

Lectures

*Analytical
Chemistry*

Soft-Modeling Curve Resolution Methods: Advantages and Disadvantages

Hamid Abdollahi

Faculty of Chemistry, Institute for Advanced Studies in Basic Sciences, IASBS, Zanjan, Iran

The soft-modeling analysis or soft modeling of multivariate data has been a core area of research in chemometrics for many years [1]. Its principles are astonishingly simple: the analysis based on the decomposition of a matrix of data into the product of two smaller matrices which are interpretable in chemical terms. Generally, one resulting matrix is related to the concentrations of the species involved in the process and the other matrix contains their response vectors. Typically, but not exclusively, we deal with multivariate spectroscopic data of a series of solutions; the spectra are written as rows of a data matrix \mathbf{D} of dimensions $n_{\text{spectra}} \times n_{\text{wavelengths}}$. According to Beer-Lambert's law \mathbf{D} can be written as a product of two matrices, $\mathbf{D} = \mathbf{C} \mathbf{A}$, \mathbf{C} containing as columns the concentration profiles of the species, giving it the dimensions $n_{\text{spectra}} \times n_{\text{species}}$, and \mathbf{A} containing as rows the molar absorptivities for the species as the measured wavelengths, giving it the dimensions $n_{\text{species}} \times n_{\text{wavelengths}}$. Soft-modeling analysis of such a data matrix \mathbf{D} consists of decomposing the matrix into the product of the two meaningful matrices \mathbf{C} and \mathbf{A} . However, the computed matrices \mathbf{C} and \mathbf{A} will generally not be chemically meaningful, i.e., they may contain elements or combination of elements that are not possible. There are natural restrictions that always apply to the matrices \mathbf{C} and \mathbf{A} ; almost universal is the restrictions that allelements have to be positive (≥ 0). Other restrictions apply for certain cases, e.g., concentration profiles in chromatography are always unimodal; in certain cases model-based restrictions to some concentrations can be imposed [2,3]. Generally, there are no restrictions in addition to non-negativity that apply to the spectra in the matrix \mathbf{A} other than possibly prior knowledge about one or more spectra. The crucial question is whether these restrictions are sufficient to impose a unique solution, and, if not, what are the ranges of feasible solutions, what are possible concentration profiles and absorption spectra that fulfill all conditions? However, applying the soft-modeling methods in analyzing the chemical data have some advantages and also disadvantages. Several basic researches and applications of soft-modeling methods have been done [5-9] in recent years in our research group which will be presented briefly in this conference.

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Plasmonic Nanomaterials: Why Should Analytical Chemists Care?

M.Reza Hormozi-Nezhad

Chemistry Department, Sharif University of Technology, Tehran, Iran.

Gold and silver nanoparticles which known as 'plasmonics nanoparticles' are a class of nanomaterials which have become widely studied because they exhibit intense size dependent optical properties. The bright colors in nanoscale noble metal particles are due to the collective oscillations of electrons in the conduction band that are excited by light of appropriate frequencies. These oscillations are termed "plasmons" or, more precisely for colloidal metal nanoparticles, localized surface plasmon resonances (LSPRs). The physical phenomenon of plasmons has helped to enhance methods of chemical analysis in recent decades, even to the point where it is possible to detect a single molecule. Though many of these methods have not yet found their way into traditional chemistry classes and labs, it is likely that many of today's chemistry and biochemistry majors will encounter plasmon-based techniques in their future. In this presentation, we examine recent advances in chemical analyte detection using gold and silver nanoparticles, with a primary focus on our own works

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Ion Mobility Spectrometry (IMS): Instrumentation and Application

M. T. Jafari

Department of Chemistry, Isfahan University of Technology, Isfahan 84156-83111, Iran

About 40 years ago, ion mobility spectrometry (IMS) under the name of "plasma chromatography" has been introduced for the trace detection of organic compounds by Karasek [1]. IMS is an accepted analytical method for determining the identity and concentration of trace substances such as explosives, chemical weapons and illicit drugs. Portability, speed, low cost, ease of maintenance, and low detection limits (~ ppb) are luring scientists to IMS. The advantage of IMS related to mass spectrometry (MS) is that IMS can be used for separation of ions under atmospheric pressure and this ability is achieved on the basis of the ion shape in addition to the ion mass and charge which are used in MS. Therefore, IMS can help users distinguish between isomeric species which it can be considered as a particularly important feature in proteomics research [2]. Ionization source is one important part of an ion mobility spectrometer which produces ions at ambient pressure. While investigations on the ion source of IMS date back to long time ago, research in this field has revitalized due to its wide range of applications especially in security organization, biological science, as well as medical applications. A variety of ionization sources including nickel (^{63}Ni), corona discharge, photoionization, electrospray ionization, and very recently low temperature plasma have been used for IMS [3-5]. The growing interest in IMS development warrants an update on the technique and its potential for environmental and medical analysis in the 2010s.

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Applied Analytical Chemistry

K.Kargosha

*Chemistry and Chemical Engineering Research Center of Iran, Tehran, P.Box. 14335-186.
< K.Ksrghosha @ccerci.ac.ir >*

Our society is changing from an industrial age, which emphasizes material, to an informational age, which emphasizes information. In this sense, Analytical chemistry is basically changed during past ten years. This means that analytical chemistry will be in a position to produce information production in the information period, corresponding to its material production in the industrial period. Nowadays these information are being produced by Academic Analytical Chemistry and Applied Analytical Chemistry (AAC). Process analytics and Industrial analytical Chemistry can be included as two principal parts of AAC. When process Analytical Chemistry (PAC) or process Analytical Technology (PAT) began some 70 years ago [1], it was largely for problem solving purposes as well as a way to determine the composition of the desired products in the process. Recently [2] PAT and PAC are defined as: - a system for the analysis and control of manufacturing Chemical process based on timely measurements of critical quality parameters and performance attributes of raw materials and in-process materials. - a process to ensure acceptable end-product quality of the completion of the processing. PAT involves, the optimal application of process analytical chemistry (PAC) tools, feedback process-control strategies and information management tools and/or product process optimization strategies for the manufacture of chemicals. PAT focuses on the principles of building quality into the product and process as well as continuous process improvement. The chemical industries has seen great change in recent years, responding to the shifts in consumer preferences, environmental pressures, the availability and cost of raw material and energy, demographic and social trends, and the overall economic and political situation worldwide. The annual growth of these industries reflect impressive development in process, formulation and application. In this impressive development and great change, the Industrial Analytical Chemistry has played a key role.

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Recent Trends in Electrode Modifications & Some Application

M. F. Mousavi

*Department of Chemistry, Tarbiat Modares University, P.O. Box 14115-175, Tehran, Iran
mousavim@modares.ac.ir, or mfmousavi@yahoo.com*

Employing nanoscience, nanotechnology, biotechnology and nanobiotechnology in preparation of modified electrodes has opened up a new horizon [1-3]. Modified electrodes with new trends have found wide spread applications including flow [4] and batch systems e.g. for electrocatalysis [5], batteries [6, 7], supercapacitors, supercapacitor-battery hybrid energy storage system, nanobiosensors [8] and ion transport & electron studies [9, 10]. In this talk after a brief overview of this issue, the ability of recent achievements in preparation of modified electrodes and surface modifications, along with some of our new findings will be discussed.

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Applications of DNA and Antigen Electrochemical Sensors for Medical and Environmental Analysis

Ali A. Ensafi

Department of Chemistry, Isfahan University of Technology, Isfahan 84156-83111, Iran.

Molecular detection has shown a great potential for rapid identification of diseases and for food and environmental monitoring. In recent years there has been an increase in the use of nucleic acids as a tool in the recognition and monitoring of many compounds of analytical interest. Nucleic acid layers combined with electrochemical transducers produce a new kind of affinity biosensor [1]. An interesting application of a DNA biosensor will be the testing of water, food, soil, and plant samples for the presence of analytes (carcinogens, drugs, mutagenic pollutants, etc.) with binding affinities for the structure of DNA. The DNA-trapped compounds can either be detected directly if they are electroactive molecules or via changes in electrochemical DNA signal [2]. The most promising biosensor technologies already finding their ways into the market include electrochemical, optical, and acoustic wave sensing technologies. Recent developments in nanotechnologies have helped the manufacturing of materials used in new devices with special capabilities due to their nanostate [3]. The claim is not far from reality that nanotechnology is making its way towards manufacturing ultra-sensitive devices for highly selective detection of biological molecules and toxic agents or systems with therapeutic targeting and screening applications. The compounds that play an important role in the identification and monitoring of critical compounds are nucleic acids [4]. Electrochemical techniques can be considered for the determination of pharmaceutical compounds as a strong alternative to the other instrumental methods. These techniques are very interesting tools for the analysis of many substances at trace level. The sensitivity and selectivity of the

electroanalytical response depend on the characteristics of the probe. There are a multitude of strategies that can be exploited for molecular detection. However, what determine the optimal solution are the functional objectives of the device that may include such goals as the achievement of the highest sensitivity possible cost minimization, or the yielding of a most mobile platform for rapid and easy-to-read results. Immunosensors (which are based on immobilization of a specific antibody on nanoparticles) or electrochemical and optical DNA biosensors are fast and inexpensive tools for drug determination [5-8]. These consist of layer immobilized over an electrochemical or optical transducer for the recognition of a nucleic acid (or a specific antibody). This layer detects changes occurring in the DNA structure while interacting with DNA-binding (or antibody-antigen) molecules [9-11]. It is the promising functions and biological activities of the interactions between nucleic acid-binding molecules and antibody-antigen that have given rise to a recently growing interest in their electrochemical and optical investigations due to. The present survey is an attempt to provide an exhaustive understanding of the versatile mechanisms that currently dominate research in DNA-based nanosensors and antibody-antigen nanosensors.

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Application of Nanostructured Materials in Preparation of Electrochemical Sensors

Saeed Shahrokhian

*Department of Chemistry, Sharif University of Technology, Tehran, Iran
Institute for Nanoscience and Nanotechnology, Sharif University of Technology, Tehran, Iran*

Electrochemical sensors and biosensors have been widely used to detect various substances due to their high sensitivity and desirable selectivity in their responses. Moreover, simplicity of surface modification of electrodes is one of the exciting developments in the field. Modification can improve the surface state of the electrode, which may lead to a significant reduction of the overpotential and increasing the rate of electron transfer process. Electrochemical sensors based on carbon nanotubes (CNTs) represent a new and interesting alternative for quantification of different analytes. Since the discovery of multi-walled carbon nanotubes (MWCNTs) by Iijima (1991) and the related single walled types (SWCNTs) in 1993, these materials have attracted enormous interest because of their unique structural, mechanical and electronic properties. Some of these properties include high chemical and thermal stability, high elasticity, high tensile strength, and in some instances, metallic conductivity. Many studies have demonstrated that the list of unique features of carbon nanotubes could be extended to include the electrocatalytic properties of carbon nanotube modified electrodes. One of the major problems in preparing sensors based on the use of CNT is their poor solubility in common solvents, which diminish the uniformity and reproducibility of the CNT film on the surface of the modified electrode. In this sense, several strategies have been proposed for immobilization of CNTs on electrochemical transducers. Some of these relied on dispersion of CNTs in special solvents, polyelectrolytes, Nafion and surfactants. The problem of agglomeration and poor dispersion of CNTs in ordinary solvents can be minimized through chemical modification or functionalization of CNT surfaces. Although such treatments cause changes in delocalized π orbital systems of CNTs, the resulting modified nanotubes are well dispersed in various solvents and form uniform and stable thin films at the surface of modified electrodes. In recent years, metal nanoparticles have attracted attention in electroanalysis because of their unusual physical and chemical properties. Metal nanoparticle-modified electrodes usually exhibit high electrocatalytic activities towards compounds with sluggish redox processes at bare electrodes. An interesting class of CNT derivatives is obtained by depositing metallic or semiconducting nanoclusters on the tubular surfaces. Such nanoparticulate hybrid materials made from inorganic solids and CNTs are highly promising for wide applications in nanoscale devices and nanoelectronics. Furthermore, uniform dispersion of metallic nanoparticles immobilised on CNT surfaces can yield ideal nanocatalysts for application in chemically modified electrodes. In this presentation nanocomposite-based modified electrodes prepared by incorporation of metallic nanoparticles decorated on carbon nanotubes at the surface of the carbon electrodes are described in electroanalysis of some biologically important compounds.

Multiphysics modeling for research and education in electrochemistry

Abolfazl Kiani

*Department of Chemistry, University of Isfahan, Isfahan
<http://sci.ui.ac.ir/~kiani>, a.kiani@chem.ui.ac.ir*

The main challenging issue in teaching electrochemistry is presenting unobservable concepts such as double layer, diffusion layer, the nature of diffusion (linear, spherical, ...), current and potential distribution in electrochemical cell and so on. On the other hand extracting kinetics and mechanistic information, getting quantitative insights from practical electrochemical data and designing new electrochemical methods is main duty of a researcher in the field of electrochemistry. The rate of an electrochemical reaction is affected by the rate of mass transfer, charge transfer and possibly homogenous chemical reactions. One can write coupled differential equations describing these phenomena and solve them analytically for simple electrochemical systems such as step potential experiment at a planner electrode. However, equations describing the physics and chemistry of a complex electrochemical system are extremely complicated and, in general, only a numerical solution of these equations is possible. With the development of computer technology, modeling has been more and more widely used in many fields of science including electrochemistry. There are some user friendly electrochemical simulation software such as Digisim[®] and DigiElch[®] which one can use for simulation in electrochemistry. They are easy to use but limited to some predefined geometries and postprocessing is rigid. Application of COMSOL[®], a general purpose software for solving many types of partial differential equations based on finite element method, has been recently introduced for modeling electrochemical systems. COMSOL[®] offers a complete modeling environment that allows one to perform all the steps in the modeling process. It could be used for any user defined geometry without need to strong computer programming background. The use of COMSOL[®] can help one visualizes

solutions and see how parameter and boundary conditions changes affect concentration profile and their corresponding fluxes for study and design of practical electrochemical systems. In this lecture, different approaches to solve mathematical equations describing electrochemical problems would be reviewed to understand the basic concepts of modeling. The details of the multiphysics modeling of electrochemical processes would be discussed. Finally, the use of COMSOL[®] multiphysics for modeling some electrochemical experiments would be illustrated; beginning from simple and ending with complex geometry. I hope this lecture will show how the efficiency of teaching and research in electrochemistry could be improved using multiphysics modeling.

Developments in hollow fiber based liquid-phase microextraction: Principles and Applications

Yadollah Yamini*

Department of Chemistry, Tarbiat Modares University, P.O. Box: 14115-175, Tehran, Iran

Liquid-phase microextraction with porous hollow fiber (HF-LPME) offers efficient alternatives to classical sample preparation techniques due to permission of high selectivity and high enrichment factors, as well as giving good possibilities for automation. In this methodology, target analytes are extracted from aqueous samples into a supported liquid membrane (SLM) sustained in the pores in the wall of a small porous hollow fiber, and further into an acceptor phase (aqueous or organic) present inside the lumen of the hollow fiber. After extraction, the acceptor solution is directly subjected to a final chemical analysis by high performance liquid chromatography (HPLC), gas chromatography (GC), capillary electrophoresis (CE), electrothermal atomic absorption spectrometry (ET-AAS) or inductively coupled plasma (ICP). This method could be performed either in the 2- or 3-phases modes. In the 2-phases mode, the organic solvent presents both in the porous wall and inside the lumen of the hollow fiber. In three phases mode acceptor phase can be aqueous resulting a system compatible with high-performance liquid chromatography or capillary electrophoresis, or the acceptor solution can be organic providing a system with two immiscible organic solvents compatible with all instruments without any limitation [1]. In three phases HF-LPME the mechanism for mass transfer of the analytes can be passive diffusion or active transport and high extraction yields as well as efficient extraction kinetics are obtained by application of a pH gradient, carrier transport and electrical potential across the supported liquid membrane [2]. HF-LPME has mostly been performed in static mode, but several studies in dynamic mode and also some automated techniques have been published both in the 2- and 3-phases modes [3]. In the dynamic process, extraction is performed by automatically movement of the organic acceptor phase in the lumen of HF using a programmable syringe pump. The dynamic HF-LPME has provided better extraction efficiency and improved reproducibility in lower extraction time as compared with the static modes. In the present speech all of the results that have been obtained since 2006 in our research group about different modes of HF-LPME will be presented.

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Coupling of micro-extraction methods with spectroscopy instruments: developing and Innovation

Farzaneh Shemirani

School of Chemistry, University College of Science, University of Tehran, Tehran, Iran

One of the problems in analytical chemistry is the direct measurement of the analyte due to matrix effects. In order to overcome this problem developing instrumental and pre-concentration methods are considered. Both developed in our research group have been considered. In recent decades, pre-concentration methods have been studied considerably. One of the oldest methods of extraction is liquid-liquid extraction with the high consumption of organic solvents. Today, in order to eliminate or reduce the use of solvents, microextraction methods such as liquid phase microextraction (LPME), Solid phase microextraction (SPME) and, etc. have been developed. In our Research Laboratory of Analytical Chemistry in University of Tehran, environmentally friendly extraction methods in order to increase preconcentration factor, extraction efficiency, user health and cost of the experiment was developed. The first reports of coupling DLLME based on organic solvents with a spectrophotometer UV_VIS and DLLME based on ionic liquids was developed in our Research group. A new homogeneous liquid liquid microextraction technique based on ILs termed cold induced aggregation microextraction (CIAME) was developed. Another interesting mode of homogeneous liquid–liquid microextraction (HLLME) based on ILs termed in situ solvent formation microextraction (ISFME) was also introduced by our group. In comparison with DLLME, no pure disperser solvent is used, which can reduce the extraction recovery. Furthermore, in order to have a cloudy system no syringe is required. With the development of nano-particles, we used magnetic nano particle, mesoporous, alumina and sulfur to increase the absorption capacity of the analyte in the sample. Develop micro-extraction techniques in biological samples using quantum dot nanoparticles of cadmium selenite is now being investigated. In the development of instrumental, a home-made microsample introduction system was used for aspiration of the extractant phase in FAAS, manufacturing thermal lens spectroscopy and use of optical fiber in UV-VIS is considered.

*Applied
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Chemistry
Education*

Research and Trends in Chemical Education

Abed Badrian

Research Institute for Education, Tehran, Iran

E-mail : ab.badrian@gmail.com

Chemistry education (or chemical education) is a comprehensive term that refers to the study of the teaching and learning of chemistry in all schools, colleges and universities. Topics in chemistry education might include understanding how students learn chemistry, how best to teach chemistry, and how to improve learning outcomes by changing teaching methods and appropriate training of chemistry instructors, within many modes, including classroom lecture, demonstrations, and laboratory activities. There is a constant need to update the skills of teachers engaged in teaching chemistry, and so chemistry education speaks to this need. Research in chemistry education was a young branch on the tree of human knowledge, much younger than research in modern chemistry. For researchers, information about the current status and trends of research in their fields is helpful for their career and academic publications. There are many journals where papers related to chemistry education can be found or published. In the field of chemical education, there has already been some systematic investigation of the research papers published in academic journals. Therefore, to provide deeper insights into research trends within a longer period, a follow-up study concerning nationality of author, research type, and research topic may be helpful [1],[2]. This study conducted a series of content analyses of the published articles. A systematic investigation of the nationality of authors who contribute to academic research, and a careful analysis of the research types and topics currently published by major journals, may provide more information about the growing internationalization in this field and be beneficial to contemporary science educators by enabling them to examine research trends.

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Content Organization of the Current High-school Chemistry Textbooks is the Result of a Revolutionary Action in the Performing of the Chemistry Curriculum

Nematollah Arshadi

Department of Chemistry, Faculty of Sciences, Zanjan University, Zanjan, Iran

narshadi@email.com

Designing effective content for each course area textbooks requires attention to both organization of the content and the instructional strategies. Content should be organized to show relationships among factual information, concepts, thoughts, and theories and so on. Since, efforts for realization of the national and international goals such as creating sustainable development, global citizenship education, etc., through different approaches have been the main concerns of the curriculum planners, content organization has known as a very appropriate tool to address the concerns. Content arrangement or organization that is an intelligent combination of knowledge, art and innovation, is the most determinative step in the textbook design. The step can be at least guaranteed the attainability of educational objectives in theory. The content reduction and organization of the high-school chemistry textbooks in Iran has known as a revolutionary action in the last decade. Although , it seems that so far it has not led to the desired results. Chemistry (I) textbook that is titled as "Chemistry for Life" was the first product of this action. The details of this unique sample including the main advantages and disadvantages of its revolutionized content organization will be presented and discussed. Also some more important barriers and several ways to improve qualitatively the content organization methods will be reviewed.

Chemistry, University, Industry, Challenges and Working out the Problems

Mahmoud paykary

Petroleum University of technology

Nowadays most of the chemists incorporate in the laboratory and use the fixed instructions in their experiments. They do not pay attention to the mechanisms of works carefully, neither do they have good efficiency as the result of having poor background and lack of motivation. Usually these persons are not important in industries and they are not well-known in comparison with many other fields. The graduations of this major are not family with the standard books and instructions and they do not have information about the way of using them. Chemists must pay attention to the following two points for being successful in different industries.

1. Educational materials must be compiled in a way that industrial basic points or similar issues in industrial units are taken into consideration to satisfy the needs of industrial units and they should clarify the guidelines for students and alumnus.
2. The chemists themselves should take actions and make efforts to find the shortages using potential powers. Also they have to decrease the challenges by studying more.

Designing: Studying on the design of each industrial unit, all of the substantial points, benefits, limitations, and shortages will be clear and the viewpoints of experts concentrate precisely on the priorities and important objects, underlying the success of individuals.

- a) **Exploitation:** the important points about advantages and disadvantages of exploitation, efficiency of system, advantages and limitations of exploitation procedures.
- b) **Use of Reference Books:** including the laboratory standards, books, instructions, mechanisms, and selection the best method in the experiments, precision in measuring, sensitivities of lab methods and the velocity of experiments.
- c) **Optimization:** the optimization of system should be suggested according to studies of planning, exploitation of laboratories, and by observing the feasibility assessment and economic studies.
- d) **Suggestion:** In order to develop the system, you can study more and prepare the reports if you like.
- e) **Energy Consumption:** Calculation of the energy balance-sheet is necessary for all of the industrial units including the consumption of fuels, water, power, steam, heat transfer, efficiency of system, efficiency of each part, the strong and weak points of system, advantages and limitations about efficiency, wasting the energy and resolving the deficiencies.

Observing the following points the chemists are not only lab technologists, but they are considered as the knowledgeable experts and supervisors. The other important subject is about management and macro planning: In this direction we suggest make a responsible organization for programming of human resources and interested persons are attracted to the universities. So their interests would not decrease and creative interested experts are trained. In the mean time the costs of studying for associate degree is 40,000,000Rls, for bachelor degree is 100,000,000Rls, for master degree is 110,000,000Rls, and for PhD is 400,000,000Rls.

Lack of precise programming cause many problems like:

1. Lack of use of efficient manpower.
2. Enormous public and private entrepreneurship without considering job market.
3. Hiring manpower without considering proper efficiency.

Comparative Advantage of the Chemical Industry in Iran and Justifications for its Development

K. Karimian

Arasto Pharmaceutical Chemicals Inc. Yusefabad, Jahanara Ave, 23rd St., No 8, Tehran 1438933743 Iran

Developing countries commit most of their financial resources to the development of industrial or agricultural segments in which they have comparative advantages. Geography and abundance of natural resources are the primary determinants in comparative advantage. Iran's proven organic natural resources are immense, second in natural gas and fifth in oil in the world. Iran also occupies 4% of the globe's land surface and therefore has also immense inorganic resources. Furthermore, because of a century-old industrial tradition in petrochemicals, nearly all equipment needed in the chemical industry are domestically designed and manufactured, including glass-lined reactors. Finally, nearly 65% of all scientific literature emanating from Iran is in chemistry and its related fields. In short, the 3Ms (material, manpower, machinery) required for the rapid development of any industry are available in abundance for the chemical industry in Iran. Unfortunately, little attention has been paid to Iran's comparative advantage in the chemical industry since the arrival of the first modern factory in Iran in 1840 during the administration of Mirza Taghikhan Amirkabir, namely the sugar factory of Ray. The result is the importation of billions of dollars of chemicals as pharmaceuticals, foodstuff, paints and resins, fertilizers, insecticides, pesticides, additives and detergents annually when Iran should be a major exporter of these commodities. Unfortunately, Iran's economic planning in the past two centuries has been, for the most part, myopic in vision, shallow in depth and narrow in width. Iran's under-developed chemical industry can be rapidly developed by avoidance from rhetoric and analysis of the present realities on domestic and global levels. To this end, the first step in the rapid development of the Iranian chemical industry is the gathering of data on domestically produced and imported chemicals by the Ministry of Industries, the Iranian Chemical Society and various syndicates representing the chemical sector. The second step is an in-depth analysis of the imported chemicals that can be manufactured from domestically manufactured building blocks (e.g. benzyl alcohol from toluene). Inadvertently, this will expand the base of the domestically manufactured chemicals, which themselves can be used to produce more complex molecules (e.g. benzyl acetate from benzyl alcohol and acetic acid). The Iranian Chemical Society can be made responsible for this study. The selected products can be distributed to universities as M.Sc. projects to graduate students in Industrial Chemistry and Chemical Engineering for process development and optimization and equipment design. The total package can be assigned to the Ministry of Industries as Amayesh Projects to identify interested investors from the private sector. The above proposal will create a dynamic and focused research environment which will succeed due to the fact that every project is market-oriented and every product has a guaranteed sale. Clearly, this will rapidly lead to the production of more complex molecules, which can be exported on a global scale. Such proposals will only succeed if government involvement is kept to a necessary minimum and within the framework of regulatory issues.

The Role of Chemistry "In Detergent Industries"

Azra Araghi

Paksan Co., Tehran, Iran

Soap is the first cleaning product known to the civilization all over the world. Gauls, Egyptian, Sumerian and Persians, for a long period used to make Soap by heating wood ashes in oil or "Trona" as natural soda ash with fat, and use it as a lux, expensive product for cleaning, cosmetic, even pharmaceutical. At the end of 18th century the efforts of chemists turned "Soap" into an everyday product for everyone. Addition Silicate and carbonate in soap making was the first revolution followed by second one, "alkyl naphthalene sulfonate" as the first created synthetic surfactant in the world. "BASF"'s chemists created this first synthetic surfactant, which had very poor wetting and detergency due to short carbon chain. In Next Steps, researching chemists succeeded to produce "butylester sulfonate" from castor oil, and then fatty alcohol sulfates which was the first real surfactant born into the world of surfactants. During the II world war by force of circumstance researchers turned their attention from animal or vegetable fat and oils to petroleum derivative resulted ABS and then LABS" still the most important surfactant, with wide application field up to now. Other surfactants, Anionics, Nonionics, Cationics and Amphoterics now are very well known and have different application in many industries. (short discussion regarding their chemistry & application). Many other chemicals than surfactants are discovered by chemists and introduced to be added into different products formula. Every chemical has appropriate duty and effect to improve product's appeal or performance. From second world war up to now detergent formulation and their physical forms had so many progressing, with some sophisticated formula in shadow of chemistry. Powder H.D or L.D. in other words T.D or NTD, liquid detergents, Tablets, many other forms of products for special purpose could be found in the market all based on surface activity, wetting, dispersing, foaming and at the end, cleaning, the main goal for producing and using detergents.

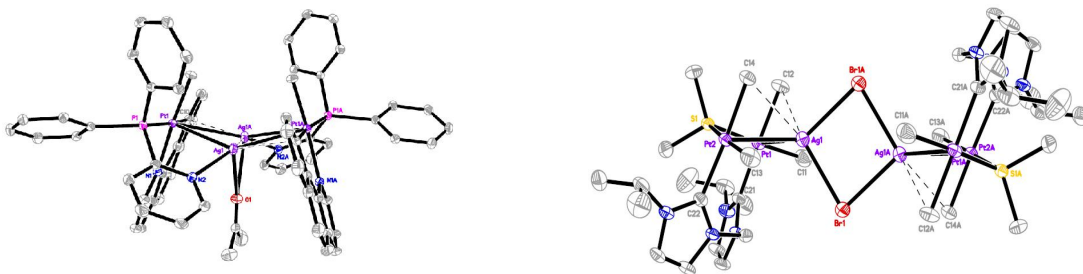
Inorganic Chemistry

Metal-metal bonding interactions in homo- and hetero multinuclear complexes containing platinum and closed shell metals (Au, Ag and Tl).

Sirous Jamali,* Zahra Mazloomi, Halimeh Abdolahi, Reza Ghazfar

Chemistry Department, Sharif University of Technology, PO Box 11155-3516, Tehran, Iran.

The study of metal-metal bonding in molecules occupies a prominent position in chemistry. Metal-metal bonding interactions play a vital role in many areas such as, cooperative reactivity, multicenter catalysis and metal-rich nanomaterials.¹ The development of synthetic approaches towards heterometallic structures is particularly attractive because of the increased challenges compared to homometallic structures and their possible relevance to modeling of interactions between substrates and alloy surfaces. Electron-rich platinum(II) complexes can expand opportunities for the formation of metal-metal dative bonds. The electron donor ability of a Pt(II) center containing a N-heterocyclic carbene and cyclometalating ligands, e.g., 2-phenylpyridine (ppy) or benzo{h}quinoline (bhq), is significantly enhanced, and this would assist in its ability to form Pt-M dative bonds. Also, it has been demonstrated that metal-metal-bonding interactions in cooperation with bridging ligands, such as bis-(phosphines), usually favor the formation of bi- and multinuclear complexes. These findings as well as our interest in synthesizing multinuclear complexes led us to incorporate appropriate bridging and electron donating ligands into one Pt(II) center and use them as precursors in the synthesis of new bi- and multi-heteronuclear complexes. Herein we describe preparation and structural characterization some of these multinuclear complexes (Figure).



Acknowledgment: Sharif University of Technology and Iran National Science Foundation are acknowledged for financial support.

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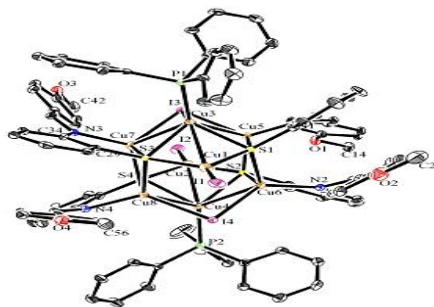
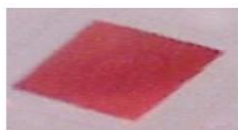
Unexpected Chemical Reactions Their Impact on the Advancement of Coordination Chemistry

Mehdi Amirasr

Department of Chemistry, Isfahan University of Technology, Isfahan, 84156-8311 Iran

amirasr@cc.iut.ac.ir

Currently, the approach to the synthesis of new material is the rational design of compounds with desired target properties. However, there are many cases that the chemical reactions lead to unexpected results which open up new avenues of research. For example, Rosenberg's serendipitous discovery of the anticancer activity of cisplatin, cis-Pt(NH₃)₂Cl₂ (Rosenberg et al., 1965) [1], initiated the development of metal based drugs as chemotherapeutic agents. These drugs are basically metal complexes with a capacity to bind nucleobases in DNA and cleave the DNA molecule hydrolytically or oxidatively [2]. Unexpected results in the field of bioinorganic chemistry, medicine, catalysis, chemistry of advanced functional materials, molecular machines and switches, etc. are numerous [3]. Solid state substitution, solvent substitution during cyclic voltammetric studies, hydrolytic cleavage of coordinated unsymmetrical Schiff base, and modification of the coordinated ligands are examples of unexpected reactions that we have observed in our research projects at IUT [4-6]. In this seminar, a brief discussion on the impact of unexpected reactions on the advancement of coordination chemistry will be presented.



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New Insights into The Chemistry of Phospha(III/V)zanes Compounds and Complexes

Abbas Tarassoli

Department of Chemistry, College of Science, Shahid Chamran University Ahvaz, Iran
(Email: tarassoli@scu.ac.ir)

Phosphorus and nitrogen form compounds of greater structural diversity than any other two elements in the periodic table. Of these compounds, phospha(III/V)zanes are known as an established system of P-N bonds and lie at the interface between organic and inorganic chemistry. The principal starting material for phospha(III)zanes is $(C_6H_5NH)_3P$ (**1**), that is prepared in very good yield by the reaction of PCl_3 with $C_6H_5NH_2$, upon which further synthetic, structural and bonding studies can be based. Thus, (**1**) is easily converted to $[(C_6H_5NH)_2P]_2NC_6H_5$ (**2**), $[(C_6H_5NH)PNC_6H_5]_2$ (**3**), $[(C_6H_5NH)PNC_6H_5]_3$ (**4**) and $[(C_6H_5NH)P_2(NC_6H_5)_2]_2NC_6H_5$ (**5**) by thermolysis and aniline elimination in a condensation reaction at suitable experimental conditions. Molybdenum complexes $[P(NHPh)_3]_2Mo(CO)_4$ (**6**), $PhN[P(NHPh)_2]_2Mo(CO)_4$ (**7**) and $[(i-PrNH)_3P]_3Mo(CO)_3$ (**8**) are synthesized and fully characterized from the reactions of these ligands with norbornadiene- $Mo(CO)_4$. The employment of phospha(III)zanes (**2**) to (**5**) for Pd(II)-catalyzed Heck-coupling reactions as both ligand and base under base-free conditions in water have also been extensively investigated and reported recently. Phosphazanes substituted with chalcogens (O, S or Se) have also prompted inorganic chemists interest in studying their coordination chemistry. We have been interested in studying those categories of P(V)-N derivatives containing oxygen because of their ease of synthesis and stability. $(C_6H_5NH)_2P(O)H$ (**9**) is prepared by the controlled hydrolysis of (**1**) or (**2**) and it has employed as a ligand. The coordination chemistry behavior of (**9**) with Al, Si, Sn, Ti, Zn and Pt has been extensively examined and the new resulted products were fully characterized. The elimination of two aniline molecules from (**9**) in the condensation reaction leads to the formation of P(V)-dimer, $[(\mu-NC_6H_5)P(H)=O]_2$ (**10**). Compound (**10**) is a very stable solid, a P_2N_2 ring with two P(O)H moieties which is the first example of P(V)-dimer and it has the potential to act as a precursor for obtaining new P-N macrocycles and complexes. The main starting material for Phospha(V)zanes is $N_3P_3Cl_6$, one of the most well studied inorganic ring systems, largely due to development of polymeric substances. $N_3P_3Cl_6$ reacted with 2,3-di(o-hydroxyphenylene)quinoxaline in the presence of a base to yield a new complex. Two diorganotin adducts with four pyrazolyl substituents have been synthesized based on functionalized $N_3P_3Cl_6$ -scaffolds. New organotin(IV) complexes with a potentially multi-sites ligands are also prepared based on the cyclotriphosphazane platform. The reaction of long-chain oxodiamines with $N_3P_3Cl_6$ lead to macrocyclic host molecules, whose conformation, cavity size and number of coordination sites depend on experimental conditions. The reaction of $N_3P_3Cl_6$ with three equivalents of salen has also been investigated and the *spiro* and *ansa* products have been characterized.

Crystallography under very Extreme Conditions: Photocrystallography, a case study on linkage isomerism

Reza Kia

Department of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran

Visiting scientist at the University of Bath & Daresbury synchrotron, station 9.8 (Crystallography and Photocrystallography), UK

E-mail: zsrkk@yahoo.com

Among the crystallographic approaches under extreme conditions such as "light-induced", "high-pressure", "very-low temperature", "under electric-field", and "high-temperature", light-induced or photocrystallography bring the fourth dimension, time, into the crystallographic analysis which makes a molecular movie in the solid-state. So, it breaks the limitations in routine-structure determination which considers time-averaged data. In photocrystallography or time-resolved X-ray diffraction, crystallographic and spectroscopic techniques are combined to pursue reaction of the solid state. Although the term photocrystallography was only coined in 1997 by Coppens, light-induced reactions in solids have been observed since the turn of the 20th century. As recalled by Schmidt in a review of photodimerization in the solid state, the field of light-induced reactions in solids went through a "heroic" era, in which physical methods for characterizing the internal structure of crystals were completely non-existent. A strong concerted effort to exploit the new crystallography to gain insight into chemical reactivity in the solid state was made by Schmidt and co-workers, starting in the 1960s. In this talk after a short review of crystallography under extreme conditions, more focus will be on photocrystallography in details. A comprehensive case study on linkage isomerism in single-crystal to single-crystal transformation of some Ni(II) complexes will be discussed which has done by the author in Daresbury synchrotron at station 9.8 in UK.

Recent progress in nanostructure metal oxide semiconductor thin films and their applications

Mohammad Hossein Habibi

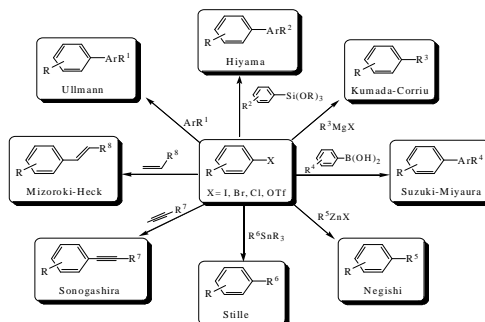
Department of Chemistry, University of Isfahan, Isfahan, 81746-73441 I.R. Iran

The aim of this paper is to present results of investigation of different metal-oxide semiconductor for application in photo-catalysis. Metal-oxide semiconductors are, today, the most promising materials for solar energy. We are working in two directions: (1) investigations of nanostructure metal oxide semiconductors thin films with the aim of optimizing their parameters and (2) investigations of new stable materials of semiconductor with visible light sensitization. The purpose of the present paper is to briefly summarize our results obtained in the last four years. As starting materials for the fabrication of nano-size semiconductor made of oxides, TiO_2 , ZnO , Nb_2O_5 , and their doped or hybrid oxides and materials have been prepared in our laboratory. Different technological methods for the preparation of nanostructure metal oxide semiconductor thin film were proposed and investigated. The effect of different parameters e.g. preparation method, coating technique, preheating, calcination temperature and dopant were investigated by X-Ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), transmission electron microscopy (TEM), atomic Force Microscopy (AFM), cyclic voltammetry (CV), energy-dispersive X-ray spectroscopy (EDAX), scanning electron microscope (SEM), ultra-violet diffuse reflectance (UV-DRS) and thermogravimetry thermal Analysis (TG-DTA).

Recent Progress in the Palladium-Catalyzed C-C Coupling Reactions

Shirin Nadri, Ezzat Raffie, **Mohammad Joshaghani***
Faculty of Chemistry, Razi University, Kermanshah, Iran
Email: mjoshaghani@razi.ac.ir

The Nobel Prize in Chemistry 2010 was awarded jointly to Richard F. Heck, Ei-ichi Negishi and Akira Suzuki for "palladium-catalyzed cross couplings in organic synthesis". This was the third Nobel Prize during this decade awarded for the application of platinum-group metals in organic synthesis and revealing the importance of this matter. Metal-catalyzed cross coupling reactions are extensively employed in a wide range of areas of organic synthesis [1], from the synthesis of complex natural products to materials science and supramolecular chemistry. The general scheme of these reactions is shown in Scheme.



Herein we present the latest finding in the palladium-catalyzed C-C coupling reactions particularly, according to mechanistic point of view.

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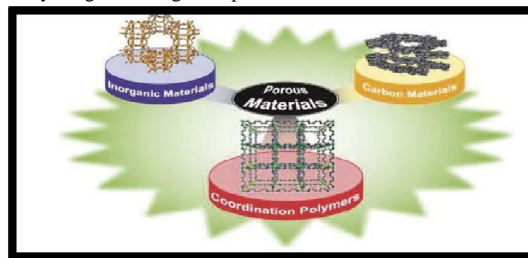
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Metal-Organic Frameworks; A New Class of Nano Porous Materials

Ali Morsali

Department of Chemistry, Faculty of Sciences, Tarbiat Modares University, P.O. Box 14115-175, Tehran, Islamic Republic of Iran

Porous materials, which have been either organic or inorganic, are very useful compounds in gas storage, adsorption based gas/vapor separation, shape/size-selective catalysis, drug storage and delivery, and as templates in the preparation of low dimensional materials.¹ Up to two decades ago, porous materials consist of activated carbons and inorganic porous frameworks, but now coordination polymers have taken an important position in the porous-materials area and added a new category to the conventional classification.^{1,2} Activated carbons do not possess ordered structures. Inorganic frameworks also suffer from a lack of diversity, as the variation of elements used seldom deviates from Al, Si and chalcogens. In order to take advantage of the properties of both organic and inorganic porous materials, porous coordination networks, also known as metal-organic frameworks (MOFs) or porous coordination polymers (PCPs), can be generated.¹ These materials are stable, ordered and possess high surface area and pore volume.³⁻⁵ The difference in nomenclature merely reflects the type of framework and the researchers who constructed it. This new class of materials shows high promise in gas storage and separation applications as well as in catalysis, gas-sensing, and photovoltaics.^{2,6-8}



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Metalloporphyrins in Organic Syntheses

Majid Moghadam

Department of Chemistry, Catalysis Division, University of Isfahan, Isfahan 81746-73441, Iran

Catalytic oxidation of hydrocarbons by oxo metalloporphyrins, in which the metal possesses high oxidation number, has attracted much attention by mimicking the function of monooxygenase enzymes like cytochrome P-450. In presence of single oxygen donors such as

iodosylbenzene, hypochlorites, amine *N*-oxides, alkyl hydroperoxides, hydrogen peroxide and sodium periodate [1-3], natural cytochrome P-450 and metalloporphyrin complexes are able to oxidize organic compounds. Homogenous metalloporphyrins readily undergo decomposition during the oxidation reaction, which leads to the formation of μ -oxo catalytically inactive dimers in solvent. Hence immobilizing these expensive catalysts on to a solid organic or inorganic support can overcome this problem [4, 5]. Although the reactivity of this heterogenized catalyst is less than the homogenized counterpart, but recovery and reusability of the catalyst makes it cost effective. Despite several reports on the application of metalloporphyrins in the oxidation of organic compounds, there are few reports on their applications as Lewis acid catalysts. High-valent metalloporphyrins, in which the metal is in its highest oxidation state, can be used as mild Lewis acids. In this respect, electron-deficient porphyrins of Cr(III), Fe(III), Sn(IV) and V(IV) have been used in organic transformations such as regioselective [3,3] rearrangement of aliphatic allyl vinyl ethers, Claisen rearrangement of simple aliphatic allyl vinyl ethers, rearrangement of α,β -epoxy ketones into 1,2-diketones, rearrangement of monoalkyl-substituted epoxides into aldehydes, highly regio- and stereoselective rearrangement of epoxides to aldehydes, epoxide ring-opening, protection of hydroxyl compounds, cyclopropanation of alkenes and olefin formation [6-11].

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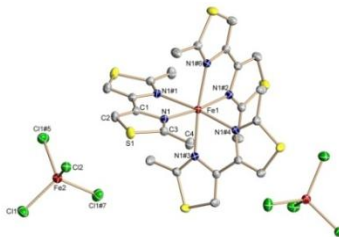
Coordination chemistry of Iron: Synthesis, characterization, mechanochromism and photochromism, magnetism and Biological properties, along with a case study of $[\text{Fe}(\text{dm4bt})_3][\text{FeCl}_4]_2$ and $[\text{Fe}(\text{dm4bt})_3][\text{FeBr}_4]_2$

Nasser Safari,^{a,d} Anita Abedi,^b Vahid Amani^a and Hamid Reza Khavasi^a

^aDepartment of Chemistry, Shahid Beheshti University, P.O. Box 1983963113, G. C., Evin, Tehran, Iran.

^bDepartment of Chemistry, North Tehran Branch, Islamic Azad University, Tehran, Iran
n-safari@cc.sbu.ac.ir

Iron is placed at the heart of table of chemical elements. It has variety of oxidation, spin and coordination geometries which make it metal of the choice for different application from biology to material science. However coordination chemistry and stepwise synthesis of its coordination compounds was not fairly explored. In this abstract some method for synthesis of iron complexes with nitrogen and oxygen donor ligands is discussed. As a case study $[\text{Fe}(\text{dm4bt})_3][\text{FeCl}_4]_2$ and $[\text{Fe}(\text{dm4bt})_3][\text{FeBr}_4]_2$ complexes (**2**) were prepared and fully characterized. Complex **1** has shown reversible mechanochromic effect in crystalline phase to powder and reversible photochromic property from yellow to green in solution upon sun light. Magnetic behaviour of the complexes was also studied at 5-300 K. At 300 K, μ_{eff} values are equal to 5.80 and 5.66 emu K mol^{-1} for **1** and **2** respectively. Upon cooling, μ_{eff} decreases where the decrease starts at around 65 K for compound **1** and at around 100 K for compound **2**, due to different counterions.

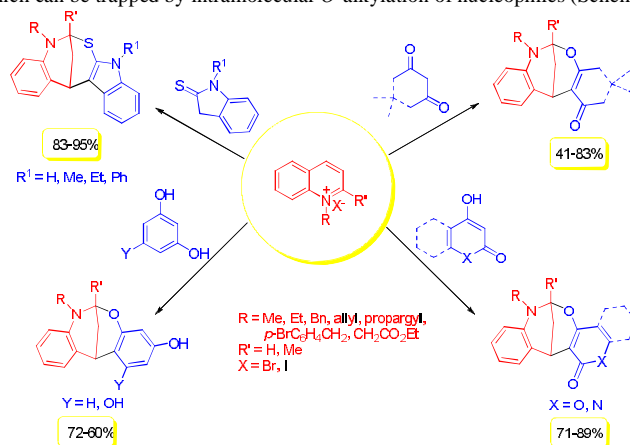


Organic Chemistry

**Tandem 1, 3-dinucleophilic addition of bifunctional nucleophiles to quinolinium salts;
new and convenient approach to heterotetracyclic benzoxazocines**
Firouz Matloubi Moghaddam

Department of Chemistry, Sharif University of Technology, P. O. Box 11155-9516 Tehran, Iran; Fax +982166012983; E-mail: Matloubi@sharif.edu

Benzoxazocines have received considerable attention because of their pharmacological properties including antidepressant, antithrombotic, antipsychotic along activity against breast cancer.¹ On other hand the construction of medium-ring heterocycles especially eight-membered rings, remains a significant synthetic challenge goal in modern organic synthesis because of entropy reasons and ring strain. However, limited attention has been given to the synthesis of medium-ring heterocycles, examples include cycloadditions, ring closing metathesis, ring expansion, Mitsunobu reactions, and metal-mediated ring cyclization.² In this work we will report the novel and efficient synthesis of a broad spectrum of polycyclic benzoxazocines via unique tandem 1,3-dinucleophilic addition of different bifunctional nucleophiles to quinolinium salts. The reaction generally involves the initial addition of nucleophiles to quinolinium salts to form enamine intermediate which can be trapped by intramolecular *O*-alkylation of nucleophiles (Scheme 1).



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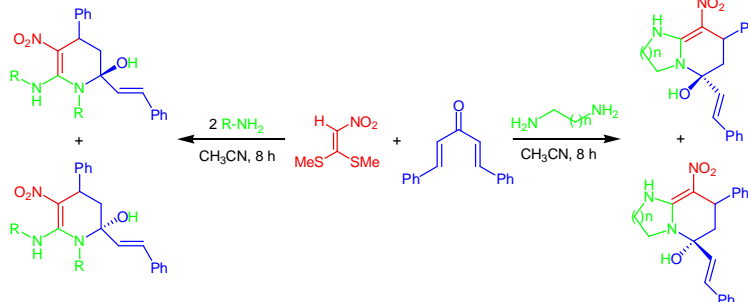
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Synthesis of Diazaheterocycles via Multicomponent Reactions

Abdolali Alizadeh

Department of Chemistry, Tarbiat Modares University, P. O. Box 14115-175, Tehran, Iran
E-mail: abdol_alizad@yahoo.com and aalizadeh@modares.ac.ir

Heterocyclic compounds are important natural and synthetic materials. The remarkable ability of heterocyclic cores to serve both as biomimetics and active pharmacophores has largely contributed to their unique value as traditional key elements of numerous drugs and designed medicinal agents in medicinal chemistry.¹ In particular, nitrogen containing heterocycles are prevalent in many drugs,² thus synthetic chemists are increasingly motivated to discover new methods for rapid construction of pharmacologically important drug-like compounds.³ In the course of our research program into design of new routes for the synthesis of a variety of active biologically nitrogen polycyclic heterocycles in our laboratory *via* one-pot reactions of enamines and amins,⁴ we describe an efficient synthesis of fully substituted pyridinols and pyrido[1,2-*a*]-fused-1,3-diazaheterocycles derivatives *via* a new and one-pot three component reaction between an nitro ketene amination derived from the addition of various primary amines or 1,*n*-diamines to 1,1-bis(methylthio)-2-nitroethene. The structures of compounds were deduced from their elemental analysis, IR, and high-field ¹H and ¹³C NMR spectra.



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Additives in the paints and coatings industry

Mohammad Bayat

Department of Chemistry, Imam Khomeini International University, Qazvin, Iran

E-mail: bayat_mo@yahoo.com

Organic coatings are complex mixtures of chemical substances that can be grouped into four broad categories: (1) binders, (2) volatile components, (3) pigments, and (4) additives [1]. Additives are materials that are included in small quantities to modify some property of a coating. Examples are catalysts for polymerization reactions, stabilizers, and flow modifiers. Additives are used to prevent defects or to achieve special properties in coating or other chemical compositions. It is almost impossible to obtain these properties using other raw materials. Additives have the reputation of problem solvers and nowadays are regularly used in all coatings and chemical formulations. They play a key role in the development of new coating systems and their importance is steadily growing as a result of higher quality standards and the switch to environmentally friendly formulations [2]. More and more additives are the components that determine whether a coating or chemical formulation is marketable or not. In the majority of cases, additives are responsible for important properties such as gloss, colour stability, adhesion or smooth surface. Wetting and dispersing additives promote pigment wetting and stabilization, prevent flooding, floating and hard settling of pigments. They ensure low viscosity at high pigment loads and improve colour strength, gloss and hiding power or transparency [3].

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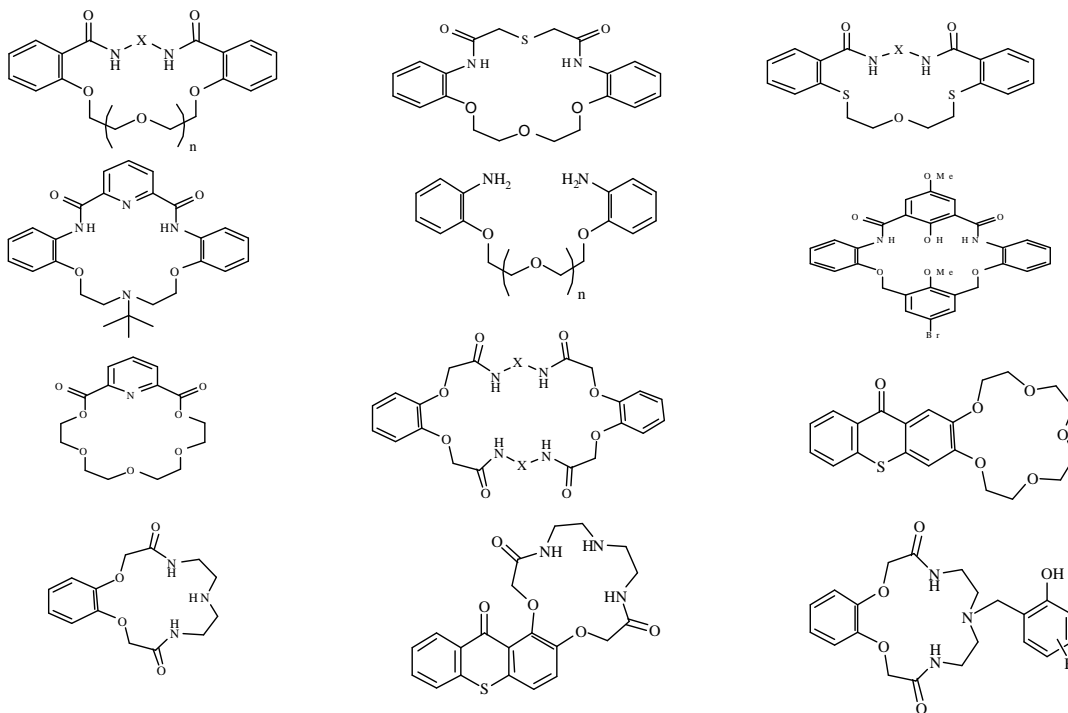
Twenty years of "Crowning" around: synthesis of crown ethers at Shiraz University

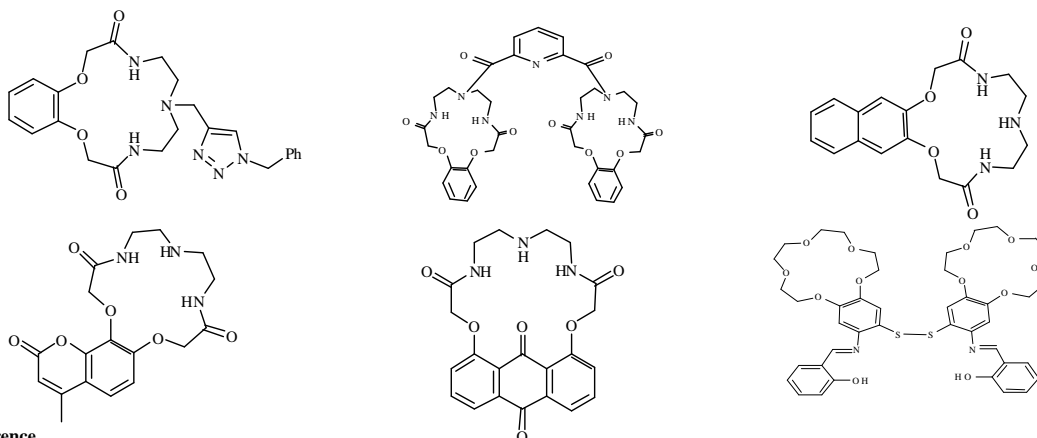
Hashem Sharghi

Department of Chemistry, Shiraz University, Shiraz, 71454, I.R.Iran

E-mail: shashem@chem.susc.ac.ir, Tel.: +98 711 2284822; Fax: +98 711 2280926

Crown ethers are cyclic ethers containing several oxygen atoms. When one or more of the oxygen atoms in crown ethers are replaced with nitrogen atoms, azacrown macrocycles result.¹ The azacrown ethers have complexation properties that are intermediate between those of the all-oxygen crowns, which strongly complex alkali and alkaline earth metal ions, and those of the all-nitrogen cyclams, which strongly complex heavy-metal cations.² Many synthetic approaches have been developed to prepare a multitude of macrocyclic ethers containing various heteroatoms and functional groups. It is not easy to find a new general method to synthesize macrocyclic ligands, especially if the method is to be applicable for the formation of new molecular topologies. Obviously, the elaboration of general and simple approaches for the synthesis and functionalization of azacrown ethers remains a very important problem for researchers working in this field. Azacrown ethers have been prepared by template effect,³ high dilution technique,⁴ reaction of diester with diamine or polyamine⁵. All of these procedures for the synthesis of macrocyclic compounds suffer from disadvantages such as: long reaction time, the use of metal salts, tedious procedures, low yields of products and use large volume solvents. This fact promoted us to apply new methods to the synthesis of crown ethers. A review of the synthesis of crown ethers at Shiraz University is presented. Topics include: azacrown ethers, thiocrown ethers, podands, fluorescent crown ethers, colour crown ethers, anthraquinone azacrown ethers, thioxantone azacrown ethers, coumarine azacrown ethers, bis azacrown ethers, and the new Mannich reaction methods to prepare lariat ethers.





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Modified Supports for Improving Activity and Selectivity of the Heterogeneous Catalysts

M. Ghiaci

Department of Chemistry, Isfahan University of Technology,
Isfahan, 8415683111, Iran
mghiaci@cc.iut.ac.ir

The drive towards clean technology, with an increasing emphasis on the reduction of waste at source, will require a level of innovation and new technology. There is a particular need to reduce the environmental impact of many processes operated by the fine and specially chemical industries. These are typically batch processes which are often unselective and inefficient, based on stoichiometric reagents and toxic solvents, require multiple separation stages and generate large volume of toxic or corrosive waste. These problems can be largely overcome if genuinely catalytic, heterogeneous alternatives to environmentally unacceptable reagents can be developed. While heterogeneous catalysis is well established in large scale vapor phase reactions, it is rarely used in liquid phase systems. Microporous materials such as zeolites have limited potential in such systems because of slow diffusion and blockage by large molecules, but many of the advantages of using porous solids should still be available through the use of mesoporous materials such as silica gel. Recent developments in the design and application of supported reagent catalysts offer considerable potential for clean synthesis. Synergistic efforts between the support material and the reagent can lead to unexpectedly high activity. Thus "Modified ZSM-5" is a potent solid acid for the Fries rearrangement of phenyl acetate when it compares with unmodified ZSM-5 [1]. This and similar zeolites and modified clay supports have been shown to have many useful applications in organic reactions. In this talk we demonstrate the value of this methodology in different areas of organic chemistry and catalysis.

Reference

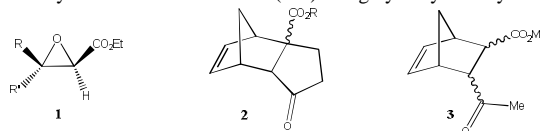
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Synthetic innovations inspired by benign methods for the preparation of biologically important products

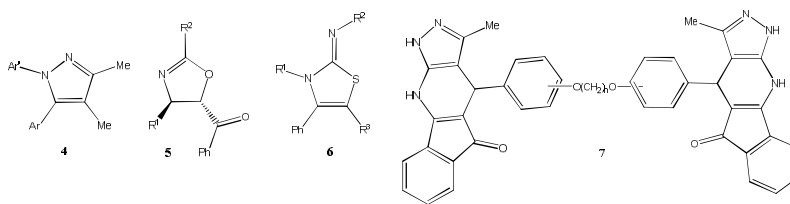
Manouchehr Mamaghani

Department of Chemistry, Faculty of Sciences, University of Guilan, P. O. Box 41335-1914, Rasht, Iran.
E-mail: m-chem41@guilan.ac.ir

The marvelously diverse architecture of biologically active natural products and medicinally important compounds offers numerous opportunities and challenges for innovation in the development and application of novel strategies and methods in organic synthesis. On the other hand, green chemistry has become a major driving force for organic chemists to develop environmentally benign routes for the preparation of organic compounds of synthetic and biological values. For example, the possibility of using biotransformations and performing reactions under ultrasonic and microwave irradiations to enhance the reaction efficiency from both economic and ecological points of view has given to this kind of procedures a remarkable synthetic value and received a great attention [1]. The first part of this lecture will be devoted to the asymmetric synthesis of novel chiroins (**1-3**) using hydrolytic enzymes and chiral auxiliaries [2].



A second part of this talk focuses on the new developments carried out in our laboratories concerning the uses of MCR reactions and clean source of energies such as ultrasonic and microwave irradiations for the synthesis of biologically important heterocycles (**4-7**) [3].



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Chemistry of *vic*-Dioximes

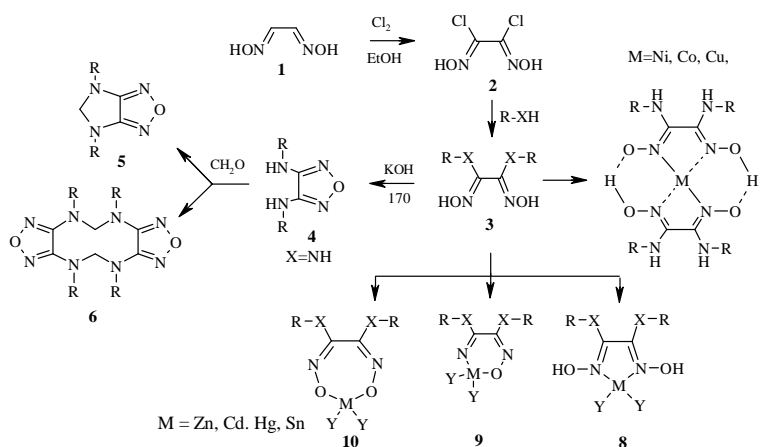
Ali Kakanejadifard*, Motaleb Ghasemian, Sakineh Omidi, Somaye Shirali

Department of Chemistry, Faculty of Science, Lorestan University

E Mail: alikakanejadifard@yahoo.com

The chemistry of *vic*-dioximes and their numerous transition metal complexes have been widely investigated as analytical reagents [1-3], models for biological systems [4], as well as catalysts in chemical processes, electrochemical and electrooptical sensors [1]. The metal containing oxime complexes [5-10] are utilized in medicine. For example, technetium (V) and copper (II) complexes containing vicinal dioxime currently are used as cerebral and myocardial perfusion imaging agents. The reaction of primary amines or thiols with dichloroglyoxime yielded various symmetrically substituted diaminoglyoxime (**3**, X=NH) or dithioglyoxime (**3**, X=S) derivatives. The reaction of N, N'-3, 4-diamino-1,2,5-Oxadiazole (**4**) was prepared by dehydration of **3** (where X=NH) in aqueous KOH at 170-180 °C. It follows from the literature, that 3,4-diamino-1,2,5-oxadiazole (**3**, X=NH, or 3,4-diamino-diaminofurazans) are weak nucleophiles [13]. We have found that condensation of the reaction of **8** with aldehyde leads to Compounds **5** or **6**. The complexation of *vic*-dioximes (**3**) in different condition leads to various structures. The structures of **3** with transition metal ions form square planar complexes (**7**) of 1:2 molar ratio of metal to ligand through N,N-chelation, while Zn(II) Cd(II), Hg(II) and Sn(II) form 1:1 tetrahedral complexes with a N, N-chelation (**8**). The novel mononuclear O,O-coordinated complexes (**10**) [M= Zn(II), Cd(II)] and its dinuclear complexes along with dinuclear N,O-coordinated complexes (**6**) of **3** have been prepared.

Scheme



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New Nanocarrier Systems Based on Peripherally Functionalized Dendrimers: Preparation and Applications

Namazi, H. and Co-workers

Research Laboratory of Dendrimers and Nanocarriers, Faculty of Chemistry, University of Tabriz, Tabriz, P. O. Box: 5166616471, Iran;
namazi@tabrizu.ac.ir

Dendrimers are a new class of polymeric materials with unique molecular architectures, which provide promising opportunities for variety of applications. Their highly branched and well defined structure, globular shape, and controlled surface functionality are important characteristics which make them excellent candidates for evaluation as nanocarrier systems. The interior cavity of dendrimers has been shown to be capable of encapsulating guest molecules. The surface functional groups of dendrimers also could be utilized for the conjugation of various molecules. Here, we present synthesis of different generations of dendritic supramolecules based on a variety of naturally occurring or biocompatible molecules such as poly (ethylene glycol) as the core molecule and citric acid or glutamic acid as the building block monomers. Meanwhile, different generations of dendritic supramolecules based on citric acid and poly (ethylene glycol) or linear citric acid glycodendrimers was prepared in moderate conditions and was applied as the drug nanocarrier agents. The capability of synthesized dendrimers as the host-guest systems has been investigated and a restricted number of guests, such as rose Bengal and some drug molecules could be encapsulated in their "dendritic box". Also new series of nanocarrier compounds as star shape biopolymer was synthesized using dendritic poly (glycerol) as the core and barbell-like dendrimers from glutamic acid dimethyl ester-PEG-glutamic acid dimethyl ester as ABA-type triblock copolymer (PGL-PEG-PGL) through liquid-phase peptide synthesis method. PEG 600 diacid was used as the core, and glutamic acid dimethyl ester as the monomers. Investigations showed that the synthesized biocompatible supramolecular compounds could trap some suitable size guest molecules and their transport capacity (TC) were significantly high and enough efficient for applications in biological systems. Also the preparation of gold nanoparticles in the presence of peripherally hydroxyl groups of citric acid-based dendrimers was evaluated.

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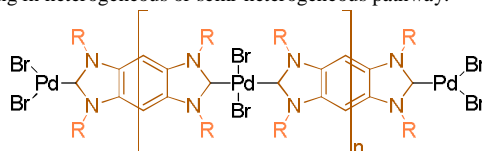
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Nano-Centipede-Like Main-Chain NHC-Palladium Polymers as a New Breakthrough in Catalyst Design

Babak Karimi

Department of Chemistry, Institute for Advanced Studies in Basic Sciences (IASBS), Gava Zang, Zanjan, 45137-6731, Iran

By analogy to natural centipede, the preparation and characterization of a number of nano-centipede-like main-chain organometallic polymers (NHC-Pd MCOP) with different N-alkyl substituted groups **R** (legs) such as benzyl, n-hexyl, n-dodecyl, and triethylene glycol is described. These materials were found to be highly active and recoverable catalytic systems in the Suzuki-Miyaura cross-coupling reaction of chloroarenes including both deactivated and hindered aryl chlorides with different types of arylboronic acids under aqueous conditions. The effect of various N-alkyl substituents on the catalytic performances of the materials will be thoroughly discussed. In this regard, we have provided several compelling evidences such as kinetic studies, poisoning experiments, microscopic analysis, dynamic light scattering (DLS), and average molecular weight determination before and after catalysis, in order to gain more insight into whether our novel catalyst systems are functioning in heterogeneous or semi-heterogeneous pathway.



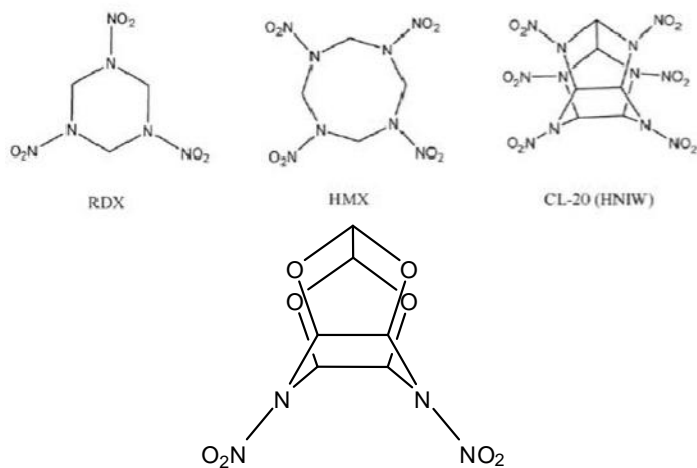
Nitramines for novel energetic materials

Yadollah Bayat

Malek-ashtar university of Technology

Aromatic and aliphatic nitro compounds are of huge industrial importance and are invaluable intermediates in organic synthesis. The replacement of amine and amide hydrogen with a nitro group via direct nitration is an important route to *N*-nitro functionality. The energetic nature of the N-NO₂ group means that *N*-nitro-based explosives are some of the most powerful explosives available and these have largely superseded aromatic *C*-nitro compounds for military applications. The energetic material containing N-NO₂ group has numerous military and commercial application and play an important role in aeronautics, civil engineering, the weapons industry and other high-tech fields at present. Cage crystal molecules containing the nitro group are important and widely are used as energetic materials due to high energetic, density, detonation pressure and low sensitivity. This lecture begins with an introduction to the energetic materials and commercial applications and after covering certain basics, focus on progress in this topics. In addition synthesis and development of the most prominent and relatively new powerful explosive (cyclic and polycyclic), containing nitramine functionalities such as 4, 10-dinitro-2, 6, 8, 12-tetraoxa-4, 10-diazaisowurtzitane (TEX), 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-

hexaazaisowurtzitane (HNIW), tetranitrotetraazacyclooctane (HMX), tetranitrocubane (TNC) examined. Also chemical characterization, crystallization, polymorphism and methods of nanosizing studied.



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*Physical
Chemistry*

Theoretical Insight to Halogen Bonding

Mohammad Solimannejad

Quantum Chemistry Group, Department of Chemistry, Faculty of Sciences, Arak University, Arak 38156-8-8349, Iran
m-solimannejad@araku.ac.ir, www.solimannejad.ir

Halogen bonding describes a directional interaction between covalently bound halogen atoms (X) and Lewis bases (A). The halogen atom is typically bonded to a carbon or another halogen atom. Halogen atoms themselves can act as Lewis bases in halogen...halogen interactions. The strong observed preference for linear D–X...A interaction parallels that known for D–H...A hydrogen bonds (HB) and preferences for the geometries at the acceptor (Lewis base) are also consistent with those observed in hydrogen bonding. Recently, more attention has been paid to halogen bond because it, like hydrogen bond, can also play a similar role in the fields of chemistry and biology [1–4]. Recently, a few articles concerning the halogen bonding and cooperativity between halogen and hydrogen bonding have been published by our research group [5–8]. In the present lecture we do our best to review different aspects of halogen bonding in theoretical point of view using results of our investigations.

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OPTICAL AND ELECTRO-OPTICAL PROPERTIES OF DYE DOPED LIQUID CRYSTALS

A. Ghanadzadeh Gilani^{a,b}

a) Department of Chemistry, Faculty of Science, University of Guilan, Rasht, Iran

b) Research Institute for Applied Physics and Astronomy, University of Tabriz, Tabriz, Iran

aggilani@guilan.ac.ir

Nematic liquid crystals are highly anisotropic materials owing to their large molecular anisotropy and intermolecular ordering [1]. Materials with nematic liquid crystalline properties are applied in electro-optical displays, optical storage devices and nonlinear optics. The wide range of optical phenomena manifested by liquid crystals has stimulated many investigations on these materials. Knowledge of the electro-optical data and the influence of chemical structure on the physical parameters of mesogenic compounds are always required. Oriented nematic liquid crystals are known to form partially ordered structure, suited as anisotropic solvents for polarized spectroscopy, and are good model systems for the investigation of anisotropic intermolecular interaction [2]. The addition of a dye to a nematic liquid crystal affects several host parameters, which is due to the strong mutual interactions between the dye and nematic molecules. Therefore, the investigations of various kinds of guest–host systems are among the most important and needed in order to understand and provide further information about the intermolecular forces in anisotropic matrix.

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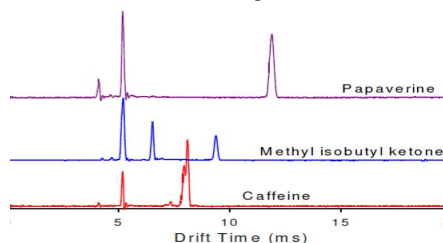
Ion Mobility Spectrometry Instrumental Developments and Applications in Analytical and Physical Chemistry

Mahmoud Tabrizchi

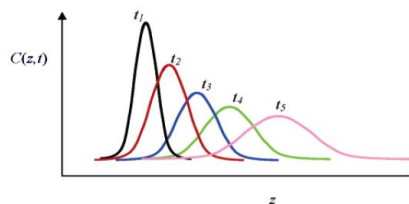
Department of Chemistry, Isfahan University of Technology, Isfahan 84156-83111, Iran

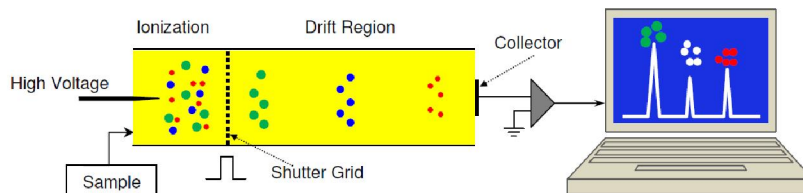
m-tabriz@cc.iut.ac.ir

Ion mobility spectrometry (IMS) has been known as a simple, inexpensive but powerful tool in the field of chemistry and physics. Over 50,000 IMS based instruments are currently employed worldwide for the detection of explosives, drugs, and chemical agents. In IMS, first the vaporized sample is ionized via atmospheric pressure chemical ionization. Ions are then moved under a constant electric field where they are separated based on their mobility. The most advantage of IMS is its operation at atmospheric pressure. Its simplicity for sample introduction, fast response and high sensitivity has increased its popularity as an analytical technique over the past decade. New instrumental developments of IMS including innovations in using different ionization sources, fundamental studies, improvement in resolution, as well as typical applications in analytical chemistry such as trace determination of different compounds will be discussed. In addition, the novel applications of IMS in thermodynamics and kinetics of ion molecule reactions as well as measuring mobility, size and diffusion coefficient of molecules will be presented.



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Ionization and Excitation of Free Atoms, Molecules and Clusters Using Synchrotron Radiation

Hossein Farrokhpour

Iranian Light Source Facility, Institute for research in fundamental sciences (IPM), Tehran, Iran
farrokhhossein@gmail.com

When electrons, at relativistic velocities, are confined to a circular orbit in a storage ring by a magnetic field, they accelerate toward the center of the circle and thus emit electromagnetic radiation which is known as synchrotron radiation. Synchrotron radiation has unique characteristics including high brightness, a wide energy spectrum from infrared to hard X-ray, polarization and pulse structure. It is an excellent spectroscopic tool to study a wide range of scientific cases. Over the past decades, the use of synchrotron radiation in the field of physics, chemistry, biology, medicine and elsewhere has expanded rapidly. Synchrotron radiation is a good mimic of solar radiation and is widely used for atmospheric chemistry studies. The number of synchrotron sources currently in operation worldwide is 50, and about 30 new facilities are under construction or being planned. Electron spectroscopic methods such as photoelectron and Auger spectroscopy are arguably the most popular techniques employed at today's ultraviolet and soft X-ray synchrotron radiation sources. The reason for its popularity is the versatile nature of the photoemission process. It allows looking at the electronic states of free atoms, molecules, clusters and solids by using the energy, angular, polarization and spin dependence of photoelectrons and Auger electrons. Also, it is possible to obtain dynamical information on the fast dissociation of molecules after core ionization or excitation by analyzing the Auger spectra. In this talk, a short summary on the synchrotron radiation sources and description of recent experiments in the field of electron spectroscopy on atoms, diatomic molecules, biomolecules and liquids performed by Iranian users will be presented. In addition a short report on the Iranian light source will be given.



General diagram of a synchrotron center

New techniques to evaluate the dynamic of phase transition at air/liquid interface

Saeid Azizian

Department of Physical Chemistry, Faculty of Chemistry, Bu-Ali Sina University, Hamedan, Iran
E-mail: saizian@basu.ac.ir

One of the most important features of surfactants is their outstanding ability to adsorb onto liquid interface. The adsorbed surfactant at air/liquid interface can appear as two dimensional structures in variety of states such as the gas (G), liquid expanded (LE), liquid condensed (LC) and solid phases [1]. The phase behavior and molecular packing at liquid interface depends on the molecular interactions. The rheological properties of a liquid surface play an important role in many physiological and industrial processes such as extension and contraction of lung surfactants, inject printing, emulsification, liquid-liquid extraction and so on. Recently, several new or improved techniques become available for the study of surfactants monolayers. Gibbs monolayers (adsorbed films) and Langmuir monolayers (insoluble films) at air/liquid interface were studied from both equilibrium and dynamic point of view. But most of the reported studies about the surface phase transitions were focused on the equilibrium states of surface phases. The purpose of the present work is to introduce some of the well known and the new techniques for studying the dynamic of phase transitions at air/liquid interface [2]. These techniques include dynamic surface tension which measures the surface tension as a function of time, external reflection FT-IR spectroscopy which is related to the vibrational frequency of a special bond in the coexisting phases at the interface, two dimensional infrared correlation spectroscopy, Brewster angle microscopy and also interfacial stress rheometer [3] which is based on calculation of the moduli of the monolayer by comparing the master oscillation of the magnetic coils with the oscillation of the rod.

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Spectroscopy of Metal Hydrides

Alireza Shayesteh

School of Chemistry, College of Science, University of Tehran, Tehran, Iran.
E-mail: ashayesteh@ut.ac.ir

Hydrogen is the most abundant element in the universe. Some diatomic metal hydrides have been found in cool stars, and their identifications have been primarily based on high-resolution laboratory spectra. For example, MgH and CaH are important molecules in astrophysics because their visible bands appear strongly in the absorption spectra of the sun and of some stars [1]. The green bands of MgH are used routinely to estimate the magnesium isotope abundances in various astronomical objects [2,3]. The orange and red bands of CaH appear in sunspots, and can be used to determine the surface gravity of cool stars [4]. On the other hand, metal hydrides are among the simplest inorganic molecules. They are favorite target molecules for quantum chemists because of the small number of valence electrons and the simplicity of metal-hydrogen bonding. *Ab initio* theoretical calculations on metal hydrides can predict reliable molecular parameters, and high quality experimental data on metal hydrides serve as benchmarks for testing the accuracy of *ab initio* methods. High-resolution spectra of metal hydrides are also useful for studying isotope effects. Three main topics regarding the spectra of hydrides will be discussed:

1. High-resolution UV-visible spectroscopy of diatomic hydrides
2. High-resolution infrared spectroscopy of triatomic metal hydrides
3. Intensity calculations and Einstein's *A* coefficients for diatomic hydrides

Some diatomic molecules of interest are CH⁺ and MgH [3], and the triatomic examples are gaseous BeH₂ and ZnH₂ [5-8].

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Ionic liquids-Solvent for Future: Thermophysical, Structure and Electronic Properties

M.H. Ghatee, F. Moosavi, A.R. Zolghadr, M. Zare, L. Pakdel N. Khanjari, M. Bahrami, R. Jahromi

Department of Chemistry, College of Science, Shiraz University, Shiraz, Iran, 71454
Email: ghatee@susc.ac.ir

Ionic liquids are the class of liquid which lately paid attention for the replacement of ordinary organic liquids. Low vapor pressure, low melting point, and high thermal stability are the main characteristics that nominate ionic liquids as green solvent for lab and industry. They are efficient electrolyte for electrochemistry in the new generation of batteries, and are known for unique durable solvent properties in biphasic organic synthesis. We will discuss thermophysical properties of bulk and interface of ionic liquids, based on experimental measurement, temperature dependence and universal behavior, and classical molecular dynamics simulation. [1-4] The results of classical and *ab initio* molecular simulation will be presented for bulk and interface of ionic liquids. A thorough understanding of the molecular orientation at the liquid/vapor interface can be gained by atoms density profiles and by molecular orientational distribution using two independent spherical polar angles. [5,6] Microscopic adsorption structures of imidazolium-based ionic liquids on the surfaces of graphene plates, coronene and circumcoronene, will be presented in detail by quantum chemical computation at the DFT/B3LYP level of theory. [6-8] The results can be used to resolve clearly the difference between hydrophobic and hydrophilic ionic liquids adsorption. Further studies unravel a different adsorption behavior shown by another important class of ionic liquids, namely pyridinium-based ionic liquids. [9]

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Physics and Chemistry of Nanostructured Materials

Elaheh K. Goharshadi

Dept. of Chemistry, Ferdowsi University of Mashhad, Mashhad 91779, Iran

Nanotechnology, the design, measuring, modeling, and manipulation of materials at the nanoscale, has the potential to deliver considerable benefits to society. The properties of materials change as their size approaches the nanoscale since the percentage of atoms at the surface of a material becomes significant. The novel properties of nanomaterials open the door to innovations in energy, environmental remediation, electronics, biomedical applications, etc.

Our research group focus on physics, chemistry, and applications of nanostructured materials, an ideal starting point for multidisciplinary science where chemical synthesis and processing techniques are combined with the characterization and application of physical properties. We have used various methods of preparing nanomaterials including insulators, semiconductors, and metals [1-3]. Our group combine novel materials synthesis with state-of-the-art characterization methods in order to fully control the chemical and physical properties of nanomaterials. A number of different properties of nanostructured materials including structural, optical, magnetic, thermal, antibacterial, rheological, environmental remediation, and semiconductor and photoluminescent properties have been investigated which lead our perspective understanding of quantum size-effect confinement [1-5].

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