezaei

Department of Chemistry, School of Science, Alzahra University. P.O.Box 1993891176, Tehran, Iran

Nanoparticles are important and versatile building blocks for the construction of functional nano-scale materials and devices [1], such as two- and three dimensional film assemblies [2] and designed colloidal aggregates [3] as well as nanoparticle-based photovoltaic [4] and sensing devices [5].

In this work we electrosynthesized Cu2S nanoparticles by cyclic potential within 0.10 to 1.50 V potential ranges in the presence of polyvinylalcohol (PVA) as stabilizer. The structure and nature of the resulting Cu2S-PVA were characterized by transmission electron microscopy (TEM) and X-ray diffraction (XRD). The results show that electrochemically synthesized Cu2S nanoparticles were homogeneously dispersed and well separated from one another with the mean diameter of about 12 nm.

References

Solvent-Free Synthesis of Xanthene Derivatives Catalyzed by Preyssler Type Heteropolyacid

Majid M. Heravi, Zohreh Daroogheha, Khadijeh Bakhtiari and Fatemeh F. Bamoharram

*a Department of Chemistry, School of Sciences, Azzahra University, Vanak, Tehran, Iran
*b Department of Chemistry, Azad University of Mashad, Mashad, Iran

Xanthene derivatives are very important heterocyclic compounds and have been widely used as dye fluorescent materials for visualization of bio-molecules and laser technologies due to their useful spectroscopic properties. [1] They have also been reported for their agricultural bactericide activity, [2] photodynamic therapy, [3] antiflammatory effect [4] and antiviral activity. [5]

The use of Heteropolyacids, HPAs, has recently received considerable attention as nontoxic, eco-friendly and environmentally benign catalysts for various organic transformations to afford the corresponding products in good yield.

We found that H$_{14}$[NaP$_5$W$_{30}$O$_{110}$] showed high catalytic activity and could be recovered and recycled several times without significant loss of activity.

\[
\begin{align*}
\text{H}^\text{14}[\text{NaP}_5\text{W}_{30}\text{O}_{110}] + 2\text{ArCHO} &\xrightarrow{\text{heat}} \text{ArO} + \text{MeO}\times\text{O} + \text{H}_2\text{O} \\
2\text{C}_6\text{H}_4\text{Me}_2\text{C}=\text{O} + 2\text{ArCHO} &\xrightarrow{\text{heat}} \text{ArO} + \text{MeO}\times\text{O} + \text{H}_2\text{O}
\end{align*}
\]

We have found a simple, convenient, straightforward and practical procedure for the synthesis of xanthene derivatives under solvent-free condition. Some advantages of this procedure are: 1) the experimental simplicity and the easy work-up procedure, 2) the compatibility with various functional groups, 3) use of the inexpensive, green, easy to handle and reusable catalyst, and 4) high yields of the products. Moreover, there is no need for dry solvents or protecting gas atmospheres.

References
Preparation and Characterization of Hydrogel Membranes Based on Crosslinked Chitosan and Blends of Chitosan/PVA for Industrial Depollution

Djamal Aliouche and Meriem Keddou
Laboratoire de Traitement et Mise en Forme des Polymères, F.S.I, M’Hamed Bougara University, Boumerdes, 35000, Algeria.
Email: aliouche_dj@yahoo.fr

Thanks to their good chemical stability, their film forming capacity and their absorbent character, the membranes of biopolymers were largely applied for the solutes diffusion and liquid separation. Among biopolymers, chitosan and poly (vinyl alcohol) are biocompatible and non-toxic, their membranes were developed for biomedical applications.

In this work, we carried out synthesis and preparation of hydrogel membranes of two types: initially glutaraldehyde crosslinked chitosan films then blend membranes of PVA/Chitosan at various percentages. All membranes were characterized by FTIR spectroscopy and SEM. Degradation and stability of membranes under UV light were studied using xenotest method. The membranes at high PVA rate show a better stability. The kinetics of swelling in water and in a physiological saline solution (0.9% NaCl) was studied for the whole of samples. A good absorbency was observed for all membranes.

Finally adsorption of a reactive dye (Bezaktiv Red) showed the capacity of the membranes for the depollution of textile wastes.
Storage of hydrogen molecules is a research topic that has deep scientific interests and enormous applications in providing a clean type of energy for the future. Probing further, we use density functional theory to study how the enclosed hydrogen molecules interact with the carbon cage. The possibility of the formation of endohedral complexes between H₂ & He and C₆₀ fullerene is discussed at the B3LYP and MP2 levels of theory using the 6-31G(d) basis set. The studied systems included benzene, bowl and fullerene. The HOMO–LUMO energy gap, ionization potential and electron affinity of studied compounds are reported and compared with experimental results. It was found that the computed electronic properties are significantly influenced by the shape and size of different host compound. The obtained results revealed that only one hydrogen molecule being incorporated inside the C₆₀ cage can form the stable complex in agreement with geometric considerations and recent experimental data.
The Synthesis of Novel Sulfamides and Cyclosulfamides Containing Phosphonate Moiety

Nadia Trad, Radia Bouasla, Malika Berredjem* and Nour-Eddine Aouf

Laboratoire de Chimie Organique Appliquée (LCOA), Groupe de Chimie Bioorganique, Faculté des Sciences, Université Badji Mokhtar. BP.12. 23000 Annaba-Algérie
E-mail: mberredjem@yahoo.fr

Phosphorus compounds containing the P-C bond are not particularly abundant in nature. Their diverse biological activity has for a long time attracted considerable synthetic and pharmacological interest. The Arbuzov reaction is regarded as the premier synthetic method in the preparation of phosphonates. This reaction is very versatile way to form P-C bond from the reaction of phosphte and halide.

In the course of our work on sulfamides and cyclosulfamides derivatives, we have prepared a number of phosphorus compounds, for which, in a recent study, biological activity properties as well as relationships between chemical structure/biological activities were investigated.

In this report we describe in detail the preparation and reactivity of sulfamides and cyclosulfamides containing phosphonate moiety starting from sulfonyl chloride and chloroethyl amine in mild conditions, then cyclisation with K$_2$CO$_3$. The obtained compounds 1 and 2 were treated by triethylphosphite to give phosphorylated compounds 3, 4 and 5.

The structures of all compounds and intermediates reported herein were unambiguously confirmed by usual spectroscopic methods: $^1$H, $^{31}$P and $^{13}$C NMR, MS and IR spectra.

References
Allylglycidylether Polymerization by Sacrificial Anodes

N-E. Djelali*, L. Daddi Oubekka

Laboratoire de Traitement et Mise en Forme des Polymères Fibreux (L.T.M.F.P.F), Université M. Bougara, Boumerdes, 35000, Algérie
E-mail: Djelnac@yahoo.fr

The cationic allylglycidylether polymerization reaction was initiated by some metallic cations obtained from sacrificial anodes (Al, Hg, V, and Cr). The reaction propagation took place even in presence of high concentrated solutions of the supporting electrolyte anions, but the anions have to be neither basic nor nucleophilic. The following anions PF$_6^-$, ClO$_4^-$, BF$_4^-$ were tested in this work. The polymers were analyzed and their weights measured. They are comparable with those obtained with other cationic polymerization methods.

Figure: Electrochemical behavior of metals in nitromethane containing 0.1 (nBu)$_4$NClO$_4$ on Pt (10 r.p.s) 1: Residual current; 2: Chromium; 3: Vanadium; 4: Mercury; 5: Aluminum.

References
Study of the Aluminum Cation Resulting from Anodic Dissolution in Non-Aqueous Medium

N-E. Djelali\textsuperscript{a}, L. Daddi Oubekka\textsuperscript{a}, G. Pierre\textsuperscript{b}

\textsuperscript{a} Laboratoire de Traitement et Mise en Forme des Polymères Fibreux (L.T.M.F.P.F), Université M. Bougara, Boumerdes, 35000, Algérie

\textsuperscript{b} Laboratoire d’Electrochimie Organique et de Photochimie Redox (L.E.O.P.R), Université J. Fourier, Grenoble, 38041, France

In this work, the oxidation degrees of the metallic cations electrochemically obtained in non aqueous media were determined with several methods: coulometry, gravimetry and atomic absorption spectroscopy. On the other hand, Al\textsuperscript{+} obtained is further oxidized into Al\textsuperscript{3+}.

\textbf{Figure 1:} Electrochemical behavior of metals in nitromethane containing 0.1 M(nBu)\textsubscript{4}NClO\textsubscript{4} on Pt (10 r.p.s) 1: Residual current; 2: Aluminum

\textbf{Figure 2:} Absorption curve, complex Al\textsuperscript{3+} - Aluminon \( \lambda = 530 \text{ nm} \); cuve: 2 mm; \([\text{Al}^{3+}] = [\text{Aluminon}] = 7.4\)

\textbf{Figure 3:} Al\textsuperscript{3+} Atomic Absorption curve
\textbf{a}: in H\textsubscript{2}O. \textbf{b}: in solution 2 % (CH\textsubscript{3}NO\textsubscript{2} + 0.1 M Bu\textsubscript{4}NClO\textsubscript{4}).

\textbf{References}

Quantum Chemistry Studies of O₃–H₂O₂ 1:1 Complexes

Hossein Roohi, Batol Makiabadi*

Department of Chemistry, Faculty of Science, University of Sistan & Baluchestan, P.O. Box 98135-674, Zahedan, Iran

Quantum chemical calculations were carried out for the O₃–H₂O₂ complexes in order to elucidate the structural characteristics and energetics of the complexes. Four complexes were found as stable structures of O₃–H₂O₂ by using B3LYP, MP2 and QCISD methods with a wide range of basis sets. The excitation energy of the O₃–H₂O₂ complexes was calculated using time-dependent density functional theory (TD-DFT). The natural bond orbital (NBO) analysis and the Bader's quantum theory of atoms in molecules (QTAIM) have been employed to elucidate the interaction characteristics of the O₃–H₂O₂ complexes. Two different intermolecular interactions were predicted that participate in the formation of complexes, namely: conventional O⋯H hydrogen bond and O⋯O contact. The NBO analysis shows that the electronic charge is transferred from O₃ to H₂O₂ in three complexes which have conventional hydrogen bond. The QTAIM results reveal that both intermolecular interactions have electrostatic character. The electron density, ρ, at O⋯H bond critical point is strongly correlated with the interaction energy and Fock matrix element Fij.
Synthesis and Characterization of some Co(II) and Ni(II) Complexes with 2-[(4-Aminophenyl)Imino]-1,2-Diphenyl-1-Ethanone

Abdusalam Hamil, Khalifa Mesbah, Amna Qasem and Arabya AbdelSalam

Chemistry department, Faculty of Science, Sebha University, Sebha Libya.
E-mail: abdsalam_1956@maktoob.com

The present work deals with the synthesis and characterization of the ligand 2-[(4-aminophenyl)imino]-1,2-diphenyl-1-ethanone and its complexes with Ni(II) and Cu(II). The synthesized complexes have been characterized by elemental analysis, electronic spectra, infrared spectra, nuclear magnetic resonance spectra and mass spectra. The metal-ligand ratio was found to be 1:1. A square planer geometry for both complexes was confirmed.
Ground water is the main source for drinking water in Hodeida city, Yemen. This study discusses the chemical and physical characteristics of nineteen ground water wells in the Al-baidh field. Thus, the measurement of water quality parameters (electrical conductivity EC, total dissolved solids TDS, pH, turbidity, color, total alkalinity, total hardness TH, NO₃⁻, SO₄²⁻, PO₄³⁻, Cl⁻, Na⁺, K⁺, Ca²⁺ and Mg²⁺ in addition to Mn, Cu, Fe and Cr) was conducted. The results indicate unacceptable levels of TDS, Cl⁻, Na⁺, Ca²⁺ and Mg²⁺ compared to the maximum tolerable concentrations given by the World Health Organization (WHO) and Yemen standards (YS). Moreover, the measurement of SO₄²⁻ and NO₃⁻ recalls values exceeding the allowable ones given by WHO and YS for most of the samples. This can be attributed to the nature of the geological and chemical structure of soil in Al-baidh field. The study included also measurements of the heavy element concentrations such as Cr, Fe, and Mn. The results show allowable values.
Removal of heavy metals from waste water is a major ecological problem (1). Chromium is present in different types of industrial effluents being responsible for environmental pollution (2). Chromium (VI) is much more toxic than chromium (III), due to both acute and chronic exposures hazards. EPA has classified chromium (VI) as a Group A, known human carcinogen by the inhalation route of exposure (3). Conventional methods for removing metals, such as chemical precipitation and sedimentation, oxidation, reduction, and separation by membranes and ionic resins may be expensive and some times ineffective depending on concentration (4). Biosorption is a process in which solids of natural origin are employed for binding heavy metals. It's a promising alternative method to treat industrial effluents mainly because of its low cost and high metal binding capacity (5). Bagasse, the fibrous material, is one of the main by-products of cane sugar manufacturing plants, which is obtained after the sugar juice is leached out of sugarcane. Removal of chromium (VI) from tannary waste by bagasse have been investigated in a batch system. The maximum removal was obtained after 3 hours. Optimum conditions were found to be (pH = 1, T=30°C, size = 0.7 mm) and chromium removal efficiency was found to be 94.25% in optimum conditions. Statistical studies on pH, temperature, size of particles of bagasse and residual chromium showed that pH and size had significant effects. The temperature effect was not as pronounced as the that of pH and size. The coefficient of determination (R2) of both Langmuir and Freundlich models were mostly greater than 0.9. This indicates that both models were valid for the experimental results. The results show that the sorption of the chromium ion on bagasse is of an exothermic nature. Characterization of biomass was carried out by FTIR spectroscopy, stability of bagasse compounds was determined before and after treatment.

References
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Quality Improvement of Recycled Chromium in The Tanning Operation by Fungi Biomass

K. Louhah*, N. Sahmoune, J. Addad, S. Barr

Laboratoire revêtement, matériaux et environnement Faculté des sciences de l’ingénieur
Université de BOUMERDES, 35000 boumerdes & ALGERIE
Email: louhab_ka@yahoo.fr

The leather industries produce daily large amounts of effluents highly contaminated by chromium salts. The use of sorption phenomenon, especially biosorption on dead residues of microorganisms produced by fermentation industries, can be an economical alternative method to depollute these effluents from heavy toxic metals. In this study we have investigated the adsorption capacity of Cr(III) present in the samples of effluents from a Algeria tannery by the mycelial by-products of filamentous fungi as Rhizopus arrhizus. Efficiency of metal ion recovery from metal-loaded biomass and subsequent regeneration of the biosorbent were also determined. The results show that, at pH 4.8, the biomass was able to adsorb 60 mg/g biomass while precipitation effects augmented these values at higher pH ranges. Adjusting the pH value to about 0 resulted in 95% and 90% recovery of Cr by using H₂SO₄ and HCl respectively. The biomass resulted from desorption processes was able to retain approximately 95% of original adsorption capacity for Cr with sixteenth repeated adsorption and recovery runs. The rate of elimination of the chromium in the effluent of the tannery is about 83% after the sixteenth cycle. The chromium recovered is reused in tannery for preparation of new tanning bath and the obtained results are similar to those obtained by the use of the conventional chromium.
A Follow-Up Study of Maternal Milk Contamination with Organochlorine Insecticide Residues

Firyal H. Abdul-Jalil Al-Obydi

Baghdad, Iraq, Email: Rolla_alazawi@yahoo.com

Contamination of human milk with residues of organochlorine insecticides represents a major environmental problem. Four mothers were the subjects of a 5-month follow-up study of the weekly variations in the levels of these pollutants in their milk. Residues detected and confirmed were those of γ-HCH, heptachlor, heptachlor epoxide, chlordane, aldrin, dieldrin and isomers and metabolites of DDT. Fluctuation in the residue levels was obvious due to variations in the daily dietary intake of residues and variations in fat content of maternal milk.
Leptin and some Biochemical Parameters in Goitrous Patients

Nahla Majeed Alsakkal

Department of Biochemistry, College of Medicine, Almustansiryah University
Baghdad, Iraq
Email: mnajjar818@yahoo.com

The results demonstrate disturbances in oxidation status in hypothyroid patients with abnormal lipid profile, which may indicate the association between oxygen derived free radicals increase in Sleptin concentration and incidence of obesity related diseases.
High Performance Liquid Chromatography Analysis of Phenolic Compounds, Amino acids and Minerals in Prosopis

Thabit Al-Azzawe

Department of Medical Biochemistry College of Medicine, Al-Mustansiriya University
Email: halla94thabit@yahoo.com

A general procedure has been fixed for the analysis of phenolic compounds by reversed phase-liquid chromatography with binary elution gradients of tetrahydrofuran (THF) and acidified deionized water (2% acetic acids). The method was applied to the separation and estimation of phenolic acids, tannin, phenolic aldehydes and coumarins from prosopis extract with detection limit of 0.1 mg/ml. Free amino acids were separated by reverse phase precolumn derivatization, using orthophthalaldehyde (OPA) derivative. Essential trace element was analyzed in the extracts.
Determination of Phthalate Esters in Jordanian Bottled Water by GC/MS and HPLC/UV

Yahya R. Tahboub, Mohammed F. Zaater and Ayman N. Al-Sayyed

Department of Applied Chemistry, Jordan University of Science and Technology
Irbid- 22110 Jordan
Email: tahboub@just.edu.jo

A reliable method was developed and validated for trace level analysis of six phthalate esters (dimethylephthalate (DMP), diethylphthalate (DEP), di-n-butylphthalate (DnBP), benzylbutylphthalate (BBP), bis(2-ethylhexyl)phthalate (DEHP) and di-n-octylphthalate (DnOP)) in drinking water. The method is based on liquid-liquid extraction with a mixture of petroleum ether and dichloromethane (80:20) and separation and detection with GC/MS and HPLC/UV. GC method involves a temperature program from 60°C to 280°C with a constant rate of 20°C for baseline separation and selected ion monitoring (SIM-MS) for detection. HPLC method involves a gradient program from water and acetonitrile for separation and UV detection at 235 and 280 nm. Runtimes were 17.0 and 30.0 minutes for both methods, respectively. Both methods were linear in the range 0.30 to 12 µg/L with average detection limits (LOD) of lower than 0.10 µg/L. Recoveries vary between 70% for DMP and 95% for DEHP. The method was applied for the analysis of phthalate esters in bottled water from Jordanian markets. Three phthlate esters, DnBP, DEHP and DnOP were detected with concentrations between 1.14-21.5 µg/L.
Perfluoroalkylation by Cross-Metathesis of Alkenes

Barbara Eignerová,a,b Martin Kotoraa,b

aDepartment of Organic and Nuclear Chemistry, Faculty of Science, Charles University, Hlavova 2030, 12843 Prague 2, Czech Republic
bInstitute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Flemingovo nám. 2, 16610 Prague 6, Czech Republic

A number of compounds with attached perfluoroalkylated chains exhibit interesting biological properties. Therefore, it is of general synthetic interest to develop new methodology that would enable to introduce perfluoroalkyl groups into various molecules under mild reaction conditions. Recently, it was shown that one such option is ruthenium catalysed cross-metathesis with perfluoroalkylated ethenes [1].

Currently, we are working on a related methodology that would allow the synthesis of arenes, ferrocenes, saccharides and steroids, bearing perfluoroalkyl substituents. Our procedure is based on the cross-metathesis of easily available 3-perfluoroalkypropenes with compounds having the terminal double bond. Effect of the substrate structure on cross-metathesis selectivity and reactivity and other mechanistic features will be presented.

\[
\begin{align*}
R^1 & \quad + \quad \text{Ru-cat} \\
& \quad \rightarrow \\
& \quad R^1 \quad R^2
\end{align*}
\]

\[R^1 = C_6F_{13}, C_3F_7, i-C_3F_7\]

\[R^2 = \begin{align*}
\text{Aromatic} \\
\text{Fe} \\
\text{OAc} \\
\text{OAc} \\
\text{OAc}
\end{align*}\]

References

Environmental chemicals are thought to adversely affect human reproductive function. Our objective is to estimate the concentration of cadmium (Cd), lead (Pb) and Zinc (Zn) concentration in serum and seminal plasma among infertile men. A sample of 70 infertile men was investigated. The relationship of trace elements concentration in serum and seminal plasma was studied in relation to sperm density, motility and sperm count. Except for Zinc, the concentration of (Pb) and (Cd) were generally higher in serum than in seminal plasma. The mean concentration of (Zn) in seminal plasma was more than 25 times higher than in serum. There were no statistical significant differences observed in the serum and seminal plasma levels of trace elements among the normospermic, oligospermic and azoospermic. It seems that no significant relationship between these trace elements and the clinical classification of the infertile men was noted. Without considering environmental conditions of life and work, way of nutrition, smoking and other possible factors, this study does not present great value.
Kinetic Study of Polyurethanes Formation by Using Differential Scanning Calorimetry

Wadie Sultan\textsuperscript{1}, Jean-Pierre Busnel\textsuperscript{2*}

\textsuperscript{1} Department of Chemistry and Chemical Technology, CST, Al-Quds University, PO Box 20002, Jerusalem
\textsuperscript{2} Polymères, Colloïdes, Interfaces, UMR CNRS, Faculté des Sciences, Université du Maine, 72085 Le Mans Cedex9, France

Kinetics of polyurethane formation between several polyols and isocyanates with dibutyltin dilaurate (DBTDL) as the curing catalyst, were studied in the bulk state by differential scanning calorimetry (DSC) using an improved method of interpretation. The molar enthalpy of urethane formation from secondary hydroxyl groups and aliphatic isocyanates is 72 ± 3 kJ/mole and for aromatic isocyanates it is 55 ± 2 kJ/mole. In the case of a single second order reaction for aliphatic isocyanates reaction, activation energy is 70 ± 5 kJ/mole with oxypropylated polyols and 55±3 kJ/mole with Castor oil. For aromatic isocyanates and oxypropylated polyols, the activation energy is higher around 77 kJ/mole.

In the case of two parallel reactions (situation for IPDI and TDI 2-4) best fits are observed considering two different activation energies.
The work deals with the synthesis of mono- and diarylidene cyclohexanone through the reactions of some aromatic aldehydes derivatives and cyclohexanone. The mechanism of the formation of the products was discussed. The structure of the synthesized compounds has been confirmed by analytical and spectral methods (C, H, N, I.R., $^1$HNMR and mass spectra). The biological activities of the resulting compounds indicate different effects on different kinds of bacteria.
Charge Transfer Complexes of some S-Methyl Heterocyclic Dithiocarbamate with $\pi$ and $\sigma$ – Electron Acceptors

Maher Mohamed Ahmed Hamed

Chemistry Department, Faculty of Science, Assiut University, 71516 Assiut, Egypt

Solid 1:1 CT complexes formed between some S- methyl heterocyclic dithiocarbamate (piperidine-, morpholino-, thiomorpholinodithiocarbamate, I–III respectively) and 2,3-dichoro-5,6-dicyano-1,4-benzoquinone (DDQ); tetracyanoethylene (TCNE) as $\pi$–electron acceptors and iodine as $\sigma$–electron acceptor are synthesized and characterized. Spectral characteristics and stability of the complexes are investigated and discussed in terms of donor molecular structure and the nature of the electron acceptor as well as the solvent polarity. It is deduced that the complexes are of weak n-$\pi$ or n-$\sigma$ type, where the sulfur thiocarbonyl group is the donor site responsible for such CT interaction\(^1\). The ionization potentials of the donors are calculated from the CT transition energies of their complexes. The obtained values can be compared with experimental data reported previously for related sulfur donors\(^3,4\).

\[
\begin{align*}
\text{X} = \text{CH}_2 (I), \text{O (II), S (III)} \\
\text{CT Complex}
\end{align*}
\]

References:
Synthesis and Spirocyclization of Some Analogs of Indole Phytoalexin Brassinin

Moussa Khlifa\textsuperscript{a} and Peter Kutschy\textsuperscript{b}

\textsuperscript{a} Sebha University, Faculty of Science, Department of Chemistry, Sebha Libya.
\textsuperscript{b} Department of Organic Chemistry, Institute of Chemical Sciences, Faculty of Science, P.J.Safarik University, Kosice, Slovakia
e-mail: khlifa72@yahoo.co.uk

Sulfur containing indole phytoalexins isolated from the plants of family Cruciferae, represent an interesting group of natural products because of their unusual structure and antimicrobial and antitumor activity.\textsuperscript{1,2} Spiroindoline representatives of this group of natural products were synthesized recently by spirocyclization of brassinin (1) and 1-methoxybrassinin (2).\textsuperscript{3}

In present contribution, the spirocyclization of amino analogs of 1-\((t\)-butoxycarbonyl) brassinin to diastereomeric products of the type \(I_a\) and \(I_b\) by dioxane dibromide and bromine mediated cyclization will be reported.

All the synthesized compounds were identified by \(^1\text{H}\)-NMR, \(^13\text{C}\)-NMR, mass spectra and elemental analysis.

\begin{center}
\includegraphics[width=\textwidth]{diagram.png}
\end{center}

References
Quantitative Determination of Fluoxetine in Pharmaceutical Formulations by Reversed-Phase Thin-Layer Chromatography

Ibrahim. A. Amar\textsuperscript{a}, T. Gondova\textsuperscript{b}, Abubaker. Sharif\textsuperscript{a}

\textsuperscript{a} Department of Chemistry, Faculty of Sciences, Sebha University, Sebha Libya
E-mail: ibr_amar@yahoo.com

\textsuperscript{b} Department of Physical and Analytical Chemistry, Faculty of Sciences, P.J. Safarik, University Moyzesova 11, SK- 040 01 Kosice, Slovak Republic

A simple, rapid, selective and precise PR-TLC densitometric method has been established for the determination of fluoxetine (FLX) in pharmaceutical formulations. The method employed RP 18-TLC plates with methanol-0.05 M phosphate buffer pH 5-triethylamine (68: 27: 5, v/v/v) as mobile phase. Densitometric analysis was performed in the absorbance mode at \( \lambda = 230 \) nm. The analytical method has excellent linearity \((r = 0.9993)\) in the working concentration range 100-1000 \( \mu g \) ml\(^{-1}\). The limits of detection and quantitation were found to be 163.5 and 545.7 ng per spot, respectively. The recoveries of fluoxetine in pharmaceutical formulations were 97.48 and 106.75\%. Statistical analysis proved that the method was precise and accurate for estimation of the drug.
Synthesis of 3-Hydroxy-Benzothiophene-2-Carboxamide Derivatives and Heterocycles Thereof

Tolaymat, I. and Geffken, D.
Institute of Pharmacy, University of Hamburg, Bundesstrasse 45, D-20146 Hamburg, Germany.

The benzothiophene moiety represents an important pharmacophore/toxophore in drug chemistry and agrochemistry[1-3]. We here report on the synthesis of novel derivatives of 3-hydroxy-benzo[b]thiophene-2-carboxamide by a facile and expedient protocol.

Successive reaction of 2-carboxymethylsulfanyl-benzoic acid methylester (1) with 1,1’-carbonyldiimidazole and various hydrazines or hydroxylamines provided 2A and 2B which upon Dieckmann reaction underwent cyclization to give N,N’-disubstituted 3-hydroxy-benzo[b]thiophene-2-carbohydrazides (3A) or N-alkoxy(araloxy)-3-hydroxy-benzo[b]thio-phen-2-carboxamides (3B), respectively in 65-87% yield. Ring closure of 3A/3B with 1,1´-carbonyldiimidazole or 1,1´-thiocarbonyldiimidazole occurred smoothly affording the novel oxazino-benzothiophene derivatives 4A and 4B in 75-90% yield.

\[
\begin{align*}
\text{O} & \quad \text{O} & \quad \text{S} & \quad \text{OH} \\
\text{O} & \quad \text{O} & \quad \text{S} & \quad \text{N} & \quad \text{H} & \quad \text{O} \\
\text{N} & \quad \text{R} & \quad \text{R} & \quad \text{O} & \quad \text{S} & \quad \text{N} & \quad \text{H} & \quad \text{O} \\
\text{N} & \quad \text{R} & \quad \text{R} & \quad \text{O} & \quad \text{S} & \quad \text{N} & \quad \text{H} & \quad \text{O} \\
\text{CDI} & \quad \text{THF} \\
\text{i : NaOMe / MeOH} & \quad \text{ii : CDI or TCDI / THF}
\end{align*}
\]

References:
Microwave Assisted Synthesis of 5-Functionalized 1,2,4-Triazolium Ylides

Khankischpur M.\textsuperscript{a} and Kurz, T.\textsuperscript{b}

\textsuperscript{a} Institute of Pharmacy, University of Hamburg, Bundesstrasse 45, D-20146 Hamburg, Germany. \textsuperscript{b} Institute of Pharmaceutical and Medicinal Chemistry, Heinrich-Heine University Düsseldorf, Universitätsstrasse 1, 40255 Düsseldorf, Germany.

1,1-Dialkyl-5-oxo-1,2,4-triazolium ylides have been described as herbicides and fungicides.\textsuperscript{1,2} Relatively few efficient synthetic strategies exist for the preparation of 1,1-dialkyl-5-oxo-1,2,4-triazolium ylides (2) and most of the reported methods are multi-step syntheses.\textsuperscript{2-5} To the best of our knowledge, only one 1,1-dialkyl-5-thioxo-1,2,4-triazolium ylide (3) has been documented in literature.\textsuperscript{3} We here report on a microwave assisted high yield preparation of 5-functionalized 1,2,4-triazolium ylides. The targeted compounds 2-4 have been obtained from the reaction of $N',N'$-disubstituted carbohydrazonamides (1) with 1,1'-carbonyl-di(1,2,4-triazole), 1,1'-thiocarbonyldiimidazole or diphenyl $N$-cyanimidocarbonate. The structure of previously unreported 5-cyanimino-functionalized 1,2,4-triazolium ylides (4) has been confirmed unambiguously by X-ray analysis.

\begin{align*}
\text{R}: \text{imidazole, 1,2,4-triazole, phenoxy}
\end{align*}

\begin{align*}
\text{1} & \xrightarrow{\text{microwave}} \text{CH}_2\text{Cl}_2 \\
2: X = O, & \quad 3: X = S, \\
4: X = N-CN
\end{align*}

\textbf{References:}
The Study of the Influence of Al-Lajoun Basin on Water Quality of Al-Mujeb Dam

Iyad A. Hailat, Waleed A. Manasreh

Department of chemistry, Mu'tah University, Al-Karak, Jordan 2008

Surface sediment and water samples were collected from different sites along Al-Lajoun basin and around Al-Mujeb dam. Content of total heavy metals (Fe, Cu, Zn, Ni and Cd) were determined using Atomic Absorption Spectrometry. The results indicate that there are elevated levels of Fe and Cd in sediment samples with 14340, 4.95 mg/kg respectively. The concentrations of Cu, Zn and Ni are 17.4, 86.6 and 37 mg/kg, respectively.

Based on the statistical analysis, it was concluded that the elevated concentrations of heavy metals are due to anthropogenic sources, especially Al-Lajoun wastewater treatment plant.

Water samples were analyzed for anions content (F⁻, Cl⁻, Br⁻, NO₃⁻, SO₄²⁻) using Auto-Suppressed Ion Chromatography and for Na⁺, K⁺ cations using Flame Photometer. Mg²⁺, Ca²⁺ were determined chemically using EDTA reagent.

The obtained results show that there are elevated levels of Chloride and Sulphate ions. These elevated concentrations are attributed to anthropogenic sources such as Al-Lajoun wastewater treatment plant and fertilizers. The concentrations of Ca²⁺ and Mg²⁺ ions are very high in water samples so that water is considered very hard.

References:
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New Route for Synthesis of Immunosuppressive Agent FTY720 and Its New Derivatives for Using in MS Therapy and Transplantation

Habibi Azizollah1*, Bayat Saadi1,2, Aghvami Madjid1, Hale Hamedifar2

1 Faculty of Chemistry Tarbiat Moallem University, No. 49, Mofatteh Street, Enghelab Ave. Tehran, Iran
2 Manager of Cinnagen Inco. No. 5 Street, Simin Dasht Industrial City, Malard Way, Karaj
* e-mail: habibi@tmu.ac.ir

FTY720 [(2-amino-2-(4-octylphenyl)propane-1,3-diol] 2 is a novel immunosuppressant for using in autoimmuno disease and transplantation [1-3]. This synthetic analogue of myriocin 1 reduces the number of blood lymphocytes by redirecting them to the lymph node. FTY720 is the first sphingosin-1-phosphate (S1P) receptor modulator. In multiple sclerosis (MS), Lymphocytes that circulate in the central nervous system (e.g. the brain and spinal cord) attack myelin sheath that surrounds and protect nerve fibers (axons). FTY720 inhibits lymphocytes (T,B cells) recirculating. Clinical results after using FTY720 showed that Fingolimode reduced the rate of relapses more than 50% and inflammatory disease activity as measured by MRI up to 80%.

In this article, derivatives of FTY720 such as H-d-Pro-FTY720, 3a; Boc-d-Pro-FTY720, 3b; H-d-Ala-FTY720, 3c; and Boc-d-Ala-FTY72, 3d; were synthesized for further pharmaceutical and neurological effect studies.
Liquid–Liquid Equilibria for Pseudoternary Systems: (Sulfolane + 2-Ethoxyethanol) + Octane + Toluene at 293.15 K

Akl M. Awwad\textsuperscript{a}\textsuperscript{*} and Amar H. Al-Dujaili\textsuperscript{b}

\textsuperscript{a}Industrial Chemistry Center, Royal Scientific Society, P. O. Box 1438 Al-Jubaiha 11941 Amman, Jordan

\textsuperscript{b}Department of Chemistry, College of Education, Ibn Al-Haitham, University of Baghdad, Baghdad, Iraq

Liquid-liquid equilibrium data, both binodal and tie-lines, are presented for the pseudo-ternary systems: \{(sulfolane + 2-ethoxyethano) (1) + octane (2) + toluene (3)\} at 293.15 K. The experimental liquid-liquid equilibrium data have been correlated using (NRTL) and (UNIQUAC) models, and the binary interaction parameters of these components have been presented. The correlated tie lines have been compared with the experimental data. The comparisons indicate that both NRTL and UNIQUAC models satisfactorily correlated the equilibrium compositions. The reliability of the experimental tie lines has been confirmed by using Hand correlation.
Synthesis, Characterization and Spectroscopic Investigation of Asymmetric Palladium PCP Pincer Complexes: \([\text{PdCl}\{\text{C}_6\text{H}_3\}(\text{CH}(\text{CH}_3)\text{PR}_2))\text{-2,6}\}], R=\text{Ph, Pr}\)

Ali Naghipour\(^a\), Zahra Haji Ghasemi\(^b\)

\(^a\) Department of Chemistry, Faculty of Science, University of Ilam, Ilam 69315, Iran
\(^b\) Department of Chemistry, Azad University of Ilam, Ilam, Iran

Corresponding Author E-mail: naghipour51@yahoo.com

Following our investigations on the application of homogeneous palladium catalysts to C-C bond forming reactions,\(^1\) we envisaged the preparation of new recyclable palladium PCP pincer complexes suitable for performing reactions at high temperatures. Among the palladium catalysts, palladacycles are a well studied class of highly active and thermally stable organopalladium complexes.\(^2\) Development of practical protocols for asymmetric synthesis of optically active compounds represents a great challenge in the area of chiral chemistry, in which the efficiency and the recycle of the chiral catalysts are key issues.\(^1-4\) Herein, we would like to report two new useful methods for the high yield synthesis of the asymmetric ligands \([\text{C}_6\text{H}_4\text{-1,3-((CH(CH}_3)\text{PR}_2))}_2\], R=\text{Ph} (1), \text{Pr}(2)\) and their palladium PCP pincer derivatives \([\text{PdCl}\{\text{C}_6\text{H}_3\}(\text{CH}(\text{CH}_3)\text{PR}_2))\text{-2,6}\}], R=\text{Ph} (3), \text{Pr}(4)\). The asymmetric PCP pincer ligands together with their palladium complexes, have been synthesized and characterized by \(\text{H}, \text{C}, \text{P}\)-NMR, Mass and C.H.N. analysis. In summary, the present poster represents two attractive and easy methods to perform methodology for the synthesis of asymmetric PCP pincer ligands and their palladium derivatives.

\[\begin{align*}
\text{PR}_2 & \quad \text{[Pd(COD)Cl]} \quad \text{Toluene} \\
\text{PR}_2 & \quad \text{Pd-Cl} \\
\text{R=Ph, Pr} &
\end{align*}\]

References
Synthesis, Characterization and Applications of New Palladium Pincer Complex in the Development of Homogeneous Catalytic Heck Coupling Reactions

Zahra Haji Ghasemi\textsuperscript{a}, Ali Naghipour\textsuperscript{b}

\textsuperscript{a} Department of Chemistry, Azad University of Ilam, Ilam, Iran
\textsuperscript{b} Department of Chemistry, Faculty of Science, University of Ilam, Ilam 69315, Iran

Transition metal complexes with pincer ligands have been prepared for numerous applications in the fields of catalysis, catalyst immobilisation, supramolecular assembly and sensor aterials.\textsuperscript{1} So far, most of the reported PCP pincer complexes are almost five-membered metalacycles, and there are few reported examples of pincer complexes with two six-membered metalacycles. Herein, first we report synthesis, characterization and spectroscopic investigation of unsymmetrical PCP pincer ligand \([\text{C}_6\text{H}_3-1-(\text{CH}_2\text{OPPh}_2)-3-(\text{CH}_2\text{OPri}_2)]\) and its palladium bis(phosphinito) PCP pincer complex \([\text{PdCl}\{\text{C}_6\text{H}_3-2-(\text{CH}_2\text{OPPh}_2)-6-(\text{CH}_2\text{OPri}_2)}\}], and then we deal the catalytic activity of the palladium PCP pincer complex with two six-membered metalacle \((\text{PdCl}\{\text{C}_6\text{H}_3(\text{CH}_2\text{OPet}_2)2,6}\}).\) The poster will show also the influence of various parameters such as type of aryl halide, base, mol\% of catalyst and solvent on the course of the reaction. The described catalyst has a very good catalytic activity in Heck coupling reactions. The results show that this complex is an ideal catalyst for coupling of deactivated and sterically hindered aryl chlorides and bromides as they are comparatively inexpensive, very easily synthesized and can be used to give high conversions at low catalyst concentrations.

\begin{center}
\begin{tikzpicture}
\node (x) at (0,0) [shape=circle,draw] {$X$};
\node (r) at (-1,-1) [shape=circle,draw] {$R$};
\node (r prime) at (1,-1) [shape=circle,draw] {$R'$};
\node (palladium) at (0,0) [shape=circle,draw] {$\text{Pd-Cl}$};
\node (phosphite) at (0,-1) [shape=circle,draw] {$\text{PPri}_2$};
\node (phosphinite) at (0,-2) [shape=circle,draw] {$\text{PPh}_2$};
\draw (x) edge (r prime);\draw (x) edge (r prime);\draw (r prime) edge (palladium);\draw (palladium) edge (phosphite);\draw (phosphite) edge (phosphinite);
\end{tikzpicture}
\end{center}

References

Analytical Study of Partially Treated Water of Commercial Stations in Hodeidah city

Mohammed Taher Majam, Badr. I. Abdul-Razzak*, and Atta. I.A

* Department of Chemistry, Faculty of Education, Hodeidah University, Yemen

This study includes the chemical and biological analysis of sixteen partially treated water stations spread in Hodeidah city of Yemen. The measurement of water quality (electrical conductivity (EC), Total dissolved solids (TDS), pH, alkalinity, total hardness (TH), NO₃⁻, SO₄²⁻, Ca²⁺, Mg²⁺, Na⁺, K⁺ and Cl⁻ content) were investigated. The results indicate that TDS of Alahlia, Almanahel, Alsalam and Tebaa are much less than the limits permissible by WHO for partially treated water. On the other hand, the results of the biological analysis show that water is within the limits permitted.
Microwave Irradiation for Accelerating the Synthesis of Heterocyclic Thioglycosides

Atta Ibrahim Atta

Medicinal Sciences College, Medicinal Laboratories, El Hodiedah University, P.O. Box 3114, Yemen- Hodiedah

Thioglycosides are important carbohydrate derivatives.\(^1\)\(^2\) There is an increasing interest in using them as glycosyl donors\(^3\)\(^4\), in addition of being promising candidates as carbohydrate mimics, potential therapeutics and enzyme inhibitors. In recent years, the use of microwave irradiation (MWI) in accelerating organic reactions is rapidly increasing due to induced short reaction times shortening, improved economic as well as environmental and operational aspects. In our laboratory, a wide range of organic reactions has been achieved using MWI. Thus, we found that the glucosyl isothiourea 1 and 2 can be successfully prepared using MWI as an energy source within 2 minutes. Reaction of 1 or 2 with different haloheterocyclic base 3 afforded 4 and 5 respectively within 4-8 min. The structures of the prepared compounds were confirmed by \(^1\)H NMR.

\[
\begin{align*}
1 & \quad Y = O \\
2 & \quad Y = NH
\end{align*}
\]

\[
\begin{align*}
3 & \quad Y = O \\
4 & \quad Y = O \\
5 & \quad Y = NH
\end{align*}
\]

References:
Approaches to Functionalized PAMAM Dendrimers

Muhanna Kamal Al-Muhanna

King Abdulaziz City for Science and Technology, Riyadh, Saudi Arabia

The primary aim of the project is to investigate the synthesis and surface functionalisation of a series of PAMAM-like dendritic macromolecules with the long term objective of preparing and developing some novel potentially bioactive compounds based on dendritic macromolecules and nanoparticles.

A number of PAMAM dendrimers has been prepared in which the core is either α, ε-diamine (NH₂(CH₂)NH₂) where 2 ≥ n ≥ 12.[1]

Dendritic macromolecules are branched structures that can be synthesised by convergent, divergent, or combinational methods.[2] There has been much interest recently in the synthesis of dendrimers containing functional cores. These include polyethylenimine dendrimers derived from a simple ammonia as well as linear polyamine cores, hydrocarbon dendrimer starting with either benzene or triptycene as interior core, polyamido alcohol dendrimer or arborols with trisbromomethylbenzene as a core, and resorcinol-derived “calixarenes”.[3] In this study a number of PAMAM dendrimers has been synthesised by convergent method in which the core is either α, ε-diamine (NH₂(CH₂)NH₂) where 2 ≥ n ≥ 12. Moreover, the synthesis of oligocalixarenes can be the first step en route to the calixarene cored-dendrimers. Calixarenes has been used for the preparation of dendrimers using the divergent method, up to the fifth generations in which the surface is covered with 64 amine groups. Calixarenes are cyclic oligomers {[1n]metacyclophanes} readily accessible by the condensation of resorcinol and an aldehyde under the basic conditions and easily functionalised in a selective manner. They have been used in supramolecular chemistry as a building block for larger and more sophisticated molecular systems.

In addition, the study the carbohydrate-carbohydrate interactions that occur between sugar groups attached to the surface of dendrimers and other sugar moieties present in solution was aimed. Many biological processes are regulated by sugars. The attachment of certain carbohydrates to the surface of dendrimers has really attracted much interest.[4] The modification of various functional groups on the surface of the dendrimers can lead to changes in some of the properties of such groups as a consequence of co-operative effects. Biological systems can identify numerous examples of molecular recognition processes enhanced by multiple interactions within the molecule.[5] For example, the carbohydrate-protein interactions which involved binding of saccharide ligends by protein receptors can be improved significantly by the clustering of the saccharide structure. Therefore, in this project

![Diagram of a dendrimer](image)
glucosyl sugar residues to these amine cored dendrimers have been successfully carried out and the resulting novel “sugar balls” characterized by a variety of spectroscopic techniques.

In the present work with a number of PAMAM dendrimers have been synthesised with different \( \alpha, \omega \) diamine cores, but using ethylene diamine and methylacrylate as extension units, in some cases up to and including the fifth generation. The use of calixerene as a dendrimer core has also been studied. Each of these materials has been fully characterised by a variety of spectroscopic techniques. The attachment of a glucose sugar residue to the outside surface of the PAMAM dendrimers has been successfully carried out.

References:
Arylselenotrimethylsilane as Efficient Arylselenating Agents in the Synthesis of Gold-Selenolate

Deeb Taher a and John F. Corrigan b

a) Department of Chemistry, Tafila Technical University, Tafila, Jordan.
b) Department of Chemistry, The University of Western Ontario, London, Ontario, N6A 5B7 Canada

Homobimetallic gold-selenolate complexes of structural type \([R_3PAuSe(C_6H_4)_nSeAuPR_3]\) (3a, \(R = EtPh_2, \ n = 1\); 3b, \(R = EtPh_2, \ n = 2\); 5a, \(R = Ph_3, \ n = 1\); 5b, \(R = Ph_3, \ n = 2\)) are accessible by the reaction of \([R_3PAuCl]\) (1, \(R = EtPh_2\); 4, \(R = Ph_3\)) with 0.5 equivalent of \(Me_3SiSe(C_6H_4)_nSeSiMe_3\) (2a, \(n = 1\); 2b, \(n = 2\)) in high yield. Complex 8b can be prepared in a two-step synthesis procedure. Reaction of \([AuCl(SMe_2)]\) (6) with \(Me_3SiSe(C_6H_4)_2SeSiMe_3\) (2b) gives \([(Me_2S)AuSe(C_6H_4)_2SeAu(SMe_2)]\), which further reacts with \(PPr_3\) (7) to afford \([PPr_3AuSe(C_6H_4)_2SeAuPPr_3]\) (8b). The new gold-selenolate complexes have been characterized by multinuclear NMR (\(^1H\), \(^{31}P\), \(^{77}Se\)) and elemental analysis. The solid state structures of 3a, 5a and 8b are determined by single X-ray structure analysis.
Polyaniline / Polyurethane Binary Blends DC Conductivity

L. A. Al-Baqeen(a), H. A. Alsalahat(b) and H. Gahnm(c)

a Jordan-Jerash, Jerash Private University, Department of Science, Faculty of Agriculture and Science, E-Mail: lamiabq@yahoo.com.
b Jordan-Alkarak, Mu'tah University, Department of Chemistry, Faculty of Science, E-Mail: salah@yahoo.com.
c Jordan-Irbid, Jordan University of Science And Technology, Department of Physics, E-Mail: hmel@just.edu.jo

Thin films of Polyaniline (PAN), and binary blends of Polyaniline / Polyurethane (PU) and Polyaniline/Polyurethane anionomers were prepared by casting from N-Cyclohexyl-2-Pyrrolidinone, and N-Methyl-2-Pyrrolidinone solution. HCl doped films are semiconductors with activation energy less than (0.30 eV). The DC conductivity of PAN blended with Polyurethane anionomers is more than that for pure PAN film (6.47x10^{-7}) S/cm, while it is the least for PAN blended with polyurethane PU 4/1, (1.18x10^{-10}) S/cm. HCl and water evolved from doped films at temperature above 70°C in case of PAN/Pu, while it is above 100°C for PAN / PU anionmer blends.
New Monoterpenes from the Jordanian Medicinal Plant *Varthemia Iphionoides*

Mahmoud. A. Al-Qudah\textsuperscript{1} and Musa. H. Abu Zarga\textsuperscript{2}

\textsuperscript{1}Department of Chemistry, Faculty of Science, Yarmouk University, Irbid- Jordan
\textsuperscript{2}Department of Chemistry, Faculty of Science, University of Jordan, Amman- Jordan

Two new monoterpenes, trans-varthemic acid (1) and cis-varthemic acid (2), were isolated from the aerial parts of *Varthemia iphionoides* (Compositea family), in addition to β-stigmasterol, 3-oxocostusic acid, velutin, Jeceidine, kumatakillin, penduletin, vanillic acid, 5,7,4\textquotesingle-trihydroxy-3,3\textquotesingledimethoxyl flavone, luteolin-3\textquotesingle-methyl ether, 5,7,4\textquotesingle-trihydroxy-3-methoxyflavone and β-sitosteryl glucoside. Structural elucidation was performed mainly by means of UV, IR, MS and (1D &2D) NMR spectroscopy.

![Structural formula of trans-varthemic acid (1)](image1)

![Structural formula of cis-varthemic acid (2)](image2)
Synthesis, Characterization and DFT Calculation of Ruthenium (II) Azoimine-Diphosphine Mixed-Ligand Complexes

Mousa Al-Noaimi, Musa I. El-Barghouthi, Mohammad El-Khateeb, Obada S. Abdel-Rahman, Helmar Görls and Robert J. Crutchley

Novel family of the general type cis-[Ru(II)(dppe)LCl2] {L= C6H5N=NC(COCH3)=NAr, Ar= 2,4,6-trimethylphenyl (L1), 2,5-dimethylphenyl (L2), 4-tolyl (L3), phenyl (L4), 4-methoxyphenyl (L5), 4-chlorophenyl (L6), 4-nitrophenyl (L7), 2,5-dichlorophenyl (L8); dppe= Ph2P(CH2)2PPh2} have been synthesized. These complexes have been characterized through analytical, spectroscopic (IR, UV/vis, and NMR) and electrochemical (cyclic voltammetry) techniques. In addition, complex 4 (where L = L4) has been further characterized by X-ray diffraction analysis. The molecular and electronic structures of all complexes have also been studied by means of density functional theory (DFT) calculations. Crystallographic, electrochemical, electronic spectral data and time-dependent DFT calculations are all consistent with azomethine ligands possessing strong π-acceptor properties. These π-acceptor properties can be “tuned” by a judicious choice of substituents on the azomethine ligand.

References
1. Al-Noaimi, M.; El-Barghouthi, M.; El-khateeb, M.; Abdel-Rahman, O.; Görls, H.; Crutchley, R. Submitted to polyhedron
Antidiabetic and Antihyperlipaemic Effects of Aqueous Neem (Azadirachta Indica) Extract on Alloxan Diabetic Rabbits

Khalil Abdullah Khalil

Faculty of Medical Sciences, Dept. Medical Laboratories, Hodeidah University, Yemen
Khalil_bioc@yahoo.Com

Extracts of various plants material capable of decreasing blood sugar have been tested in experimental animal models and their effects confirmed. Neem or Margose (Azadirachta Indica) is an indigenous plant believed to have antiviral, antifungal, antidiabetic and many other properties. This paper deals with a comparative study of effect of aqueous Neem leaves extract alone or in combination with glibenclamide on alloxan diabetic rabbits. Administration of crude aqueous Neem extract (CANE) alone (1.5 ml/kg/day) as well as the combination of CANE (1.5 ml/kg/day) with glibenclamide (0.25 mg/kg/day) significantly decreased (P<0.05) the concentrations of serum lipids, blood glucose and lipoprotein VLDL and LDL, but significantly increased (P<0.05) the concentration of HDL. The change was observed to be significantly greater when the treatment was given in combination of CANE and glibenclamid than with CANE alone.
Synthesis, Characterization and Anti-HIV and Antitumor Activities of New Coumarin Derivatives

Yaseen A. Al-Souda, Haitham H. Al-Sa’doni, Houssain A. S. Amajaour, Kifah S. M. Salih, Mohammad S. Mubarak, Najim A. Al-Masoudi, and Ihsan H. Jaber

\textit{a} Department of Chemistry, College of Science, University of Al al-Bayt, Al-Mafraq, Jordan \\
\textit{b} Department of Chemistry, College of Science, University of Jordan, Amman, Jordan \\
\textit{c} Formerly Fachbereich Chemie, Universität Konstanz, D-78457 Konstanz, Germany

A new series of coumarin and benzofuran derivatives were synthesized as potential non-nucleoside reverse transcriptase inhibitors (NNRTIs) by reacting, separately, 4-bromomethylcoumarins, their sulphonyl chlorides, and ethyl 3-(bromomethyl)-6-methoxy-1-benzofuran-2-carboxylate with different imidazoles and their benzo analogues. The antiviral (HIV-1, HIV-2) properties of the newly synthesized compounds were investigated \textit{in vitro} and all compounds were found to be inactive, except 10 which showed inhibition of HIV-2 with EC50 > 0.51 \textmu g\text{mL}^{-1}. The \textit{in vitro} cytotoxicity of 17 and 19 was assayed against a panel of tumor cell lines consisting of CD4 human T-cells.
In this study, the fluorescence of plasticized and non-plasticized poly (para-methoxystyrene) solid films was measured. Strong excimer fluorescence and weak monomer fluorescence were observed.

Thermal degradation of this polymer was investigated in this work. Thermal heating of the non-plasticized and plasticized poly (para-methoxystyrene) at temperature range below their transition temperatures, causes a thermal quenching of the polymeric fluorescence as well as thermal degradation of the used polymers in solid films. To speed up the thermal degradation from these polymers, solid films were heated for several hours at the following temperatures 323, 343 and 353 K. As a result of this heating, a change in the polymer fluorescence spectral structure was obtained, also a gradual disappearance in the excimer fluorescence of the polymer was observed. Thermal degradation of poly (4-methoxystyrene) and plasticized poly (4-methoxystyrene) with dimethyl terephthalate were verified using infrared spectroscopy upon heating at 353 K for 48 hr.