In The Name Of Allah

Dear participant

Welcome to 18th Iranian Seminar of Organic Chemistry (18th ISOC). the seminar will be held during March 7-9, 2012(Esfand 17-19, 1390),at the department of chemistry, faculty of science, University of Sistan and Baluchestan with the collaboration of the Iranian chemical society to expand upon the knowledge and technology in organic chemistry, dependent fields and applications in industries, nanotechnology, environment, etc.
The scientific programs cover a wide variety of topics in organic chemistry, including synthesis, methodology, physical organic chemistry, stereochemistry, spectroscopy, polymer, nano-chemistry and all subjects related to the organic chemistry.
The scientific and organizing committee would like to express their deep gratitude to all authors for their contribution in this seminar.
We hope that you will enjoy the 18th Iranian seminar of organic chemistry alongside it's scientific and relaxing social programs. Also, we hope that you will have a wonderful experience in zahedan city and beautiful University of Sistan and Baluchestan that will stay in your memories forever.
With the best regards,
We would like to heartily appreciate the Chancellor, Finance Vice Chancellor, and Research Vice Chancellor of the University Of Sistan and Baluchestan, and also the Iranian chemical society, scientific committee, department of chemistry, and organizing committee for their valuable contribution and organizing the seminar.
With the best regards,

N. Hazeri

Associate Professor In Organic Chemistry

The chairman of the 18th Iranian seminar of Organic Chemistry

تنها تنها، در بی چراغی شب ها می رفتم
دست‌هایم از یادِ مشعل‌ها تهی شده بود
همه ستاره‌هایم به تاریکی رفته بود
مُشتِ من ، ساقه خشکِ تپش‌ها را می‌فشرد
لحظه‌هایم، از طنینِ ریزش پیوندها پُر بود
تنها می‌رفتم، می‌شنوی؟ تنها
ناگهان......
قطره‌هایِ ستاره‌ای در تاریکیِ درونم درخشید
و سرانجام در آهنگ پُر تلالو زمزمه‌هایش
اِی فرهیخته، ای مرزِ بی انتهای دانش، ترا پیدا کردم
و من در پیدایش تو رفتم و می‌رفتم...........
تا با تکیه‌ی به تو و هم اندیشی‌ات در پایانِ خود فرو اُفتم.

تقدیم به همه اندیشمندان شرکت کننده در هجده مین سمینار
شیمی ایران
اسفند ماه ۹۰

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- دکتر نورا... حاضری	دبیر سمینار
- دکتر ملک طاهر مقصودلو	عضو هیئت علمی
- دکتر حمیدرضا شاطریان	عضو هیئت علمی
- دکتر رضا حیدری	عضو هیئت علمی
- دکتر علیرضا مدرسی عالم	عضو هیئت علمی
- دکتر ابراهیم ملاشاهی	عضو هیئت علمی
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- اسماعیل ناروئی	کارشناس گروه
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- نسرین محمود آبادی

Formation of 2H-Pyran-2-ones from 1,3-Dicarbonyl Compounds, Acetylenic Esters and Sodium O-Alkyl Carbonodithioates

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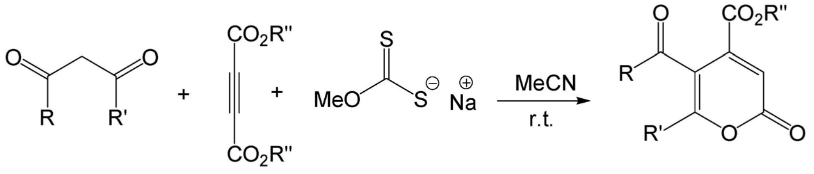
Introduction:

The pyran-2-one motif is found in a large number of naturally occurring compounds, many of which have interesting pharmacological properties [1, 2]. For this reason, pyran-2-ones have long been recognized as important synthons for organic synthesis and medicinal chemistry and their reactivity has received substantial attention. Pyran-2-ones are useful as Diels-Alder dienes, and therefore cycloadditions comprise much of the literature pertaining to these compounds. Deils-Alder reactions with pyran-2-one are facile with alkynes in addition to alkenes [3, 4].

Results and discussion:

As part of our current studies on the development of new routes in heterocyclic synthesis [5], we report an efficient synthetic route to 2H-pyran-2-ones. Thus, the reaction of 1,3-dicarbonyl compounds **1** with dialkyl acetylenedicarboxylates **2**, in the presence of sodium O-methyl carbonodithioate (**3**) at room temperature in MeCN as a solvent, produced 2H-pyran-2-ones **4** in good yields



1 **2** **3** **4**

In conclusion:

we have developed a convenient, one-pot method for the preparation of functionalized 2H-pyran-2-ones from 1,3-carbonyl compounds and dialkyl acetylenedicarboxylates in the presence of sodium O-methyl carbonodithioate. The simplicity of the present procedure makes it an interesting alternative to complex multistep approaches.

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Phenolic Compounds of Stachys Byzantina from Northwest of Iran

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The Vascular plants are able to synthesize a multitude of organic molecules as phytochemical, referred to as secondary metabolites. These molecules are involved in a varity of roles in the life span of plants ranging from structural ones to protection [1]. Phenolic compounds are regarded as one such group that are synthesized by plants during development and in response to conditions such infection, wounding and Uv radiation etc. Approximately 8000 naturally occurring compounds belong to the category of phenolics [2].

Phenolic compounds are known to act as antioxidants not only because of their ability to donate hydrogen or electrons but also because they are stable radical intermediates [3].

Phenolic acids are also well-known inhibitors of seed germination and interact synergistically to enhance the inhibitory effect [4].

Phenolics have an array of health promoting benefits, they are current interest due to their important biological and pharmacological properties, especially the anti-inflammatory, antioxidant, anticarcinogenic activities [5].

In this study, at the first step, our main aim was extraction and separation these phytochemicals with pharmacological effects. For this purpose, the aerial parts of this plant (leaf) were collected in May 2010 at Euromieh, Provience of Western Azarbaijan. The air dried leafs are extracted with ethanol. The ethanolic extracts are used for extraction of phenolic acids. Phenolic acids purified with preparative thin layer chromatography, and 5 different type of phenolic acids were analyzed by mass spectrometry (MS) and Infrared spectroscopy (IR).

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Chemical Constituents of the Essential Oil of Stachys Byzantina from Northwest of Iran

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The Vascular plant genus Stachys Byzantina considered as one of largest genera of the Lamiaceae, which grow wild in Turkey, Armenia and Iran. More than 270 Species of genera Lamiaceae is known in the world [1]. The stachys genus is one of the largest groups of this family. Plants of this genus have included more than 34 species in Iran [2]. Stachys Byzantina belongs to aromatic plants that grow in North and North-West of Iran. Plants of this genus have long been applied in folk medicine of NW Iran (Khoi, Euromieh) approved for healing wounds, treating abdominal pains, and as disinfectant. The other phytochemical that recently attracted the attention of many scientists, are essential oils [3]. Many papers on the biological activities as antimicrobial, antiviral, antifungal and antinoceptive were introduced [4, 5]. In this study the essential oils of air dried leaf evaluated by steam distillation. After extraction of essential oils with Dichloromethane, steam distilled of Stachys Byzantina oils were analyzed by a Heweltt-Packard 5973 mass selective detector connected with HP 6890 gas chromatograph, and 23 compounds were detected.

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Synthesis and Thermodynamics of Binding in the interaction of a water soluble and anti-cancer Platinum (II) complex with Calf Thymus DNA

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A new platinum (II) anticancer complex of [Pt(phen)(pyr-dtc)] (where phen is 1,10 phenanthrolin and pyr-dtc is pyrrolidindithiocarbamate) was synthesised and the interaction of this complex with Calf Thymus DNA was studied by isothermal titration method in 30mM Tris_HCl buffer solution (pH=7.0) at 300 and 310K.

There is a set of 6 binding sits(g) for the complex on the DNA with positive cooperativity in binding. n,the Hill coefficient (as a criterion of cooperativity) find out to be 3 at 300 K and 5at 310K respectively. K_{app} the apparent equilibrium constant are 42.5 mM^{-1} and 49.5 mM^{-1} at 300K and 310K respectively.

The above compound can denature the DNA and the concentration of this ligand in the midpoint of transition ($[L]_{1/2}$), is decreased by improving temperature, from 0.093 mmol/L at 300K to 0.087 mmol/L at 310K. the conformational stability of DNA in the interaction with ligand ($\Delta G^0{}_{H2O}$) determined to be 23.4 kJ/mol and 25.9kJ/mol at 300K and 310K respectively.

Presence of ligand led to less stability of the DNA . values for m, (a measure of ligand strength for DNA denaturation) are 0.65 and 0.79 (kJ/mol).$(mol/L)^{-1}$ at 300K and 310K respectively.

Enthalpy of DNA denaturation by the complex ($\Delta H^0{}_{coformation}$ or $\Delta H^0{}_{denaturation}$) in the range of 300K and 310K is find out to be 6.3 kJ/mol. In addition, the calculated entropy ($\Delta S^0{}_{H2O}$) of DNA denaturation by complex is -0.17 kJ/mol at 300K. the negative value of entropy change is related to the more disorder of denatured DNA with respect to the native DNA.

Keywords: Thermodynamic Studies, anti-cancer Palladium (II) complex

Investigation of plasticizing properties of ABA triblock copolymers based on PEG in cementitious systems

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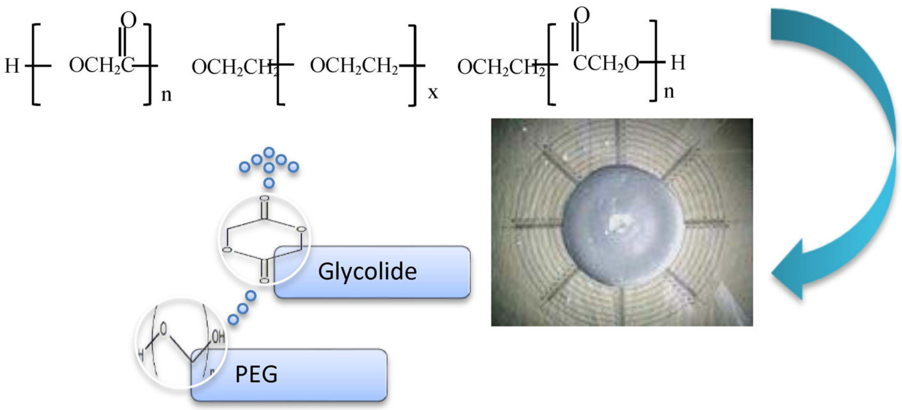
Plasticizers in cementitious systems are additives that uppon addition at a low dosage can change the workability, mechanical strength and other properties of cement paste effectively.[1] Plasticizers cause dispersion of cement particles and increase their mobility by two mechanisms: steric hindrance and electrostatic repulsion between cement particles by adsorption of negative functional groups on the plasticizer molecules.[2]

Slump retaining agents control the rate of setting of cement paste, so they can retain the workability of cement long enough for placing and finishing operation.

In this study, triblock copolymers based on poly ethylen glycol (PEG) was synthesised and their applications in the cementitious systems was investigated. The main purpose was verification of plasticizing effects of these copolymers in the cement paste. Ability of plasticizers depends on their structure, dosage and the water to cement ratio (W/C).[3]

ABA triblock copolymers with PEG (1000 and 1500 g/mol) as B block, poly caprolactone (PCL) and poly glycolide (PGA) (with different weigth ratio) as A block was synthesised via ring opening polymerization with stannous octanoate as catalyst. Their plastisizing effects and rheological properties was studied by mini-slump test and cylinder-cup rheometer. The Results show that by adding these copolymers to cement paste, the flowability increases, with PGA-PEG-PGA showing the highest performance. In this case the time of setting of hydraulic cement was also determined by Vicat Needle instrumen

Although these copolymers are not as efficient as commercial superplasticizer, they provide more insight into possibility and mechanism of plasticizing effects by non-ionic copolymers.



$$H\left[OCH_2\overset{O}{\overset{\|}{C}}\right]_n OCH_2CH_2\left[OCH_2CH_2\right]_x OCH_2CH_2\left[\overset{O}{\overset{\|}{C}}CH_2O\right]_n H$$

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Synthesis of novel pyrimido[4,5-b]quinolines using ionic liquid as catalyst

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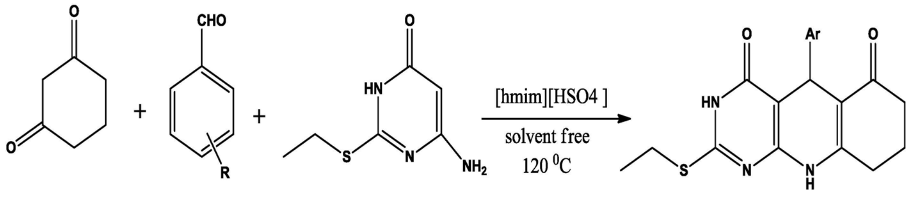
Multi-component reactions (MCRs) by virtue of their convergence, productivity, ease of execution and generally high yields of products have attracted considerable attention from the point of view of combinatorial chemistry [1]. On the other hand pyrimido[4,5-b]quinolines are important compounds because of their biological properties which are known to depend mainly on the nature and position of the substituent [2]. Quinoline derivatives display a broad range of biological activities such as anti-malarial [3], anti-tumor [4] and anti-bacterial [5]. Thus, considerable attention has been focused on the development of new methodologies to synthesize many kinds of pyridoquinoline systems.

Following our continued interests in the synthesis of biologically important heterocycles [6], in this research, we wish to report a very simple and highly efficient one-pot method for the synthesis of novel pyrimido[4,5-b]quinolines via a three-component cyclocondensation of equimolar amounts of 1,3-cyclohexadiene، aromatic aldehydes and 6-amino-2-(ethylthio)pyrimidin-4(3H)-one derivatives in the presence of ionic liquid [hmim][HSO4] (Scheme 1).



1 2 3

Scheme 1

4

This efficient method furnished the desired products (**4**) in high yields (75-95%) and short reaction times (10-30 min). High yields and ease of recovery and reusability of ionic liquid with consistent activity, makes this protocol efficient and environmentally benign.

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Theoretical study on the H-bonded complexes between 8-oxoguanine and formamide

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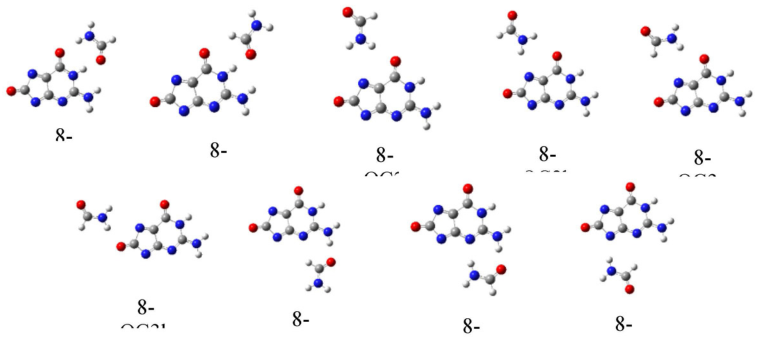
Hydrogen bonding is one of the most important concepts in chemistry because it is decisive to understand many different interactions both in the gas phase and condensed media [1]. Intramolecular and intermolecular bonds for the interaction between nucleotide bases and the folding pattern of proteins. Therefore, hydrogen bonds between biomolecules and the effects of hydrogen bonds on their properties are of great interest. 8-oxoguanine (8-OG) is one of the most abundant bases generated when DNA is attacked by reactive oxygen species, which are produced by cellular oxidant [2]. Formamide, also known as methanamide, is an amide derived from formic acid. Its formula is $HCONH_2$ or CH_3NO. The aim of this work is to find the complexes formed from interaction between 8-OG and formamide. All the structures studied in this work were optimized by using B3LYP method with 6-311++G(2d,2p) basis set by Gaussian 98 program package [3].



There are six positions in 8-OG for interaction with formamide. We found nine major structures for interaction of 8-OG with formamide on the potential energy surface. All optimized complexes have cyclic structures (with the exception of 8-OG3b). In all structures (with the exception of 8-OG2a and 8-OG3b complexes) there are two H-bonds interactions. In 8-OG2a and 8-OG3b complexes there are one and three hydrogen bonds interactions respectively. The calculated binding energies (kJ/mol) for complexes at B3LYP/6-311++G(2d,2p) level of theory have been computed as a difference between the energy of the complex and the sum of energies of monomers. All complexes are more stable than the monomers. The relative stability order of the complexes is: 8-OG1a>8-OG5a>8-OG1b>8-OG5b>8-OG4>8-OG3a>8-OG3b> 8-OG2a>8-OG2b

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One-Pot synthesis of hexahydroquinoline derivatives using $AlPW_{12}O_{40}.XH_2O$ catalyst

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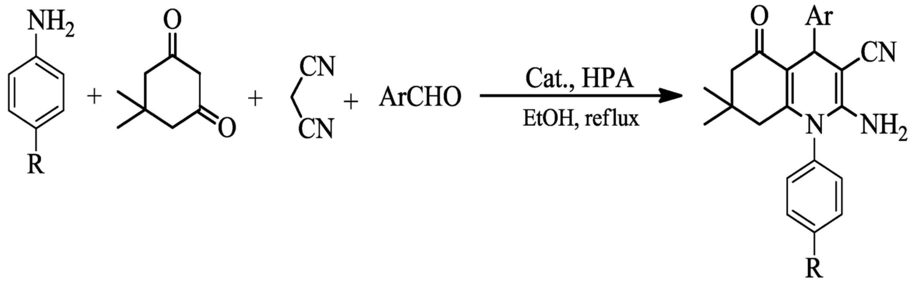
In recent years, an increasing interest has been focused on the synthesis of 1,4-dihydropyridine (DHP) compounds owing to their significant biological activities.[1] Quinolines having a 1,4-dihydropyridine nucleus are very important compounds because of their pharmacological properties such as antitumalarial, anti-inflamatory, antiasthamatic, antibacterial and antihypertensive.[2] Alternative strategies for their synthesis involving different catalysts and conditions have been developed.[3,4] However, some method suffer from drawbacks like some longer reaction times, unsatisfactory yields, harsh reaction conditions. In continuation of our investigations on the synthesis of 1,4-dihydropyridine,[5] herein we describe a novel and efficient one-pot method for the preparation of 2-amino-7,7-dimethyl-5-oxo-1,4-diaryl-1,4,5,6,7,8-hexahydroquinoline-3-carbonitrile derivatives from cyclo-condensation of aldehydes, malononitrile, anilines and dimedone in reflux of ethanol as solvent and HPA as catalyst. This new one pot method has the advantages to give high yields, to be completed in short reaction times, with simple product isolation procedure.



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Evaluation of the origin of conformational and tautomeric preference of N-formylformamide and its thio and seleno derivatives

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The amide functional group is the fundamental unit of proteins, peptides, and other biologically important molecules and has been traditionally characterized by a restricted C—N bond rotation, coplanarity of the attached atoms, short C—N bond lengths, and protonation at oxygen rather than nitrogen [1]. N-Formylforamide, as the simplest members of β-diamides, can participate in the amide↔imidic acid equilibrium (Fig.1) which interconverts by classical and quantum mechanical paths. Moreover, the imidic form of this molecule involved in O-H...O intramolecular hydrogen bonds that strongly coupled with π-electron delocalization and belong to the resonance assisted hydrogen bonds (RAHB) systems [2]. In the present study, we evaluated the origin of conformational and tautomeric preferences of N-Formylforamide with its thio (S) and seleno (Se) analogues. Moreover, the local and global minimums of potential energy surface, proton transfer process and intramolecular hydrogen bonding were also investigated.

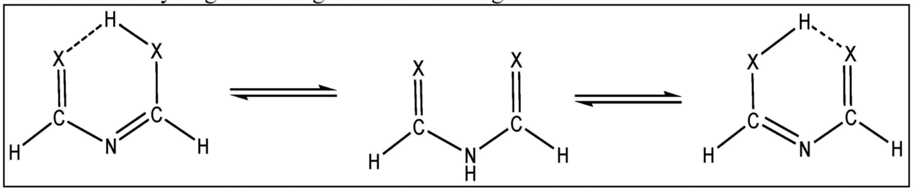

Fig.1. Amide↔imidic acid tautomeric equilibriums in title molecules (X= O, S, Se)

The geometrical optimization for all of the local minimums and transition structures were carried out by HF, B3LYP and MP2 methods with the standard 6-311++G(d, p) and 6-311++G(3df,3pd) basis sets. The optimized Structures were used to obtain the appropriate wave function files for AIM and NBO analyses. At all of theoretical levels, the amide forms and its chalgogen derivatives have more stability with respect to the imidic conformers. The NBO analysis show that the origin of tautomeric preference is mainly due to the electron delocalization in amide tautomers, especially LP(N)→π*C=X charge transfer.

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Fe(DS)$_3$-Catalyzed Synthesis of 2-Substituted Benzoxazoles

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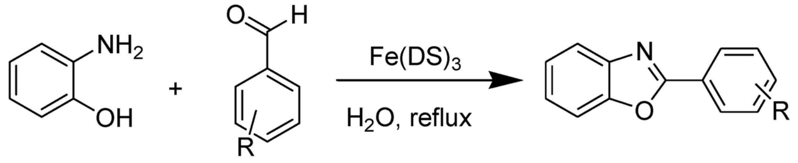
Synthesis of 2-substituted benzoxazoles has attracted interest in diverse areas of chemistry.[1] These heterocycles have shown different pharmacological activities such as antiviral, antimicrobial, anti-Parkinson, anticancer, and antibiotic properties.[2] The benzoxazole scaffold is also found in many biologically active compounds such as elastase inhibitors[3] and H_2 antagonists.[4] There are different methods for the synthesis of 2-arylbenzoxazoles based on substituted 2-aminophenols as starting materials.[5] Many of the procedures produce toxic or environmentally problematic by-products, often involve laborious workup procedures, or suffer from poor yields. Therefore, development of more convenient, environmentally friendly, and practical synthetic methods for benzoxazoles still remains an active area of research.

Therefore, we wish to report an efficient synthesis of 2-substituted benzoxazoles using of 2-aminophenol and various substituted arylaldehydes by Fe(DS)$_3$ in H_2O at reflux temperature (Scheme 1). The advantages of this method are higher reaction yields, short reaction times and use of H_2O as an environment friendly solvent(Scheme 1).



Scheme 1

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One-pot synthesis of 2,4,6,8,10,12- hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane in ionic liquids

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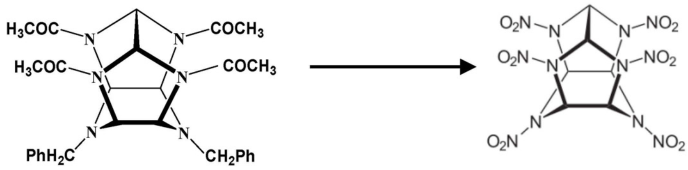
One of the most powerful explosives recently manufactured worldwide on a semi-commercial scale known as CL-20 or HNIW or 2,4,6,8,10,12- hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane. Also CL-20 is a potential candidate to replace HMX[1].

There has been much literature about the synthesis of HNIW,and several synthetic routs for the preparation of HNIW have been introduced.

Among all of the precursors, the following compounds are thought to be worthy for synthesis of HNIW:TADB(tetraacetyldibenzylhexaazaisowurtzitane),TADE(tetraacetyldiethylhexaazaiowurtzitane),TADF(tetraacetyldiformylhexaazaisowurtzitane),TAIW(tetraacetylhexaazaisowurtzitane), and HAIW (hexaacetylhexaazaisowurtzitane). All of the known methods for producing HNIW are based on the same starting material, 2,4,6,8,10,12-hexabenzyl-2,4,6,8,10,12-hexaazaisowurtzitane (HBIW), which is prepared by reacting benzylamine and glyoxal in an acetonitrile solvent at 25°C. In the synthesis of HNIW, HBIW is first reductively acylated to form TADB. The remaining benzyl groups can then be removed either by reductive formylation,with formation of TADF, or by nitrosation, leading to tetraacetyldinitrosohexaazaisowurtzitane (TADNSO), which both are easily converted to HNIW by nitration with different nitrating systems[2].

The first method for synthesis of HNIW from TADBIW is the reaction that used (NOBF4) as a nitrosing agent . This reaction affords a product of high purity, which is the highest in comparison with other methods. A disadvantage of this method, however, is its moderate yield that is up to 55% and a high price of the nitrosing agent,nitrosotetrafluoroborate[3]. Debenzylation of TADB in presence of larger quantity of palladium catalysts yields another nitrolysable precursor TAIW,which can be easily nitrated to CL-20with common nitrating agent.Both these debenzilation reactions make use of expensive palladium catalysts[1]. In The other two methods dinitrogen tetroxide is used as a nitrosing agent[3,4] . N_2O_4 has a low boiling point and work with it ,is hard.



Most of these reactions carried out within two stages. In this work, we used ionic liquid media,for synthesis of HNIW from TADBIW. HNIW was synthesized by the one-pot method described in this paper. We optimize the reaction parameters affect on synthesis of HNIW for obtaining high yield.

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An efficient , simple and green method for the synthesis of N-benzylphthalimide

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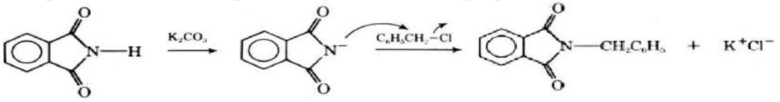
N-alkylating phthalimides are important intermediates in synthesizing the fatty primary amine and α-amino acid and are used as drugs[1- 2]. In the classical method for the synthesis of this drug, the N-alkylating phthalimides, was synthesized in N,N-dimethylformamide (DMF) by the reaction of halogenated compound with the salt, which was prepared by the reaction of phthalimide and KOH[3].

N-benzylphthalimide was firstly synthesized catalyzed by the alkaline reagent K_2CO_3-Al_2O_3 under microwave irradiation in 2002. In this reaction, a higher yield of 98% was obtained within a shorter time of 420s. However, it took about 6-7h to prepare the catalyst (alkaline reagents K_2CO_3-Al_2O_3) and 3h to purify the product after the completion of the reaction. Although the reaction time is only 420s, the work up is far from simplicity[4]. In this respect, the preparatory method was further improved.

The methods have been established for N-alkylation of phthalimide are associated with one or more of the following drawbacks: (i) long reaction time, (ii) moderate yield, (iii) the use of solvents such as DMSO and DMF that the workup of reaction is not only cumbersome, but also the green aspect of reaction is annihilated using these solvents. In addition, these reactions often are performed at high temperature[5].

The process could be expressed by the following equation:



We present here an efficient and simple method for the synthesis of N-benzylphthalimide in the presence of K_2CO_3 under microwave irradiation (MW) in good to excellent yield (99%) and short reaction times (360s). The reported method does not require the use of solvent. The experimental conditions were optimized and Several influence factors on the product yield were investigated, such as the proportion of reagents,the irradiation time, Phase transfer catalysts and the quantity of them.

All operation cycle took only about 20min. The method was very easy to operate, not only energy used was greatly saved, but also the reagents were reduced, which brought the highest economic value. In addition, pollution could be further reduced.

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Silica Sulfuric Acid/HNO$_3$ as a Novel Heterogeneous System for the Nitrolysis of DADN to HMX under Mild Conditions

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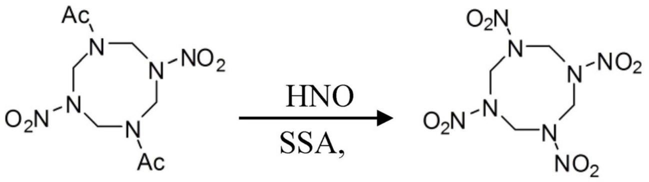
1,3,5,7-Tetranitro-1,3,5,7-tetraazacyclooctane (HMX), also referred to as octogen or cyclotetramethylenetetramine, is a highly energetic material that is useful in variouse explosives and propellants for military and non-military applications[1–3].
Some procedures are described for preparing HMX from hexamine. The first know process for the manufacture of HMX was developed in 1940's as Bachmann process [4]. This process typically provides yields of 80-84% which only about 10-40% is HMX. There are several drawback in this process and a great amount of another explosive, hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) is produced. For improving of these problems another synthetic routs involving various intermediates for making HMX have been proposed. Some intermediates that have been use to produced HMX are 3,7-dinitro-1,3,5,7-tetraazabicyclo [3,3,1] nonane (DPT), 1,3,5,7-tetraacetyl 1,3,5,7-tetraazacyclooctane (TAT) , etc. One of these intermediate involving 1,5-diacetyl-3,'7-dinitro-l,3,5,7-tetraazacyclooctane (DADN) gives a better yield of HMX than the established Bachmann process.



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The present investigation focuses on a new method for nitrolysis of DADN to HMX by developing a new nitrolysis process involving the use of nitric acid catalyzed by Silica Sulfuric Acid (SSA). In order to optimize the process parameters for synthesis of HMX to obtain higher yield and purity, a study was carried out with variation of some parametric conditions like time, mole ratio of SSA and nitric acid. This method gave us a green and mild conditions for nitration reaction.

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Tetramethylguanidinium triflate: An efficient catalyst solvent for henry reaction

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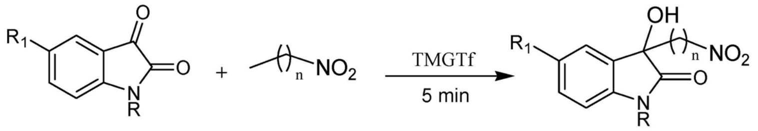
Several carbon-carbon bond forming reactions have been discovered and well reported in the literature.[1] The most prominent ones are aldol reaction, Gringnard reaction, … and Henry reaction.[2] Henry reaction is a classic-carbon-carbon bond-forming reaction and has been applied extensively in organic synthesis of β-nitroalkanols which are versatile intermediates for the preparation of nitro alkenes, 2-amino-alchohols, 2-nitro-ketones and biological compounds including fungicides, insecticides, natural prouducts and certain antibiotics.[3] Isatin is an active carbonyl compound, which like aldehydes can take part in henry reaction. Being prompted by recent interests in the synthesis of indolin-2-ones from isatin derivatives, we planned to investigate the possible improvement of henry reaction of isatin and nitro alkane for synthesis of 3-hydroxy-3-nitromethyl-oxindole. Based on our literature survey, there are only two reports on the henry reactions of isatin derivatives.[4,5] Thus, the development of simple and efficient reaction condition is an active area of research and there is a scope for further improvement towards milder reaction conditions, short reaction time and higher product yields. Ionic liquids, by virtue of their organic and ionic nature, are potent solvents, exerting nearly all kinds of interactions on reacting species, including transition states, whereupon sometimes give rise to improved yields and rate enhancements.[6] Structural variation of ionic liquids gives more flexibility to their applications, as provides fine tunning of their miscibility to merit phase-separation from products. In conclusion an efficient and convenient route to the synthesis of the title compounds was introduced here. Tetramethylguanidinium triflate ionic liquid plays as a catalyst solvent and can be recovered for reuse several times. Another advantages of the present method may be; requiring no metal catalysts or additional solvent.



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accelerated aging of epoxy nanocomposite based on response surface method: Dynamic mechanical behavior and nano-addition effect

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Epoxy resin based materials are thermosetting polymers widely used for structural applications, adhesives, organic coatings, electrical engineering and aeronautics[1]. When considering composites for long-term applications, it is necessary to know how the materials will behave during the intended service life. [2-3] almost all resins are adapted with various additives and fillers to pick up the process ability and the mechanical, thermal and electrical properties. additive are commonly mixed with the monomer in order to prevent premature reaction and increase the shelf life [7].they used not only favor the casting but also extend the storage life of the resin system. Recent studies show that nano silica has been attracting increasing attention due to its fascinating properties and potential applications. [4], as they are stable in most solvent environments.

Having known all this, in the present work, it is planned to accomplish a methodical experimental of study, to assess the performance characteristics of the epoxy nano composite, an epoxy resin containing different proportion of Fumed silica (Aerosil 200) and the results of the study were compared with epoxy resin without nano filler content. Results are presented from accelerated ageing in natural sea water.

Response surface methodology is a collection of statistical and mathematical techniques useful for the modeling and test analysis of in which a relevant response is influenced by several variables and the objective is to optimize this response. its use has been widely adopted in texts on chemometrics. [5] Experimental design and statistical analysis was performed using Design-Expert 7 computer software (trial version, Stat-Ease Inc., USA).

In this study, the effect of three identified process variables such as: different amount of nano silica(0-4%wt), aging time(1-3 month), temperature(20°-60° C)of aging were investigated and optimized with RSM. three quadratic polynomial equations were fit for loss module, Tg (from DMTA data) and mass gain(by periodic weighing with precision 0.1 mg)

also thermal aging and moisture absorption were described by Raman spectroscopy

Keywords: epoxy composite , accelerated aging, Response surface method, nano sillica, Raman

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A simple and efficient procedure for the synthesis of 1H-Pyrazolo[1,2-b]phthalazine-5,10-dione Derivatives

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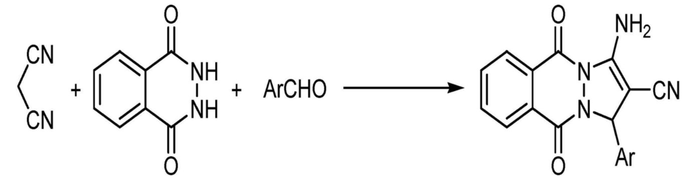
After the discovery of multicomponent reactions (MCR), the concept has stimulated substantial interest in organic chemistry because it provides useful products in a single step by the creation of several new bonds in one pot. In drug discovery as well as 'green chemistry', MCR are the preferred techniques due to high throughput synthesis of compounds in a cost- and time-effective manner.[1,2]

Multicomponent reactions of malononitrile, an aldehyde and nucleophilic compounds have recently attracted the interest of the synthetic community because the formation of different condensation products can be expected on the specific conditions and structure of the building blocks.

Heterocycles containing the pyrazole ring are important targets in synthetic and medicinal chemistry because this fragment is a key moiety in numerous biologically active compounds, among them such prominent drug molecules as celecoxib, pyrazofurine, and many others. Similarly, heterocycles containing a phthalazine moiety are of interest because they show some pharmacological and biological activities.[3,4]



we report the synthesis of 1H pyrazolo[1,2-b]phthalazine- 5,10-dione derivatives via the simple, efficient, one-pot, and three-component condensation reaction of malononitrile, phthalhydrazide and aromatic aldehydes in the presence of a catalytic amount of **solid acid** in ethanol as solvent at 70 °C. The structures of all products were confirmed using physical and spectral (NMR and IR) data.

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H-bonded complexes between uracil and nitrous acid: An ab initio study

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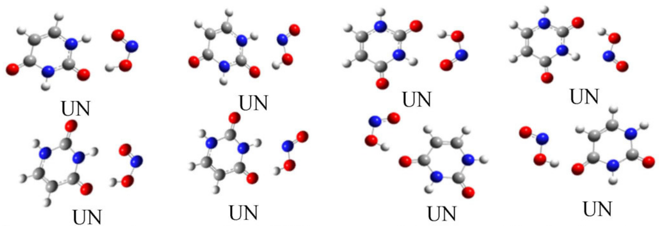
The nucleic acid bases have tremendous versatility in the formation of hydrogen bond complexes because of the presence of numerous hydrogen bond donor and acceptor groups [1]. Because of the simple structure of uracil, the theoretical analysis of its interaction with one or several water molecules has received a great deal of attention during the past years [2]. Nitrous acid, HONO, is one of the most important odd nitrogen species that plays an important role in atmospheric chemistry [3]. It is known as one of the most important sources of the OH radical in the atmosphere during the day, especially during sunrise, according to the dissociation channels. The OH radical has been known as the primary oxidant in the daytime chemistry [4]. The aim of this work is to study H-bonded complexes between uracil and nitrous acid. There are four positions in uracil for interaction with glycine. For the study of interactions between uracil and nitrous acid (UN), computations were carried out using B3LYP, B3PW91 and MP2 methods whit the 6-311++G (2d,2p) basis set.



The counterpoise procedure (CP) was used to correct for basis set superposition error (BSSE) in the calculation of binding energy. All optimized complexes have cyclic structures with two H-bond involved in the interaction. The structures UN1, UN3, UN5 and UN7 are eight-membered cyclic complexes. In eight-membered structures UN1, UN3, UN5 and NU7 the O atom of nitrous acid and one C=O group of uracil act as proton acceptors and C-H bond of nitrous acid and N-H uracil (with the exception of C-H bond in UN8) as proton donors. In seven-membered structures UN2, UN4, UN6 and U8 the N atom of NO group acts as proton acceptor. The electronic binding energies (D_e) range from -46.30 to -33.19 kJ/mol. The relative stability order of the seven complexes is UN1> UN2> UN3> UN4> UN5> UN6> UN8> UN7. The structure UN2 is the most stable and UN7 structure is the less stable.

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Tetramethylguanidinium triflate: An efficient catalyst solvent for henry reaction

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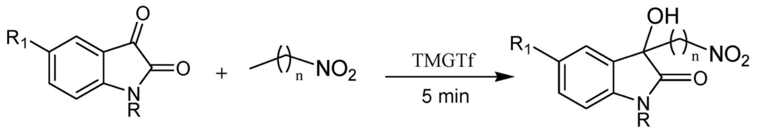
Several carbon-carbon bond forming reactions have been discovered and well reported in the literature.[1] The most prominent ones are aldol reaction, Gringnard reaction, … and Henry reaction.[2] Henry reaction is a classic-carbon-carbon bond-forming reaction and has been applied extensively in organic synthesis of β-nitroalkanols which are versatile intermediates for the preparation of nitro alkenes, 2-amino-alchohols, 2-nitro-ketones and biological compounds including fungicides, insecticides, natural prouducts and certain antibiotics.[3] Isatin is an active carbonyl compound, which like aldehydes can take part in henry reaction. Being prompted by recent interests in the synthesis of indolin-2-ones from isatin derivatives, we planned to investigate the possible improvement of henry reaction of isatin and nitro alkane for synthesis of 3-hydroxy-3-nitromethyl-oxindole. Based on our literature survey, there are only two reports on the henry reactions of isatin derivatives.[4,5] Thus, the development of simple and efficient reaction condition is an active area of research and there is a scope for further improvement towards milder reaction conditions, short reaction time and higher product yields. Ionic liquids, by virtue of their organic and ionic nature, are potent solvents, exerting nearly all kinds of interactions on reacting species, including transition states, whereupon sometimes give rise to improved yields and rate enhancements.[6] Structural variation of ionic liquids gives more flexibility to their applications, as provides fine tunning of their miscibility to merit phase-separation from products. In conclusion an efficient and convenient route to the synthesis of the title compounds was introduced here. Tetramethylguanidinium triflate ionic liquid plays as a catalyst solvent and can be recovered for reuse several times. Another advantages of the present method may be; requiring no metal catalysts or additional solvent.



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An investigation on the curing behavior of epoxy resin based on bisphenol A (DGEBA), in the presence of nano filler

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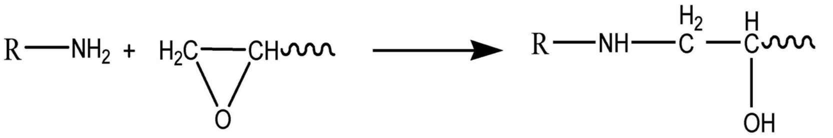
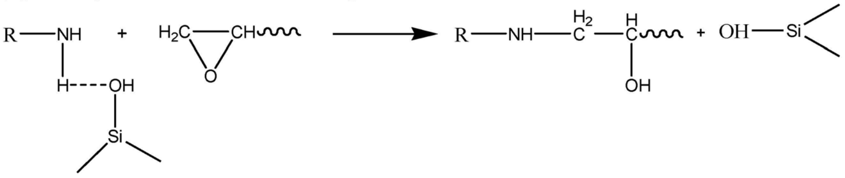
Epoxy resin has been developed rapidly since invented, and are widely used in modern life [1–3]. The most important and industrialized epoxy is bisphenol A. In this study, the cure process of epoxy resin based on bisphenolA (DGEBA) with polyamine hardener in presence of nano silica investigated through Differential Scanning Calorimetry (DSC) and Fourier Transform Infrared (FT-IR) [4]

In this study, the cure process of epoxy resin based on bisphenolA (DGEBA) with polyamine hardener (equation 1) in presence of fumed silica investigated through Differential Scanning Calorimetry (DSC) and Fourier Transform Infrared (FT-IR) [1]



(1)

The total reaction enthalpy (the maximum produced heat of reaction during curing) and glass Transition (Tg) was measured by DSC scans from 25 to 200 °C at rate of 10°C/min. All results were compared to those of bare epoxy resin. Fumed silica contains surface hydroxy groups, which can act as catalysis (equation 2) so the rate of reaction and Tg increases.



(2)

As a consequence of DSC, total reaction enthalpy decrease, Therefore, some of epoxy rings residue in the matrix as a result FT-IR spectra shows epoxy ring peak (the band at 914 cm^{-1}) after curing with the same amount of hardener . This may related to cover some amine active hydrogen with nano particles [5,6].

By preparing composites with different percent of fumed silica, nano composites with 1 wt% of SiO2 have a good dispersion of nano particles, within fully cured DGEBA matrix were easily produced through the proposed synthesis route. By increasing amount of fumed silica, cure kinetics reduces. Cure activation energy is not influenced by the silica presence.

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Thermal curing comparison of epoxy resin with amine and amide curing agents

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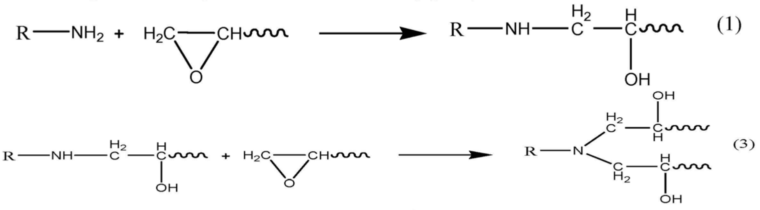
Abstract

Epoxy composites have extensive applications, for instance in adhesive, medical devices, optical component owing to their admirable resistance compared many materials [1-3]. The type of curing agent for modifications of epoxy resins can influence the curing chemistry, the curing rate, crosslink density, morphology, etc. So the choice of curing agent is very essential and requires to be considered very carefully. Epoxy resins can be cured with a wide variety of curing agents. Aliphatic and aromatic polyamines, polyamides, and their derivatives are the commonly used amine type curing agents. In this study, influence of different curing agents on thermal curing process of epoxy composite is investigated. Therefore the curing process of epoxy resin based on diglycidyl ether of bisphenol F (DGEBF) in the presence of amine and amide curing agent is determined through differential scanning microscopy (DSC) that were performed from 25 to 250 K at 10°C. Moreover, Fourier Transform Infrared Spectroscopy (FT-IR) was used to discuss the complete curing of composites. The FTIR results revealed that epoxy resin cross linked with amine curing agent more completely than amide curing agent. Because the epoxide ring is strained (unstable), polar groups (nucleophiles) can attack it. The amine groups react with matrix after completing the curing process of DGEBF and the epoxide ring peak is disappeared (figure1). The curing process with using polyamide curing agent due to presence of electron acceptor groups of oxygen which attract the nitrogen nonbonding electrons is more difficult (figure2).



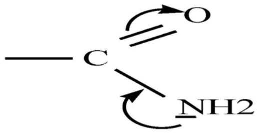


Figure 1: the curing process of amine curing agents

Figure 2: amide functional group

DSC results showed higher glass transition temperature (Tg) and total reaction enthalpy (the maximum produced heat of reaction during curing) of polyamine system. Therefore polyamine system has more thermal stability than polyamide system. Furthermore crosslinking decrease is due to increasing flexibility of epoxy/ polyamide that depends on lower Tg. On the basis of obtained results, the curing behavior of epoxy composite depends on the type of curing agent.

Keywords: epoxy resin, thermal curing, polyamine, polyamide

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Synthesis and Study of the Solvent Effect on Self-Assembly in a Novel Tripeptide Molecule contained unusual amino acid using Molecular Dynamics Simulations.

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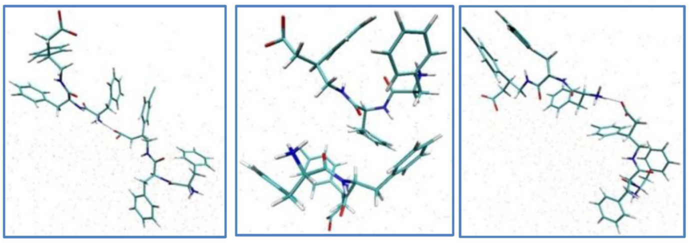
The diphenylalanine dipeptide is a suitable building block for molecular self-assembly. It is well reported that misfolding of the peptidic chain may produce unwanted processes that provoke fatal diseases. One of these problematic processes could be peptide assembly or aggregation. For instance, amyloid proteins may suffer conformational changes during folding processes leading to intermediate misfolded structures that can evolve into amyloid assemblies. These assemblies may precipitate as plaques over important parts of the body such as neural tissues and produce the so called amyloidogenic diseases[1]. We were encouraged to synthesis some novel peptides which contained γ- amino acids in their backbones. Gabapentin and baclofen were the best candidates for this approach. Baclofen is a muscle relaxer and an antispastic agent. In this article, we focused on the synthesis of some peptides. Between the synthesized peptides, H-Phe-Phe-Baclofen-OH was selected due to the existence of aromatic moiety in the structure of baclofen which is responsible for self-assembly via π-π stacking.

The realm of applications of computational chemistry is considerably expanding owing to steady advances in computer power. An ab initio quantum mechanical calculation was performed on H-Phe-Phe-Baclofen-OH tripeptide using Gaussian 03 package. The gas phase energy of the tripeptide was optimized at the HF/3-21G level. Molecular Dynamics Simulations were carried out with explicit solvent (water) using Gromacs 4.0.7 package. The details of simulations will be reported. Figure 1 shows screen captures in trajectory of the MD simulation of the tripeptide in bulk solvent. Different possible ways of self-assembly such as H-bonding, π-π stacking and T-Stacking can be seen in this Figure. The details about the self assembly of these compounds will discuss in the conference.



Keywords: Phenylalanine, Baclofen, Hydrogen bonds, Synthesis of tripeptide, Molecular Dynamics

Acknowledgment: We thank Iran Nanotechnology Initiative Council for financial support.

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Synthesis of Some New Small Molecules Towards OLED Application

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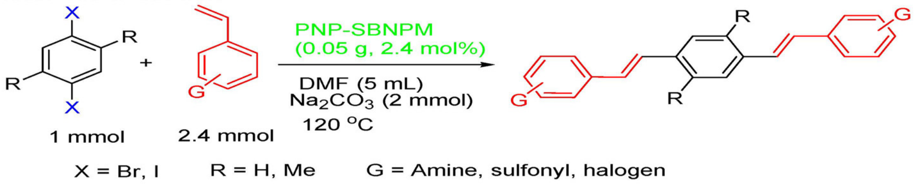
There is widespread interest in the use of conjugated organic materials in emerging optoelectronic technologies.[1] Conjugated materials such as small molecules and polymers have appeared that emission from organic-based light-emitting diodes (OLEDs) covers the entire visible spectrum.[1,2] In contrast to conjugated polymers, conjugated small molecules are desirable because their relatively simple structure enables straight forward structure-property relationships to be determined and thus regular structure films of specified thickness can be created by using evaporation techniques in a pure form.[3]

Some new 1,4-distrylbenzene derivatives were synthesized by using immobilized palladium nanoparticles on silica bonded N-propyl morpholine (PNP-SBNPM) as a heterogeneous catalyst. These one-pot reactions afforded a range of stereoselective symmetrical (E)-1,4-distyrylbenzene derivatives with high yields (78–90%). The green catalyst system is recyclable and allows facile product isolation. The recycled catalyst could be reused four times without appreciable loss in the catalytic activity. Single layer organic light emitting diodes (OLEDs) based on 1,4-distyrylbenzenes using thermal evaporation under vacuum condition has been fabricated and their optical properties such as electroluminescence (EL) and photoluminescence (PL) have been investigated. Fabricated OLEDs had EL emission in visible spectrum from 480 to 600 nm.



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Synthesis of Some Novel 4-Pyridyl-2-Aminothiophene and Related Schiff-Bases

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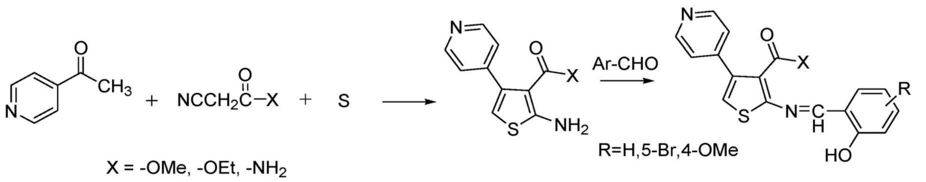
Thiophene derivatives exert broad applications such as functional materials in dyes, liquid crystals, molecular wires, organic light-emitting diodes, field-effect transistors and agrochemicals [1] They can also be used as selective site-directed inhibitors of various biological targets [2] On the other hand, Schiff bases derived from aromatic amines and aromatic aldehydes are very important class of organic compounds because of their applications in many fields including biological, inorganic and analytical chemistry [3].

In view of aforesaid points, we decided to extend our research [4] and have synthesized some novel 4-pyridin-2-amino thiophene by reaction of a ketone and elemental sulfur with methyl-, ethyl cyanoacetate or cyanoacetamide in the presence of morpholine, which followed by reaction with aromatic aldehydes to prepare related Schiff-bases (Scheme 1.). ^{1}H NMR and IR spectra together with UV spectroscopy data were used to identification of these compounds.



Scheme 1.

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An efficient approach to the synthesis of polyfunctionalized amino acids

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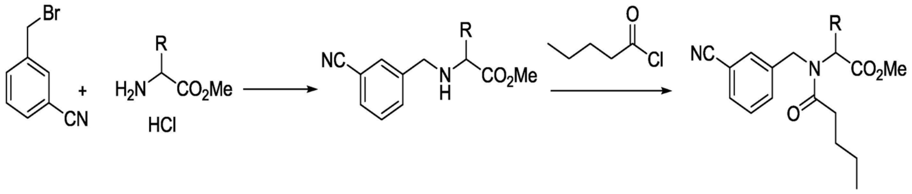
Functionalized amino acids are ubiquitous in many important biologically active molecules, synthetic drugs and drug candidates. For instance, Valsartan which is a nonpeptide, orally active, and specific angiotensin II receptor blocker acting on the AT_1 receptor subtype has been used in treatment of hypertension, heart failure and in left ventricular dysfunction post myocardial infarction (heart attack)[1,2]. The existence of the different functional groups can affect the chemical behavior of the molecule and may increase transforming potential of desired products.
In this approach we wish to report the synthesis of a series of amino acid methyl ester. The synthesized amino acid methyl esters are then carried to the next step to undergo coupling with aryl halides and carboxylic acids or acyl halides respectively. The products have different functional groups which could be used for further transformation. The general reaction is shown below.



The products could be used in different reactions, such as addition of azide, hydrolysis and reduction of nitrile groups. The details about this research project will be discussed in the conference.

Key words: Functionalized amino acids, hypertension drugs, Tertiary amides,

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New Sequential Ugi/Click Reaction for the Synthesis of Functionalized Pseudopeptides

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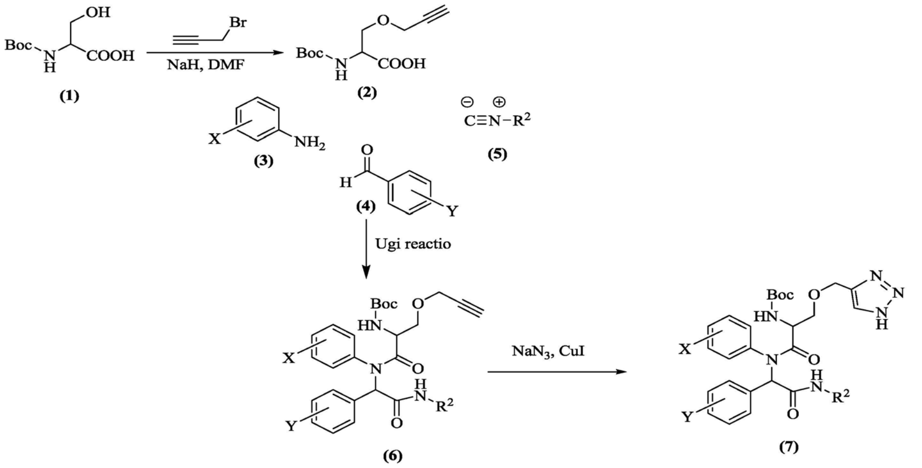
Multi-component reactions have huge potential for the rapid generation of small molecules libraries. However, there is a continuous need for designing and carrying out the reactions with novel starting materials in organic synthesis [1]. Ugi-4CR based on isocyanide is an efficient approach for the synthesis of structurally functionalized diverse complex molecules and they could supply the feedstock for advanced research in chemical biology [2].

In this approach, we would like to introduce protected N-tert-butoxy carbonyl O-propargylated -L-serine **(2)** as a starting material in Ugi-4CR.

Reaction of N-tert- butoxy carbonyl O-propargyl -L-serine **(2)**, aromatic aldehyde **(4)**, primary amines **(3)**, and isocyanides **(5)** leads to synthesis of pseudopeptide **(6)** which could be used for click reaction with Natrium azide in the presence of cuprous iodide. The existence of acetylenic moiety in the structure of product could add the huge potential for the synthesis of new small library.



Scheme1: Synthesis of functionalized pseudopeptide

Acknowledgment
We gratefully acknowledge K. N. Toosi University of Technology research council for financial support.

Key word: pseudopeptide, Ugi/click reaction, N-tert- butoxy carbonyl O-propargyl -L-serine.

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Highly efficient Suzuki Cross-Coupling Reactions catalyzed by heterogeneous palladium porphyrin

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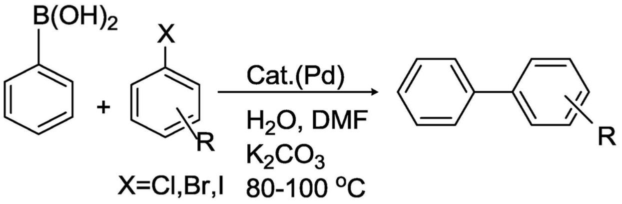
Suzuki cross-coupling reaction represents a powerful method for the C-C bond formation [1-3]. Construction of biaryl compounds via the palladium-catalyzed Suzuki reaction is an interesting area in organic synthesis. The importance of biaryl units as molecular components in pharmaceuticals, herbicides and natural products, as well as in engineering materials such as conducting polymers, molecular wires and liquid crystals, has attracted enormous interest [4-6]. The reaction represents an attractive alternative over other methods using organometallics because organoboranes are air- and moisture-stable with relatively low toxicity. With various metals being employed in coupling reactions, palladium is the most versatile metal in promoting or catalyzing reactions involving C-C formation due to its excellent catalytic efficiency in this type of reactions [7-10]. A control experiment indicated that the coupling reaction did not occur in the absence of catalyst.

In the present work, we have prepared heterogeneous tetrakis(4-aminophenyl)porphyrinatopalladium(II) and its catalytic activity was tested for the Suzuki cross-coupling reactions under various conditions. The catalyst exhibits high catalytic activities for the coupling of various aryl halides with organoboronic acid providing excellent yields of desired product [11]. The catalyst was characterized by various physicochemical and spectroscopic techniques.



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Efficient Synthesis of Polyfunctional N-Substituted 1,4-Dihydropyridines

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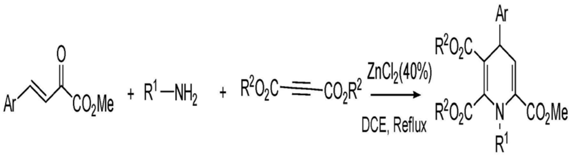
1,4-Dihydropyridine derivatives (1,4-DHPs) have interesting pharmacological and biological properties. It is clear that 1,4-DHP nucleus serves as the scaffold of important cardiovascular drugs and act as calcium channel blockers. It was shown that the activities of these compounds are related to the substituents and especially the number of ester functional groups [1].Due to the biological activity of 1,4-DHPs, we wish to report herein an efficient approach for the synthesis of polyfunctional 1,4-DHPs with three alkyl ester groups.

Aryl methylidene methylpyruvates were used as starting material which could be synthesized via reaction of pyruvic acid and aromatic aldehydes in the presence of Potassium hydroxide. Three-component reaction of arylmethylidene pyruvates, dialkylacetylene dicarboxylates and primary amines in the presence of Zinc choloride (40%) as Lewis acid, leads to form polyfunctional N-substituted 1, 4-dihydropyridines in 42-87% yields.

The synthesized novel 1,4-DHPs bearing three alkyl ester groups at C-2, C-5, and –C-6, which could be used for further transformation.



It seems that the existence of more alkyl ester functional groups could add the interaction activity of these compounds with lipase enzymes[2].The investigation of the biological activity of these compounds is in progress.Reaction could follow via these procedures:

a) Formation of enaminone via reaction of dialkyl acetylene dicarboxylate.
b) Addition of enaminone to activated aryl methylidene pyruvates.
c) Cyclization and finally dehydration.

In conclusion, this work describes a convenient and efficient process for the synthesis of functionalized 1,4-dihydropyridines via 3-MCR.The details will discuss in the conference.

Key words: N-substituted 1,4-dihydropyridines, Alkyl Aryl methylidene pyruvates, calcium channel blockers

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Effect of Synthesis Procedure on The Dynamic Properties of two Types Hydroxy Terminated Poly Butadiene (HTPB) base Polyurethane

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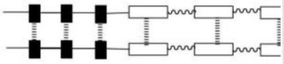
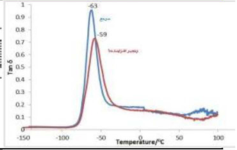
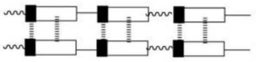
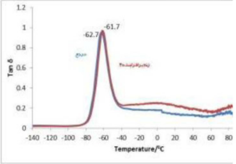
Application of polyurethane elastomers under cyclic loading (dynamic) is depend on to its structure and morphology [1]. In this study, we have prepared two types of polyurethane by using a one shot and prepolymer procedures [2]. In the first method all ingredient (HTPB, Chain extender (bis N,N (hydroxyl ethyl) cyanoactamide ,IPDI) is reacted in one stage and in the latter ,we prepared an isocyanate terminated prepolymer (reaction of bis N,N (hydroxyl ethyl)cyanoactamide and IPDI (1:2)) and react it with HTPB. In both methods the ratio of NCO/OH is equal .Our results have shown that the polyurethane is produced in one shot process have pseudo filler effect, so it show better dynamic properties (less Loss Compliance (J”)) than the polyurethane elastomers are obtained by a prepolymer method [1, 3, 4].

Procedure	Structure	Morphology*	Properties
One shot	NCO/OH=1 (HTPB, Chain extender (bis N,N (hydroxyl ethyl) cyanoactamide ,IPDI)		
Prepolymer	NCO/OH=1 (bis N,N (hydroxyl ethyl) cyanoactamide and IPDI (1:2)),HTPB		

*morphology abbreviation

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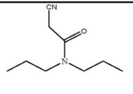	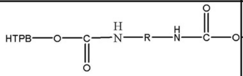	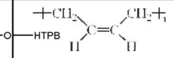	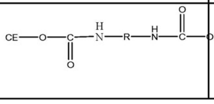	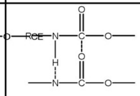

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Synthesis and Characterization of a New Chairal Composite from Polymerization of (+)-2-sec-Butylaniline-(+)-camphorsulfonate under Solvent-free Condition

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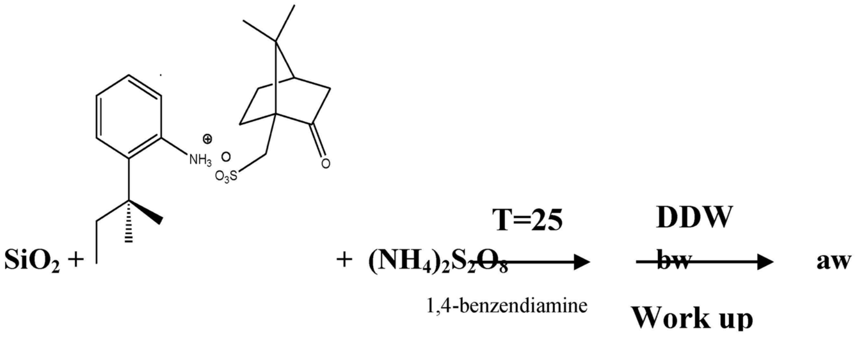
Conductive polymeric materials containing conjugated bonds have attracted much interest in scientific and technological areas in recent years.The conductivity in these polymers can be varied by doping them with different protonic acids or by using functionalized protonic acids.Among all the conducting polymers, polyaniline has received a great deal of attention owing to its simple synthesis, good environmental stability, ability to dope with protonic acids and moderately high electrical conductivity [1]. The most common method of chemical synthesis includes oxidation of the monomer with an oxidizing agent, e.g. ammonium persulfate, which is added to monomer solution. The resulting polymer is typically obtained in form of an amorphous suspension [2]. In recent years, polyanilines have received great attention due to their environmental stability, ease in preparation, exciting electrochemical, optical and electrical propertiesw [3,4]. This class of conducting polymers has also been postulated as potential candidates for numerous applications inelectrochromic displays, rechargeable batteries, microelectronics devices, biosensors, protective coatings and chemical sensorsw [5].

In this work, salt of (+)-2-sec-butylanilinum-(+)-camphorsulfonate, as monomer, was polymerized to form a new composite by in situ oxidative polymerization in the presence of ammonium peroxodisulfate as oxidant and silica under solid-state (solvent free) condition for the first time. The resulting composite was characterized using Fourier transform infrared (FT-IR)and ultraviolet-visible (UV-vis) spectroscopy.The morphology of composite was determined using scanning electron microscopy (SEM).



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Preparation of a New Chiral Nanocomposite from Polymerization of (+)-2-sec-Butylaniline-(+)-camphorsulfonate in the Presence of Nanosilica under Solid-State Condition

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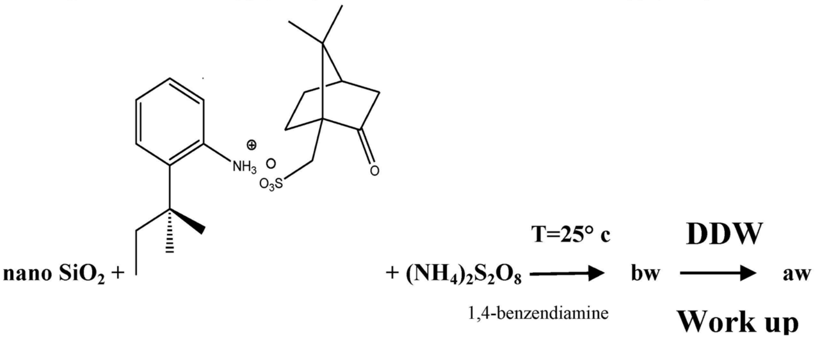
Conducting polymers and silica (SiO_2) are very important materials for a wide range of technological applications. Electrical properties of polymers are modified by adding inorganic particles within the polymer matrix. Composites containing organic polymers and inorganic particles regime provide a completely new class of materials with novel properties [1,2]. Among them, many PANI/inorganic polymer composites have been prepared recently. These composites based on polyaniline have been harvesting several intriguing properties within themselves due to the mutual influence of the individual constituents and synergism of their properties [3]. Nanocomposites are a special class of materials originating from suitable combinations of two or more such nanoparticles ornanosized objects in some suitable technique, resulting in materials having unique physical properties and wide application potential in diverse area. The development of nanocomposites is a topic of great current interest.

In this work, salt of (+)-2-sec-butylanilinum-(+)-camphorsulfonate was separated from its diastereomer (-)-2-sec-butylanilinum-(+)-camphorsulfonate by resolution method in solution. The former, as monomer, was polymerized to form a new chiral nanocomposite by in situ oxidative polymerization in the presence of ammonium peroxodisulfate as oxidant and nanosilica under solid-state (solvent free) condition for the first time. The resulting nanocomposite was characterized using Fourier transform infrared (FT-IR) and Ultraviolet-visible (UV-vis) spectroscopy. The morphology of nanocomposite was determined using scanning electron microscopy (SEM) and transmission electron microscopy (TEM).



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Synthesis and characterization of novel thermally stable and aromatic PAI/TiO_2 nanocomposites under ultrasonic process

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In the recent years, the preparation of polymer nanocomposite materials has been extremely considered due to their comparatively remarkable properties [1]. Titanium dioxide (TiO_2) nanoparticles have unique properties such as higher stability, safe, inexpensive and shown antibacterial activity [2]. TiO_2 nanoparticles have been especially the center of attention for their photo-catalytic activities. This makes TiO_2 nanoparticles applicable in many fields such as self-cleaning, anti-bacterial agent, UV protecting agent, environmental purification [3]. In this study, the novel poly (amide-imide) (PAI) with flame retardancy property was synthesized from the polymerization reaction of a novel diacid with 4,4′-methylenebis(3-chloro-2,6-diethylaniline) using molten tetrabutylammonium bromide (TBAB) and triphenyl phosphite (TPP) as solvent and activating agent. As well TBAB/TPP was used as easy, safe and nontoxic method for the preparation of PAI. The obtained polymer and inorganic metal oxide nanoparticles were used to prepare PAI/TiO_2 nanocomposites through ultrasonic irradiation. The resulting materials were characterized by ^{1}H-NMR, fourier transform infrared spectroscopy, elemental analysis, powder X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM) and thermogravimetric analysis (TGA) techniques. TEM and FE-SEM images showed that the nanoparticles were uniformly dispersed in the polymer matrix. FE-SEM of pure PAI and PAI/TiO_2 nanocomposites (15 wt %) showed in Fig. 1. TGA data demonstrated that new synthesized PAI/TiO_2 nanocomposites are more thermally stable than pure PAI.

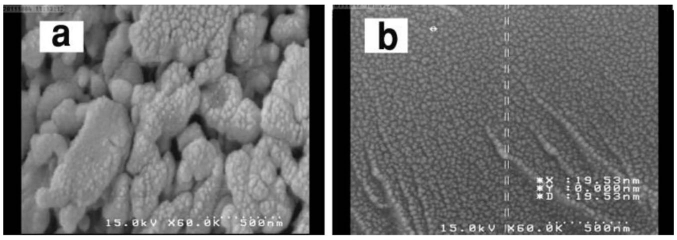

Fig. 1. Pure polymer (a), PAI/TiO_2 (15wt %) (b)

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Synthesis and Polycondensation of N-phenyl-N′-(1,2,4-triazolidine-3,5-dione-4-yl) thiourea with diisocyanates

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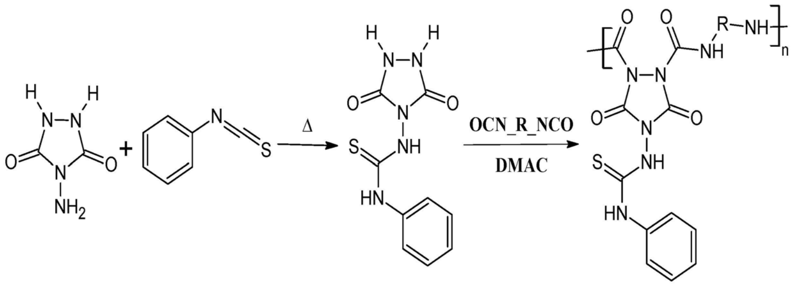
Some Urazole derivatives were found to be potent cytotoxic agents in murrain and human cancer cell lines. Other pharmaceutical properties of Urazole derivatives are hypolipidemic activity via lowering serum, cholesterol, and triglyceride levels [1], pesticides [2] and insecticides[3]. Preparations of thermoplastics, production of heat resistant coatings[4], tire rubbers with high gripability and melamine resins, are among the applications in the field of polymerization of urazole derivatives. Among a large variety of nitrogen-containing heterocyclic compounds, p-urazine (4-amino-1,2,4-triazolidine-3,5-dione) is interesting because It is used as a laboratory reagent for the synthesis of novel heterocyclic and organometallic compounds. In this work, we present synthesis of new polymers based on 1-phenyl-2-(1,2,4-triazolidine-3,5-dione-4-yl)thiourea.

p-Urazine was prepared according to a common procedure [5]. The mentioned compound was reacted with phenylisothiocyanate to its phenylurea-derivative directly. The phenylurea -derivative was introduced to various aliphatic and aromatic diisocyanates, as a DMAC solution. Some physical properties and spectroscopic data of the resulting polymers (4-7) were reported.



Diisocyanates: HMDI, IPDI, TDI,DPMDI

Polymers(4-7)

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Chemical Oxidative Synthesis of a New Composite of Poly(o-methoxyaniline) under Solvent-Free Condition

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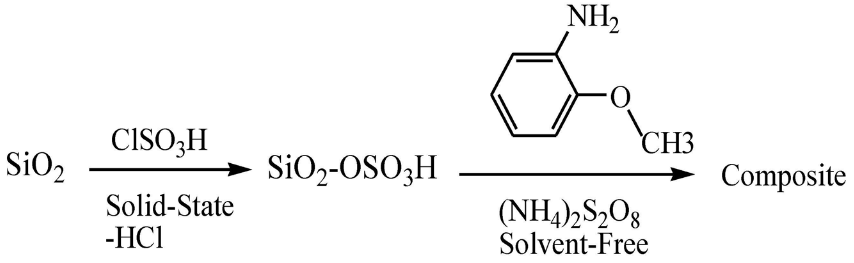
Recently, many research efforts have been made indeveloping polymer-silica hybrid composites [1–3].The combination of superior properties of polymers such as flexibility, dielectric, toughness and process ability, and that of oxides which have high thermal stability, good mechanical and optical properties, can lead to product of highly functionalized materials with desired properties to meet the demands of many industrial and high technology applications [4]. Organic/inorganic composite materials have been extensively studied for a long time. Organic/inorganic composites are generally organic polymer composites with inorganic nanoscale building blocks. They combine the advantages of the inorganic material (e.g., rigidity, thermal stability) and the organic polymer (e.g., flexibility, dielectric, ductility, and processability).

The compound ortho-methoxyaniline can be polymerized by both chemical and electrochemical methods. ortho-methoxyaniline or o-anisidine was chosen because of the potential effect of the methoxy group on chain solubility. The ortho-isomer was used instead of the meta because of the ortho-para directing nature of the methoxy group. With the ortho-isomer no one position is highly activated and a linear chain polymer is more likely [5].

In this work, we prepared a new composite from POMA by polymerization of 2-methoxy aniline in the presence of ammonium peroxydisulfate as under solvent free-condition. The UV-vis absorption spectra of composite were obtained in N-methyl-2-pyrrolidinone (NMP). The FT-IR spectra of composite were obtained from compressed KBr pellet. SEM image of composite particles has been used to determine the morphology and average size of the particles.



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Synthesis and Polycondensation of N-phenyl-N′-(1,2,4-triazolidine-3,5-dione-4-yl) thiourea with diisocyanates

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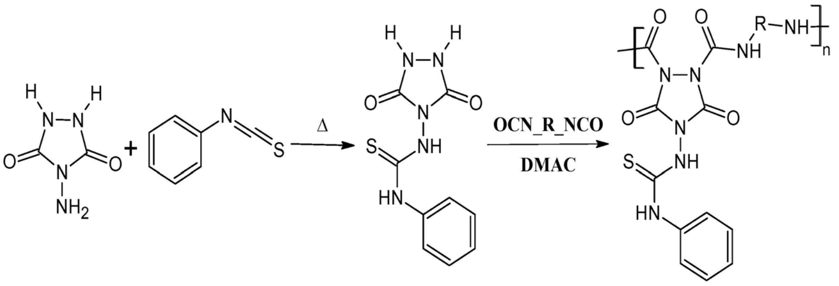

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Chemical Oxidative Synthesis of a New Composite of Poly(o-methoxyaniline) under Solvent-Free Condition

Ali Reza Modarresi-Alam[a*], Ilnaz Shariati[a]*, Tahere Akhondi[a], Sakineh Zafari[a]
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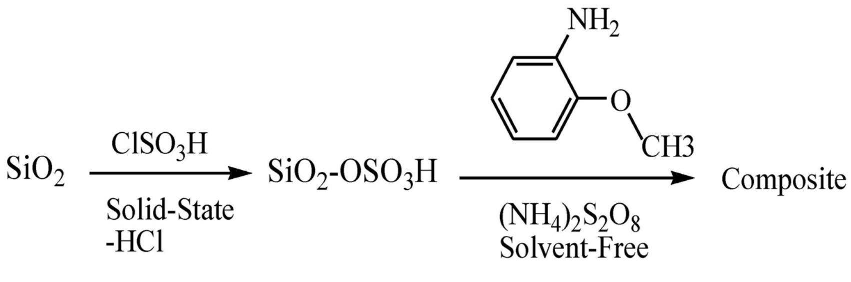

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Synthesis and Characterization of Aromatic tetra-Functional Methacrylate as Cross-linker for UV-Curable Coatings

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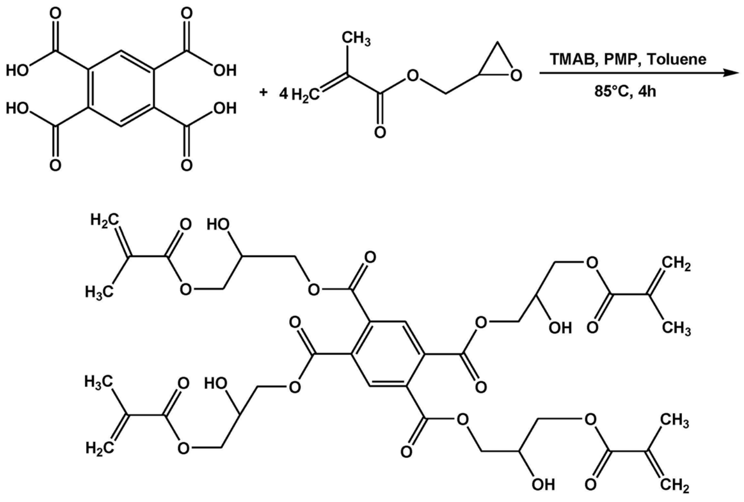
Aromatic tetra-functional methacrylate (ATM) can be used as a cross-linker in UV-curable coatings. The ATM was synthesized by 1,2,4,5 benzenetetracarboxylic acid and glycidyl methacrylate in present of tetramethylammonium bromide (TMAB) as catalyst, p-methoxy phenol (PMP) as radical inhibitor and toluene as solvent in 85°C for 4h. ATM was formulated in epoxy dimethacrylate as binder, benzophenone and N-metyl diethanol amine as photoinitiator and co-initiator, respectively. Curing time and film properties such as hardness, gloss, impact and adhesion have been evaluated after ultraviolet radiation curing.



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Synthesis of New Composite of Poly(anilinum hydrochloride)-Silica Under Solvent-Free Condition

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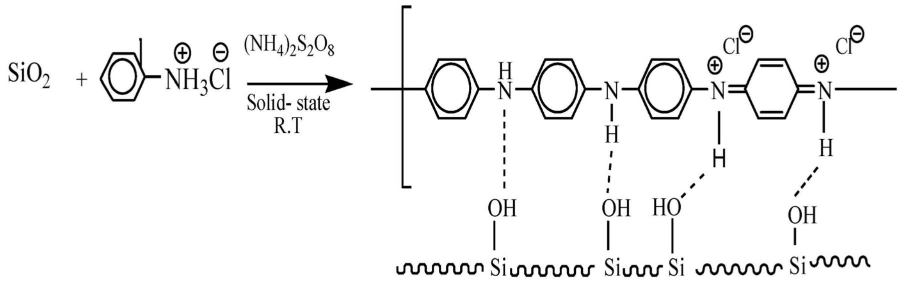
As a key material in the family of conducting polymers, polyaniline (PANI) has attracted intensive interest due to its promising electrical, electrochemical and optical properties [1]. In recent years, composites of PANI and inorganic compounds have been synthesized in order to get new materials with modified properties [2,3].

One way of making composites involves synthesizing the conductive polymer inside the matrices of conventional polymers (for example, inorganic polymers such as silica) or incorporating the inorganic component into the conducting PANI matrix using chemical or electrochemical polymerization [4]. Among those inorganic materials, silica (SiO_2) has received great attention because of its unique properties and wide applications [5].

In the present work, a new composite, poly (anilinum hydrochloride), with silica (SiO_2) was synthesized under solid-state or solvent-free condition. Ammonium peroxydisulfate was used as oxidant. The resulting composite was characterized by the UV-vis, FT-IR spectroscopy and Scanning electron microscopy (SEM) was done to study the morphology of composite.



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Synthesis and Characterization of Crosslinked CMC-Chitosan Full-Polysaccharide Biodegradable Films

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Introduction

During the past decades, researches on biopolymers have become an interesting area because of their versatile applications in various fields such as medical applications and nano-biocomposites [1,2]. Polysaccharides constitute the majority of the natural based biodegradable films because of their exceptional properties, i.e. biocompatibility, biodegradability, renewability, and non-toxicity. Carboxymethyl cellulose (CMC) is a renewable and biodegradable natural polymer that is used in a variety of commercial applications because of its capacity for gelatinization. Chitosan is a biodegradable copolymer composed of D-glucosamine and N-acetyl-D-glucosamine [3]. Chitosan is currently receiving enormous interest in medical and pharmaceutical applications since it is a safe and friendly substance for the human organism and because it has beneficial intrinsic properties [4]. The aim of the present work was to synthesize a biodegradable and biocompatible film that can be used in some applications such as tissue engineering and drug delivery systems.

Results and discussion

CMC-Chitosan full-polysaccharide hydrogels were prepared by crosslinking of chitosan with CMC polyaldehyde and subsequent reductive alkylation. CMC polyaldehyde molecule was prepared by periodate oxidation of CMC and then applied as a crosslinking agent to form a new hydrogel network. The swelling behavior of the polymer was studied at various pH values between 2.0 and 10.0 at room temperature. The swelling of the hydrogel decreased with increasing pH from 1 to 10. The dynamic swelling behavior of the hydrogel was determined with certain particles size (40–60 mesh) in water at room temperature. The equilibrium swelling was achieved after 20 min. Power law behaviors are obvious from the data and they may be well fitted with a Voigt-based equation.

Conclusion

CMC-Chitosan full-polysaccharide hydrogels were prepared by crosslinking of chitosan with CMC polyaldehyde and subsequent reductive alkylation. The structure of the hydrogel was confirmed by FTIR spectroscopy, scanning electron microscopy (SEM), and thermogravimetric analysis (TGA). Swelling and deswelling measurements of the synthesized hydrogel in different salt solutions showed good swelling capacity. The polymer will most probably possess high biodegradability due to the presence of natural polysaccharides and low toxicity since no toxic material is used in the synthesis process. This practical approach may be preferred as a relative “green process”. The synthesize polymer has potential applications in the controlled delivery of bioactive agents and for
wound dressing application in the form of sheets or film.

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Synthesis of poly(3,4-ethylenedioxythiophene)/silver nanocomposites in the presence of sodium dodecyl sulfate in aqueous medium

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Nanocomposites formed by metal nanoparticles (NPs) dispersed in electrically-conducting polymers, such as polyaniline, polypyrrole, or poly(3,4-ethylenedioxythiophene) (PEDOT), have received attention in the past few years [1]. The polymer and metal nanoparticles in these hybrid nanomaterials are expected to display several synergistic properties, making them potential candidates for application in several fields: catalysis [2], sensors and biosensors [3] and memory devices [4]. In polymeric core-shell nanohybrids, the polymer shell protects the metal core from oxidation and corrosion, allowing good performance to be maintained. In the present research, we report a novel one-step synthesis of PEDOT-coated silver nanocomposites with core-shell morphology by aqueous chemical oxidative dispersion polymerization and an electron exchange of PEDOT with silver nitrate. This discovery substantially broadens and extends the scope of core-shell particle syntheses.

Firstly, 3,4-ethylenedioxythiophene (EDOT) (0.85 mL, 8 mmol) was added to a colloidally-stable Ag NPs with sodium dodecyl sulfate (SDS) as the colloidal stabilizer. The mixture was then stirred at 25 °C FOR 1 h. Next, the solution of $FeCl_3$ oxidant (3.2442 g, 20 mmol) in distilled deionized water (DDW) (20 mL) was added dropwise to the reaction vessel. The final mixture was stirred for an additional 24 h. Secondly, to compare the results obtained; a pure sample of PEDOT in the presence of SDS was also prepared in a similar manner. Note that the SDS used in the first work plays simultaneously the role of both the dispersant of the nanosilver particles and the creator of micelles in polymerization step. The SDS used in the next work, however, acts only as an emulsifier. The resulting products were characterized by IR, UV-vis, X-ray diffraction (XRD), scanning electron microscopy (SEM), and thermogravimetric analysis (TGA). In addition, the homogeneously-dispersed silver nanoparticles in the matrix of polymeric sample were obviously observed by transmission electron microscopy (TEM).

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Synthesis and Characterization of Wholly Aromatic Poly (amide-imide), Thermally Stable and Organosolubl Based on Trimellitic acid

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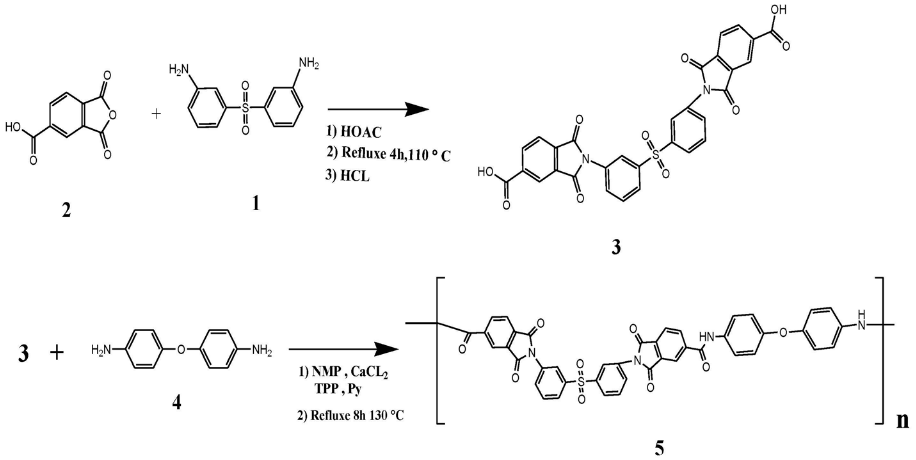
Poly (amide-imide) s (PAI) s as high performance materials (excellent thermal stability and mechanical properties) have been noted in new century [1], however, it has some defects such as low solubility and processing that cause difficulty for synthesis [2]. The use of aromatic groups in poly (amide-imide) s has been shown better resistance compared to ones containing nonaromatic groups but these groups are rigid and may decrease solubility. The use of some flexible groups (such as -O- ,$-SO_2-$, $-CH_2-$) may improve these deficiencies. In this project, new monomer (3) was synthesized with condensation reaction between 3, 3'-diamino diphenyl sulfone (1) and trimellitic acid (2), it was fully characterized by FTIR spectroscopy, elemental analysis and melting point successfully in high yield (90%). The poly (amide-imide) (5) was prepared reaction of diacid (3) and 4, 4'-diamino diphenyl ether (4) by direct polymerization at the presence of triphenyl phosphite, $CaCl_2$ and pyridine in N-methyl-2-pyrolidone (NMP), the structure of this organosolubl PAI was determined by FTIR spectroscopy, elemental analysis, thermal gravimetric analysis (TGA and DTG) and inherent viscosity of this polymer is 0.3 dLg^{-1} in high yield (97.77%). The resulting PAI was shown excellent thermal stability (T_5: 285.18 °C, T_{10}: 340.63 °C) since existence a lot of aromatics groups in it (see figure-1), and this PAI has been shown so high solubility due to there are flexible linkage groups like $-SO_2-$ and -O- in the main chain of PAI. This new soluble poly (amide-imide) could be considered as new processable high-performance polymeric material.



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Fabrication and study on morphology and properties of biodegradable poly(amide-imide)/organo-montmorillonite/modified ZnO nanoparticles

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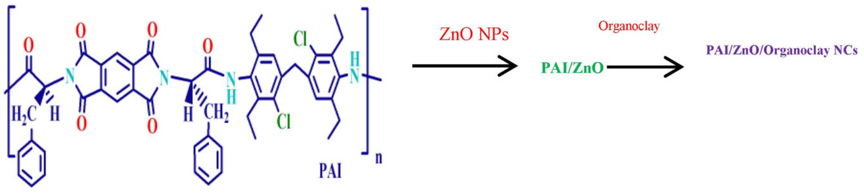
Polymer nanocomposites (NCs) are a very interesting material because of their remarkable mechanical properties like elastic stiffness, strength and thermal stability with a small amount of the nanoadditives [1-3]. Whether the nanocomposites would have high thermal stability and improved mechanical property, when two types of nanomaterials are incorporated into the polymer matrix [4]. The objective of this study was to investigate the effect of addition of organoclay on the properties of the Poly(amide-imide) (PAI)/zinc oxide (ZnO) NCs. At first optically active PAI was synthesized from the direct polycondensation reaction of N,N-(pyromellitoyl)-bis-L-phenylalanine diacid with 4,4-methylene bis(3-chloro-2,6-diethylaniline) under green media using tetrabutylammonium bromide/triphenyl phosphite. Subsequently dispersion of ZnO nanoparticle in a PAI matrix was performed using ultrasonic system. Then, PAI/organoclay/ZnO NCs with 1, 3, 5, 7 and 9% of organoclay content were prepared via a solution intercalation technique (Scheme-1). The morphostructural properties of the synthesized materials were studied by X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), FT-IR spectroscopy and thermogravimetric analysis techniques. It was found that the PAI/organoclay/ZnO NCs exhibit considerably enhanced thermal properties compared with the PAI/ZnO NCs. XRD analysis showed that organoclay layers are exfoliated during the solution intercalation process in NCs with 5 wt% organoclay loading. This exploration presented a favorable method for preparation of environment-friendly biodegradable polymer NCs with two nanomaterials of organoclay and ZnO.



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Preparation and characterization of phtoluminescent polyimide/titania(TiO_2) hybrid nanocomposites by sol-gel processes

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In the past two decades, organic/inorganic nanocomposite materials obtained by sol-gel process have drawn a vast deal of consideration in material science owing to their unique properties [1]. In inorganic nanoparticles, TiO_2 is one of the most potential materials in research and application fields because of its versatile functions. Due to the expected properties of TiO_2, considerable attention has been devoted to the manufacture of well-dispersed TiO_2 in polymer matrix used as interference filter, antireflective coating, and optical waveguides [2,3]. These polymer/inorganics hybrid materials can effectively increase the mechanical and thermal properties by the microstructure of inorganics particles well-dispersing in polymer matrices. In this study, when titanium alkoxide is added into polyimide (PI) matrix, the gelation and phase separation occurred easily due to the relatively fast hydrolysis rate to create precipitates of titanium alkoxides. Thus, the use of acetylacetone (ACAC) chelating agent is necessary in order to control the reactivity of titanium alkoxides of the resulting nanocomposite materials [4,5]. PI/TiO_2 hybrid films via sol-gel process in situ preparation show higher glass transition temperature, an increase and flattening of the rubbery plateau modulus, and a decrease in crystallinity and could be dried afterwards without any post-treatment utilized in gas separation.

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Synthesis and polymerization of new anthracene -Based diamine

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The overall goal of this ongoing research is to modify the structure of aromatic polyimides to attain solubility in common organic solvents without substantially decreasing the rigidity of their backbone [1,2]. Solubility is sought to allow processing in the imide form and, thus, avoid the many problems associated with handling poly(amic acid) (PAA) precursors [3,4]. This is especially important in microelectronic and optical applications where the imidization conditions for PAAs used during processing can dramatically affect the final material properties [5,6]. The objective of this research was to investigate the effects of introducing pendent anthracene groups along the polyimide backbone. Thus, the new diamine was to be synthesized and polymerized with a series dianhydrides. The resulting polyimides were to be thoroughly characterized. In particular, the effects of the anthracene groups on the solubility of the polymers and the optical properties of their films were to be carefully determined.

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Preparation and characterization of phtoluminescent polyimide/titania(TiO_2) hybrid nanocomposites by sol-gel processes

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Synthesis and polymerization of new anthracene -Based diamine

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Magnetic Hyperbranched Polymer Based on Carbon Nanotube

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Carbon nanotubes (CNTs), discovered by Iijima [1], have attracted more and more attention for their unique structure and excellent mechanical, electrical and thermal properties [2]. Due to their fascinating nanoscale dimensions and high surface areas, CNTs are considered as an ideal carrier to direct assembly of inorganic nanoparticles (NPs) which have special properties [3]. Among these inorganic NPs, iron oxide nanoparticles (Fe3O4 NPs) are of great importance for their good magnetic properties which endow them with potential applications in color imaging, magnetic recoding media, soft magnetic materials and for Adsorption of Dyes [4]. the modification of surface of CNTs which is based on chemical reactions on the sidewall and tips of CNTs. Different chemical reactions have been used to conjugate variety of molecules on the convex walls and tips of CNTs [5,6].
In summary, we reported a facile method to prepare magnetic MWMTs/Fe3O4 NPs/PCA composite nanotubes through a two-step process. We first in situ synthesize Fe3O4 NPs on the surface of MWNTs and then coated the nanocomposites with PCA layer via polycondensation reaction. SEM and TEM images confirmed the core-sheath nanostructure and the attachment of Fe_3O_4 NPs on the surface of MWNTs. However CNT-g-PCA is probably the biocompatible nanocomposite which is soluble in the water freely.The combination of these properties in a nanocomposite makes it promising material for nanomedicine applications.
The molecular structure and composition of MWNTs/Fe_3O_4 NPs/PCA nanotubes were characterized by Fourier transform infrared spectra (FTIR, X-ray diffraction (XRD) and Raman spectra. UV–vis spectra confirmed the existence of PCA.

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Micelle-assisted one-pot preparation of polyaniline/Ag nanohybrids in a water-based nanofluid

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It has been demonstrated that the incorporation of metal nanoparticles (NPs) could effectively improve the electrical, optical and dielectric properties of polyaniline (PANI) composites [1-3]. Composites of PANI with silver NPs have been prepared in three ways: (1) template Ag NPs were embedded into PANI during its conventional polymerization using APS oxidant (2) presynthesized PANI was used as a reductant of silver salts to metallic silver, and (3) the oxidation of aniline with silver ion as oxidant yielded a composite of PANI and metallic silver [1-3].

In the present work, we tried to apply the first approach in a new form. In the first step, a stable water-based nanofluid of metallic silver was prepared using silver nitrate, sodium iodide and sodium borohydride in the presence of sodium dodecyl sulfate (SDS) surfactant, which plays only the role of a dispersant in this step. The concentration of SDS was willfully selected upper than its critical micelle concentration (CMC), able to provide micelles for the next step. To acidify the medium (PH=1), hydrochloric acid was added. Aniline and ammonium peroxydisulfate (APS) were then added dropwise into the resulting nanofluid, respectively. The molar ratios of APS oxidant to monomer and monomer to surfactant were 1.2 and 5.0, respectively. The emulsion polymerization reaction was allowed to proceed for 48 h, while stirring at room temperature. Acetonitrile was added to the green dispersion to destroy the micelles. The suspension was filtered, and the solid was washed with the corresponding acid solution and acetone to remove residual monomer, SDS, oxidant as well as other low molecular weight oligomers. A thorough final washing with acetone also prevents the aggregation of PANI precipitate during the drying stage so that the product is obtained as a fine powder. The product was characterized by IR, UV-vis, X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and thermogravimetric analysis (TGA). In sum, it could be concluded that this novel micelle-aided one-pot strategy provides an exceptional method to prepare PANI/Ag nanocomposites with the best nanoparticle distribution, optical, morphological and thermal characteristics.

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Probing effects of employing binary organic solvents in synthesis line of poly(3-methylthiophene)/SiO_2 nanocomposite using surfactants

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Unlike polythiophene, poly(3-alkylthiophene)s are both readily soluble in many organic solvents and melt processable. This class of materials has good chemical and environmental stability with excellent electronic and optical properties suitable for various applications in advanced technology [1-3]. Chemical oxidative polymerization technique, which kindly provides a large scale of it in each batch process,has a notable limitation associated with low organosolubility of the oxidant used. The most commonly used oxidant to prepare poly(3-alkylthiophene)s is ferric chloride. It has been demonstrated that the least concentration of this oxidant that should be present in the reaction vessel is two times of mole ratio relative to the monomer. However, solubility of $FeCl_3$ in chloroform, as the usual solvent for preparing these types of polymers is too little to be ideal. Accordingly, the plan of employing binary organic solvents in synthesis line of the most important poly(3-alkylthiophene)s namelypoly(3-methylthiophene) seems to be very useful if performed well. Meanwhile, this ingenious plan for the first time was successfully exercised by Im et al. [4]. On the other hand, it is well-accepted that the embedment of nanosized particles such as nano-Ag, Au, TiO_2 and SiO_2 into the matrix of these polymers has some exceptional results that develops their applicationextensively.

Here, we report a unique chemical oxidativemethod using two kinds of miscible organic solvents including acetonitrile and chloroform for thesynthesisof poly(3-methylthiophene)/SiO_2nanocomposite.To prepare ahomogeneous nanofluid from nanoparticles of $SiO_2$by sonication in chloroform, two dispersants including sodium dodecylbenzenesulfonate (SDBS) and sodium polystyrene sulfonate (SPSS) were separately used. Firstly, a solution of $FeCl_3$ oxidant in CH_3CN was added slowlyto the stabilized $CHCl_3$-based nanofluid while stirring. In this modified technique, we could reach five for the molar ratio of $FeCl_3$ to 3-methylthiophene, which this had some positive effects on the composite optical and thermal behavior according to UV-vis, XRD, SEM, TEM and TGA results. Polymerization was carried out at room temperature with 24 h stirring. To compare the results, a sample of poly(3-methylthiophene)/SiO_2nanocomposite was also prepared in its classical form under the same conditions without the use of CH_3CN.In both cases, the composite suspensions were filtered out, washed with methanol and then dried at 50 °C under vacuum. Obviously, it should be noted that the employing binary solvents to preparepoly(3-methylthiophene)/SiO_2nanocomposite using surfactantsopensa new window toward us in the field of nanotechnology.

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Controlled drug delivery of Phenobarbital using of melamine modified poly(vinyl acetate-alt-maleic anhydride)hydrogel

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Hydrogels are hydrophilic three dimensional swellable networks that can be obtained by chemical and/or physical crosslinking of polymers. They show a wide variety of applications as medical devices and in the field of pharmaceutics.[1]

Hydrogels have been developed as stimuli-responsive materials, which can undergo abrupt volume change in response to small change in environmental parameters: temperature, pH, ionic strength, etc.[2-4]

In these work we synthesized pH sensitive hydrogels base on poly (vinyl acetate-alt-maleic anhydride). The melamine was grafted on backbone of poly (vinyl acetate-alt-maleic anhydride) in various ratios. The cloudy point of prepared polymer in aqoues solution respect to pH was measured and the pHs of sol-gel transitions were in about 7.5. The swelling index of prepared polymers was measured. Then the Phenobarbital drug was loaded on prepared hydrogel and in-vitro drug release behavior of drug-adduct hydrogel was investigated.

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Preparation of 1,2-bis-(2-hydroxy ethyl)-4-tetrabromo phthalimido-1,2,4-triazolidine-3,5-dione of p-urazine

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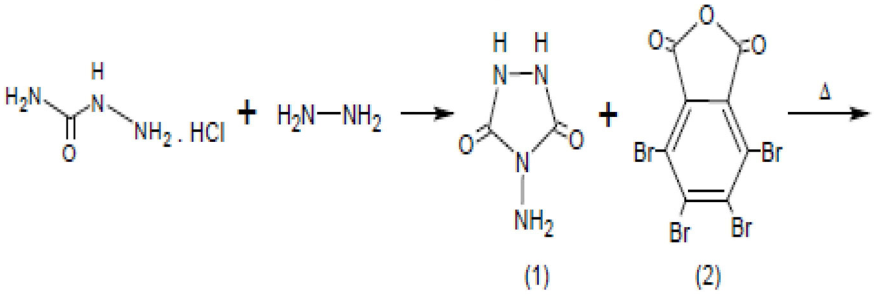
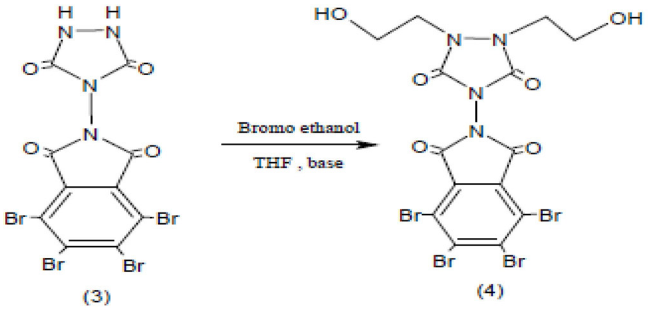
Heterocyclic nitrogen-containing molecules constitute the largest portion of chemical entities, which are part of many natural products, fine chemicals, and biologically active pharmaceutical compounds, vital for enhancing the quality of life [1]. Among a large variety of nitrogen-containing heterocyclic compounds, p-urazine (4-amino-1,2,4-triazolidine-3,5-dione) **(1)** is interesting, because it is used as a laboratory reagent for the synthesis of novel heterocyclic and organometallic compounds [2]. In this work, we present synthesis of 1,2-bis-(2-hydroxyethyl)-4-tetrabromo phthalimido-1,2,4-triazolidine-3,5-dione. p-Urazine was prepared according to a common procedure [3]. The mentioned compound was reacted with tetraboromophthalic anhydride **(2)** to its related phthalimid derivative **(3)** directly. tetraboromophthalimido-1,2,4-triazolidine-3,5-dione reacted with excess amount of 2-bromoethanol. as the result, 4-phthalimido-1,2,4triazolidine-3,5-dione was introduced to 1,2-bis-(2-hydroxyethyl)-4-tetra bromo phthalimido-1,2,4-triazolidine-3,5dione **(4)**, was produced. The resulted molecule was identified by varius spectroscopic methods. Polymerization reactions of the mentioned product is under investigation.





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Synthesis of Conductive blend based on Polyaniline/ Ciricacid grafted copolymer

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In recent years, polymer-polyaniline (PANI) conductive polymeric blends have received considerable attention because of their potential applications in electrodes, biosensors, batteries, antistatic coatings, gas sensors, membranes and light emitting diodes[1-3].

Citric acid grafted Poly(styrene-alt-maleic anhydride) was synthesized by ring opening graft reaction of citric acid on poly(styrene-alt-maleic anhydride) copolymer with various molar ratio in THF as solvent. The prepared copolymer was characterized by FT-IR and H-NMR spectroscopy. Conducting polyaniline (PANI) nano particles doped with HCl was synthesized by a sonochemical method. Polyaniline/citric acid modified Poly(styrene-alt-maleic acid) blend with different polyaniline content were developed by solution-dispersion blending method. The influence of citric acid Poly(styrene-alt-maleic acid) concentration in blend structure was also investigated. The blend dispersed solution in water/ethanol cast to fabricate conductive films with evaporation of the solvent. With only a mixing procedure and without any dispersant added, the PANI nanoparticles were well dispersed in the matrix polymer as indicated by AFM images. The conductivity of obtained blends was measured with four probe technique. The obtained blend characterized by FT-IR and UV-Vis spectroscopy.

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Synthesis and Characterization of a New Composite of Polyaniline by Doping Polymer with Silica Sulfuric Acid under Solvent-Free Condition.

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Polyaniline (PANI) is a very important polymer owing to its diversified chemistry and interesting physical properties [1]. Polyaniline can be doped and undoped on exposure to an acidic or alkaline environment without changing the number of π-electrons in the polymer [2]. This aspect of doping and undoping makes polyaniline and its analogous highly suitable for industrial applications. Various organic and inorganic acids and salts can dope polyaniline [3,4]. In this work, a new composite of polyaniline-silica sulfuric acid (PANI-SSA) was synthesized at room temperature and under solid-state or solvent-free condition [5,6], Scheme. In fact, we used a new solid polymeric acid dopant (silica sulfuric acid) in doping polyaniline.

The resulting composite was characterized by FT-IR and UV-vis spectroscopy and its doping was confirmed by means of comparison with prepared polyaniline emeraldine base. In other words, the doping process has been proved via FT-IR and UV-vis spectroscopy. The morphology of composites was determined using Scanning Electron Micrographs (SEM). The conductivity of the synthesized samples was measured by means of a four-probe device.

$$SiO_2 \xrightarrow[\substack{\text{solid-state} \\ \text{-HCl}}]{\text{ClSO3H}} SiO_2\text{-}OSO_3H \xrightarrow[\substack{\text{solid-state} \\ \text{R.T}}]{\text{PANI-EB}} \text{Composite SSA-PANI}$$

Scheme

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Silica-Supported Sulfuric Acid as Effective Solid Dopant Acid in Doping of Polyaniline Emeraldine Base for Synthesis of a New Composite of Polyaniline in Solid-State

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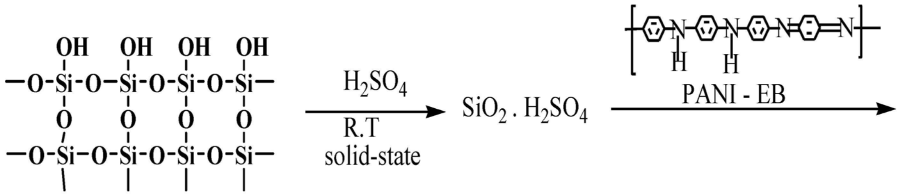
Polyaniline (PANI) is one of the most promising conducting polymers due to its straightforward polymerization and excellent chemical stability combined with relatively high levels of conductivity [1]. The conductivity of PANI can lead to change and increase when PANI is doped or protonated with acidic compounds such as HCl, H_2SO_4, or some organic sulfuric acids such as silica-supported sulfuric acid (SSSA) [2]. Also it is possible to modify the electrical properties of PANI by adding inorganic particles within the polymer matrix. So composites containing organic polymers and inorganic particles such as silica (SiO_2) provide a new class of materials with novel properties [3].

In the present work, a new composite of PANI-EB with SSSA was synthesized under solid state or solvent-free condition. The solvent–free reactions are industrially important due to reduced pollution, low costs, and simplicity in process and handling [4,5], Scheme.

The resulting composite was characterized by FT-IR and UV-vis spectroscopy and its doping was confirmed by means of comparison with prepared polyaniline emeraldine base. In other words, the doping process has been proved via FT-IR and UV-vis spectroscopy. The morphology of composites was determined using Scanning Electron Micrographs (SEM).



Composite PANI-EB-Silica supported sulfuric acid

Scheme

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Investigating the effects of starch phosphates on flowability of Portland cement slurries

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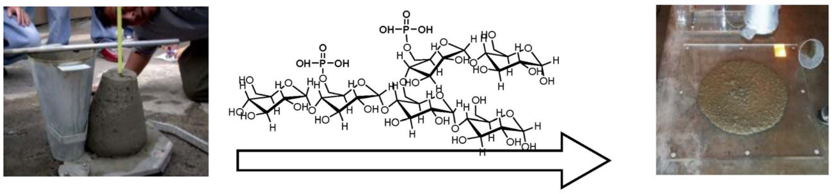
In the construction industry, it is very important for fresh concrete to be fluid enough to provide facile transportation and placing. To achieve this, the so-called water-reducing agents are used, which interact with the surface of cement particles and decrease their natural tendency to coagulate in aqueous systems [1]. Many conventional water-reducing agents are the condensation or addition polymers of synthetic origin. To avoid undesirable environmental effects of these petrochemical based materials, many investigations on water reducing agents based on the starch or cellulose were carried out [2,3].

In this study, an attempt has been made to enhance the flow and stability of Portland cement slurries by utilization of phosphorylated starch [4]. Consequently, we directed our efforts toward studying the rheological parameters of cement slurries, investigating the influence of molecular weight and DS value upon viscosity and yield stress of slurries, and also explored the possibility of using the starch phosphate as a stabilizer to enhance the paste stability and reduce bleeding.



Commercial cornstarch was acid hydrolyzed to yield various number-average molecular weights depending on the conditions of hydrolysis. The products were then phosphorylated using sodium dihydrogen phosphate and sodium hydrogen phosphate.

The phosphorus content of the starch phosphate was determined by a spectrophotometric method and the degree of substitution of the modified starch was calculated from the phosphorus content. It was shown that DS has an important role in enhancing the paste stability and flowability, so that bleeding rate and yield stress are reduced with increasing DS values.

Measurement of viscosity and yield stress of slurries by a rotary rheometer (Physica MCR-300) with shear rates from 0.01 to 100 S^{-1} suggested that best results were obtained only when the hydrolysis is mild. The progress of hydrolysis severely deteriorates the flow of the slurries.

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Synthesis, Characterization, and Properties of Novel Polyamides with Preformed Ester Structure

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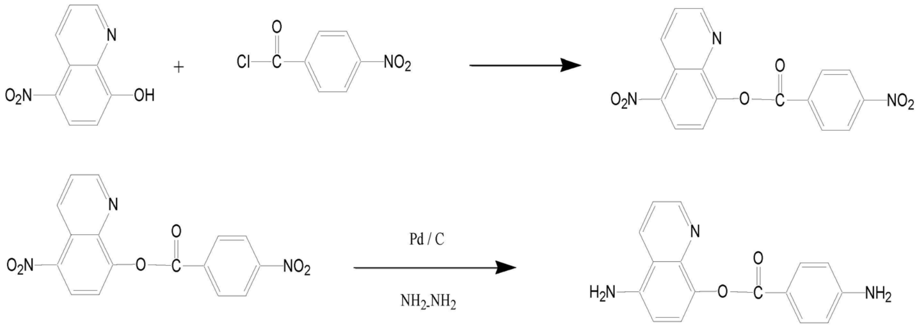
Aromatic polyamides are one of the most important classes of high temperature polymers that have good chemical and physical properties. But their industrial uses are limited by their difficult processability due to their high melting point, high glass transition temperature and limited solubility in most organic solvents [1,2]. Some certain properties could be introduced to the polymers by structural modification. Copolycondensation is one of the possible ways for modification of polymer properties. Modification of the properties of polyamides by incorporation of ester groups has been investigated and poly (ester amide) s have been studied extensively [3]. Therefore, much attention has been paid to different synthetic methods in this area for improving their solubility and processability (including introduction of flexible groups, bulky groups and disruption of symmetry and regularity of main chain) through the design and synthesis of new and specific monomer to obtain polymers with improved solubility while maintaining thermal stability. In this research, a new diamine was prepared via reaction of 8-hydroxy-5-nitro quinoline with 4-nitrobenzoyl chloride and subsequent reduction of nitro groups, and used as a monomer for the preparation of related polyamides with preformed ester unit.



Polycondensation reaction of this monomer with different aromatic diacid chlorides in the presence of propylene oxide (as an acid scavenger) led to preparation of different polyamides.

The prepared monomer and all the polymers were characterized by conventional methods. Thermal and physical properties of the polyamides including thermal stability, thermal behavior, solution viscosity, and solubility behavior in addition to crystallinity, and molecular weights were studied. They showed nice balance of properties including enhanced solubility, and heat-resistant that extends their application in various industries. Structure-property relations of the prepared polyimides were also studied.

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Novel poly(keto ether imide)s: as a new generation of soluble, heat-resistant polymers

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Aromatic polyimides are thermally stable polymers that generally show excellent mechanical strength and stability. Due to the increased performance characteristics demanded on polymers in various fields including the aerospace, automobile, and microelectronic industries, the use of these aromatic polymers in growing steadily [1]. However, one of the drawbacks to the employment of these high performance polymers is the difficulty in processing due to their high melting temperatures or high glass transition temperatures.[3] Therefore, some significant synthetic efforts, in the area of high-temperature resistant polymers, have been focused on improving their processability and solubility through the design and synthesis of new monomers [2,3]. Aromatic polyimides that contain aryl ether linkage generally have greater tractability, lower glass transition, and greater chain flexibility than their corresponding polymers without these groups in the repeat units. The improved solubility and lower glass transition temperatures are attributed to the flexible linkages that provide a polymer chain with a lower energy of internal rotation.

The present article deals with preparation a new diamine monomer containing ether and carbonyl flexible units and resulting poly(keto ether imide)s there from.

Monomer and polymers were fully characterized and the physical and thermal properties of the polymers including thermal stability and behavior, molecular weight, crystallinity, solubility, and mechanical properties were studied. As expected, polymers were high heat-resistance that was related to the fully aromatic nature of these polyimides and avoid of any weak linkages. Also, enhanced solubility of these polyimides was attributed to the high contribution of flexible groups (ether and ketone) in the backbone of these poly(keto ether imide)s.

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The effect of titanium dioxide nanoparticles on their physical and thermal properties of heterocyclic polyimides

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Nowadays, polymer-inorganic hybrid materials have become a popular topic in material science because of their unique properties [1-3]. This is related to their diphasic structure, leading to multifunctional materials. However, increasing interest in nano-size systems (ie systems of size range 0.5-100 nm) in recent years seems to be determined both by some distinctive properties of nanoparticles themselves and by anomalous cooperative properties of systems consisting of these moieties [4]. Polyimides (PI)s, which can be prepared from a variety of starting materials by a variety of synthesis routes and posses high thermal stability, high chemical resistance and excellent mechanical properties are a promising candidate type for the matrix of these hybrids [5,6]. The high glass-transition temperature of PIs would be expected to further stabilize the nanoparticles by decreasing their mobility, thereby preventing their agglomeration into large particles. In this study, the titanium alkoxide is incorporated into PI matrix through a simpler process and good quality and well-dispersed PI/titania hybrid films with relatively high titania content are prepared. Moreover, the characteristics of morphology, optical, mechanical, and thermal properties for the hybrid films are also investigated.

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The Role of Silica-Supported Camphor Sulfonic Acid in Doping and Synthesis of a New Composite under Solid-State Condition

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Conductive polymeric materials containing conjugated bonds have attracted much interest in scientific and technological areas in recent years. The conducting polymers such as polypyrrole, polythiophene, poly(p-phenylene), polyaniline and poly(o-methoxyaniline) have commonly been used in scientific and industrial studies and in various applications as rechargeable batteries [1,2], sensors [3–6], diodes, in transistors and microelectronic devices [7]. Among all the conducting polymers, polyaniline has received a great deal of attention owing to its simple synthesis, good environmental stability ability to dope with protonic acids and moderately high electrical conductivity [8]. The conductivity in thesepolymers can be varied by doping them with different protonic acids or by using functionalized protonic acids,these functionalized acids make polymer conducting as wellas render the resulting polymer complex soluble in common organic solvents such as m-cresol, toluene, xylene and chloroform[9,10].

In this work, a new composite was synthesized by doping of poly(o-methoxyaniline – emeraldin) base (POMA-EB) using of silica-supported camphor sulfonic acid. This method differs from the in situ polymerization because POMA-EB was prepared in a separate step and then doping was done by solid acid above . The resulting composite was characterized using Fourier transform infrared (FT-IR) and Ultraviolet-visible (UV-vis) spectroscopy. The morphology of composite was determined using scanning electron microscopy (SEM).

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Influence of nano-ZnO on polycondensation of UV-curable unsaturated polyester

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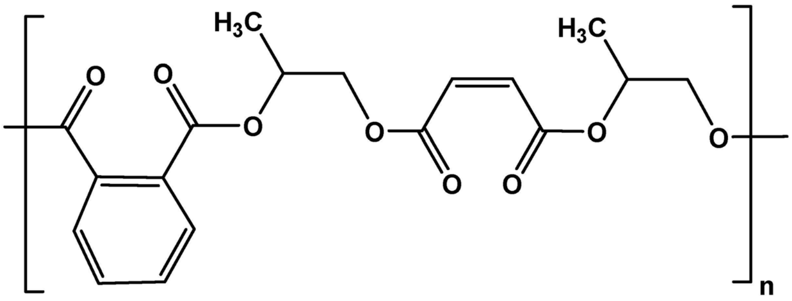
We have been synthesized UV-curable unsaturated polyester that can be used for wood coatings. The polyesterification of phetalic anhydride, maleic anhydride and propylene glycol was achieved in the presence of nano-ZnO. Unsaturated polyester was diluented by trimethylol propane triacrylate (TMPTA) and hexandiol diacrylate (HDDA). The diluented unsaturated polyester was formulated by benzophenone and N-methyl diethanol amine as photoinitiator and coinitiator, respectively. The formulated resins were cured by ultraviolet radiation. The effects of nano-ZnO on the mechanical properties of film coatings after UV radiation were evaluated by hardness, adhesion and gloss.



UV-curable linear unsaturated polyester

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Effect of nanosilica on the morphology and mechanical behavior of epoxy nanocomposite

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Among polymeric materials, thermosetting epoxy resins are commonly used in adhesives, coating, optical components and etc. due to their superior properties and low cost [1]. Depending on the specific desires for certain physical and mechanical properties, combinations of epoxy resin and some filler can usually be formulated. In the past decade, spates of research activities have been reported for improving mechanical properties of epoxy composites. Nanoparticles can significantly alter the mechanical properties of the polymer close to the particle surface due to changes in polymer chain mobility. Several recent investigations on nanocomposites of glassy polymer matrices reported enhance of strength and toughness [2-5]. As the matter of fact, silica has played an important role in reinforcement components due to nanoscale effects [6].

In this study, the mechanical properties of epoxy resin based on bisphenol A (DGEBA) with amine curing agent, in the presence of silica filler in comparison of different nanoscale concentrations were determined. Ultrasonic cavitation technique is one of the well-organized tools to disperse nanoparticles into a polymer [7]. Ultrasonic processor (Sartorius Labsonic® P, 105 W/cm2) was used to obtain a homogeneous mixture of epoxy resin/fumed silica and thereby helped to increase their interfaces. The mechanical properties of epoxy nanocomposites were measured via tensile test that were performed on dog-bone specimens (ASTM D3039 with crosshead speed of 1mm/min). Scanning electron microscopy (SEM) analysis was shown the agglomeration event in higher percentage of nanofiller. On the basis of obtained results, the epoxy nanocomposite contains 1 Wt. % of nanosilica showed sufficient disparity and highest strength and yang modulus.

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Investigation of plasticizing properties of ABA triblock copolymers based on PEG in cementitious systems

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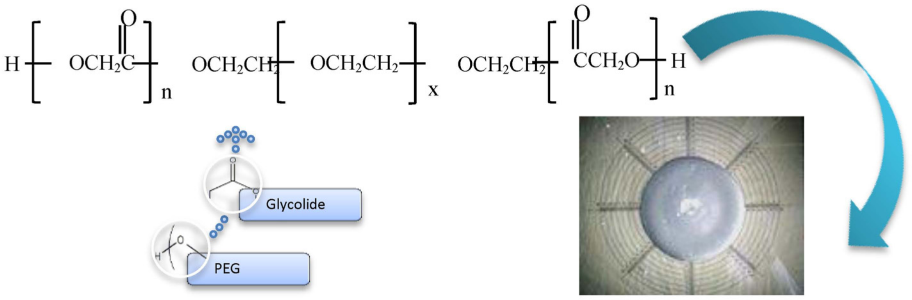
Plasticizers in cementitious systems are additives that uppon addition at a low dosage can change the workability, mechanical strength and other properties of cement paste effectively.[1] Plasticizers cause dispersion of cement particles and increase their mobility by two mechanisms: steric hindrance and electrostatic repulsion between cement particles by adsorption of negative functional groups on the plasticizer molecules.[2]

Slump retaining agents control the rate of setting of cement paste, so they can retain the workability of cement long enough for placing and finishing operation.

In this study, triblock copolymers based on poly ethylen glycol (PEG) was synthesised and their applications in the cementitious systems was investigated. The main purpose was verification of plasticizing effects of these copolymers in the cement paste. Ability of plasticizers depends on their structure, dosage and the water to cement ratio (W/C).[3]

ABA triblock copolymers with PEG (1000 and 1500 g/mol) as B block, poly caprolactone (PCL) and poly glycolide (PGA) (with different weigth ratio) as A block was synthesised via ring opening polymerization with stannous octanoate as catalyst. Their plastisizing effects and rheological properties was studied by mini-slump test and cylinder-cup rheometer. The Results show that by adding these copolymers to cement paste, the flowability increases, with PGA-PEG-PGA showing the highest performance. In this case the time of setting of hydraulic cement was also determined by Vicat Needle instrumen

Although these copolymers are not as efficient as commercial superplasticizer, they provide more insight into possibility and mechanism of plasticizing effects by non-ionic copolymers.



$$H\left[OCH_2\overset{O}{\overset{\|}{C}}\right]_n OCH_2CH_2\left[OCH_2CH_2\right]_x OCH_2CH_2\left[\overset{O}{\overset{\|}{C}}CH_2O\right]_n H$$

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Kinetics and Thermodynamics of Isothermal Curing Reaction of Epoxy - 4, 4'-Diaminodiphenylsolfon Reinforced with MWCNT Epoxy Functional

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Multiwall carbon nanotubes were functionalized with epoxy groups by chemical modification in four stages [1]. At each stage the compound was characterized by Fourier transform infrared spectroscopy and scanning electron microscopy. Epoxy composite samples were prepared by mixing diglycidyl ether of bisphenol A-based epoxy resin and synthetic epoxy functionalized multiwall carbon nanotube (E-MWCNT) with different percentages (1, 3, 6, 9, 12, 15 %) in acetone. Ultrasonic dispersion was used to produce homogenous blends. The optimum ratio of the reacting components (9%) was investigated by total enthalpy of the curing reaction from differential scanning calorimetry (DSC) thermograms. The kinetics of the curing reaction for epoxy composites with 4, 4'-diaminodiphenylsolfon as a curing agent was studied by means of a DSC isothermal technique [2]. The Kamal autocatalytic-like kinetic model was used to estimate the reaction orders (m, n), rate constants (k_1, k_2), and active energies (E_a) of the curing reaction [3]. However, the existence of E-MWCNT with hydroxyl groups in the structure catalyzes the cure reaction and influence the rate of reaction and therefore kinetics parameters. The E_a of cure reaction of DGEBA/DAS systems showed a decrease when E-MWCNT were present, therefore the rate was increased. Using the rate constants from the kinetic analysis and transition state (TS) theory, thermodynamic parameters such as enthalpy ($\Delta H^{\#}$), entropy ($\Delta S^{\#}$) and Gibbs free energy ($\Delta G^{\#}$) changes were also calculated [4]. The thermodynamic functions were shown to be very sensitive parameters for evaluation of the cure reaction.

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Small-Bandgap Conducting Polymers Based on Poly(heteroarylene methylenes) and Poly(heteroarylene methines). Synthesis, and Properties

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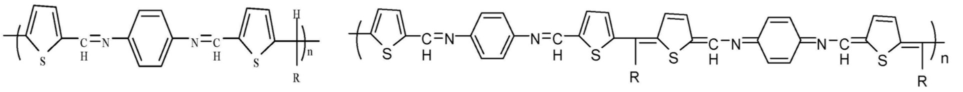
Currently known conducting polymers are prepared from π-conjugated polymers by a chemical or electrochemical process called doping which enhances the electrical conductivity of the pristine conjugated polymer by many orders of magnitude from the semiconducting to the metallic range (10^{-7} to 106 S/cm) [1]. However, it was also thought that control of the E_g value of a polymer by molecular design would allow the control of its optical, electronic, and optoelectronic properties [2]. There are a number of theoretical [3] and experimental [4] approaches to achieving small-bandgap conducting polymers. Along this, we wish to focus on the novel conjugated poly(N,N'-Bis(2-thienylmethylene)benzene-1,4-diamine methines) (I) and poly(N,N'-Bis(2-thienylmethylene) benzene-1,4-diamine methylenes) (II). Thus herein we report the synthesis and characterization of the poly(N,N'-Bis(2-thienylmethylene) benzene-1,4-diamine methines) and poly(N,N'-Bis(2-thienylmethylene)benzene-1,4-diamine methylenes). The theoretical and experimental characterization of relatively small band gap methines and methylenes –bridged derivatives is performed. AM1 and the modified extended Hückel theory were used to explore the ground-state geometric and electronic structures of these polymers.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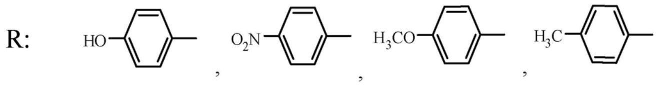

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Synthesis of salep phosphates and superabsorbent hydrogel networks based on Poly(acrylic acid) grafted onto salep phosphate for Controlled Release of Fertilizers

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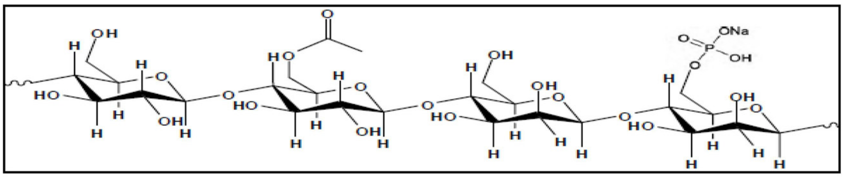
The preparation and applications of functional polymers is one of the most important research areas in polymer science. Incorporation of specific functional groups into polymers influences the physical, chemical, mechanical and rheological properties of materials [1]. Incorporation of vinyl monomers onto the backbone of natural polysaccharides helps in improving some properties of the polysaccharides and also allows the product copolymers to be used in novel applications, for example, as hydrogels. A hydrogel is a superabsorbent macromolecular compound that can absorb pure water up to hundred or thousand times of its dried weight [2].

Agrochemicals are bioactive agents that improve production of crops both in quality and quantity. contamination of ground water by agrochemicals becomes a great problem. One of the most alarming problems is nitrate leaching and subsequent pollution of ground water. Thus, the application of nitrate loaded carrier with a technology based on the controlled release of nitrates by the swelling of a polymeric carrier could prove to be a suitable technology against pollution of ground water [3].

In this study, salep phosphates with different phosphorus contents were prepared via reacting salep with a mixture of primary and secondary sodium phosphates under weak acidic conditions in a semi dry process. Effect of phosphorylaion of salep in swelling behavior and controlled release potential of superabsorbent hydrogels based on salep phosphates grafted with Poly(acrylic acid) is described. For a structural characterisation of salep phosphates FTIR spectra were recorded. The phosphorus contents of modified salep were determined using a standard wet chemistry method. The new superabsorbent hydrogel biopolymer was synthesized via radical crosslinking and graft copolymerization of acrylic acid monomer onto salep phosphates backbones. In our procedure, ammonium persulfate (APS) as a water-soluble initiator and methylenebisacrylamide (MBA) as a suitable crosslinking agent were used and the best synthesis conditions described.



Salep phosphates:

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Synthesis and characterization of novel chiral nanostructured poly(amide-imide)s from N-trimellitylimido-L-amino acids and 3,5-diamino-N-(thiazole-2-yl) benzamide under green condition

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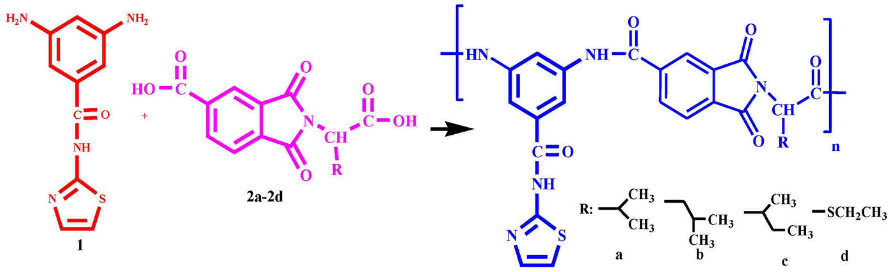
Recently poly(amide–imide)s (PAIs) have received much attention due to their favorable balance between process ability and performance. The PAIs have excellent thermal, physical and mechanical properties [1]. Functional macromolecular materials using biological chiral resources such as amino acids have been drawing much interest due to their biocompatibility and biodegradability easing the ecological trouble because amino acid residues can be targeted for leaving by different enzymes [2]. Thiazoles are reported to possess a broad range of antitumour, antibiotic, antibacterial, antifungal and antiinflammatory activities [2]. In the study a new series of optically active PAIs with moderated inherent viscosities in the range of 0.25-0.35 dL/g were synthesized from the direct polycondensation reaction of N-trimellitylimido-L-amino acids (2a-2d) with 3,5-diamino-N-(thiazole-2-yl)benzamide (1) in green medium consisting of tetra-n-butylammonium bromide and triphenyl phosphite (Scheme 1). At first N-trimellitylimido-L-amino acids were synthesized by the condensation reaction of trimellitic anhydride with two equimolars of various L-amino acids in acetic acid solution. Then, 3,5-dinitro-N-(thiazole-2-yl) benzamide (1) was prepared from the 3,5-dinitrobenzoyl chloride and 2-aminothiazole and it was reduction by using FeOOH/ hydrazine monohydrate. The resulted materials were fully characterized by means of by fourier transform infrared spectroscopy, ^{1}H-NMR spectroscopy thermogravimetry analysis, X-ray powder diffraction, UV-Vis spectroscopy and field emission-scanning electron microscopy.



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Synthesis and characterization of new aromatic polyesters

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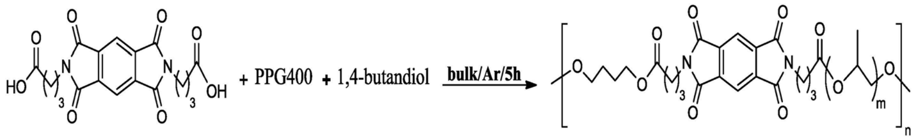
Polyesters are one of the most versatile polymers. They contain widely different materials with large applications, which are produced by a variety of manufacturing techniques [1]. They have in common the ester group –CO–O– in the main chain, which is a polar group and brings about inter and intramolecular chain interactions that may reflect in some properties such as low solubility, mobility of the chain and melting characterizations.[2]

Aromatic polyesters are of considerable interest both scientifically and commercially because of their excellent mechanical properties, chemical resistance and thermal stability [3, 4].

Dicarboxylic acid monomers were synthesized from the reaction of amino acids with anhydrides. Different polyesters with various molecular weights were synthesized from these carboxylic acids and diols with different stoichiometric molar ratios by polycondensation reaction. The obtained polymers were characterized by Fourier transform infrared spectroscopy (FT-IR), GPC, H-NMR and differential scanning calorimetric (DSC).



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Synthesis of N-methyl imidazol grafted poly(styrene-alt-maleic anhydride) copolymer and its application in phenol adsorption from aqueous solution

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Contamination of surface water and groundwater with aromatic compounds is one of the serious environmental problems human being today [2]. Phenol and phenolic compounds were listed as priority pollutants by the environmental protection agency (EPA) of United States and other countries and commonly present in industrial wastewater from oil refineries, petrochemical plants, ceramic plants, coal conversion processes, phenolic resin industries, pharmaceuticals, etc[1]. The permissible concentration of phenolic contents in potable water is $1\mu g\ L^{-1}$ according to the recommendation of world health organization (WHO) so it is toxic even at low concentration [3]. Various treatment methods have been applied to remove phenolic compounds from aqueous solution. In this work we select the adsorption method for removing of phenol from aqueous solution. For this propose the poly(styrene-alt-maleic anhydride) was synthesized by free radical polymerization. Then the alternative copolymer were modified by step by step grafting reaction of N-methyl imidazole and ethylene diamine as crosslinking agent on the poly(styrene-alt-maleic anhydride) backbone. The various ratio of N-methyl imidazole to poly(styrene-alt-maleic anhydride) were used in preparation of modified copolymers. Fourier transform infrared spectroscopy (FT-IR) was used for characterization of prepared polymers. The prepared copolymers were investigated in phenol adsorption from aqueous solutions. The prepared copolymers showed good capacity in adsorption of phenol.

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Synthesis of a New Chiral Composite of Poly(aniline-*co*-(±)-2-*sec*-butylaniline) in the Presence of Silica Sulfuric Acid in Solid-State

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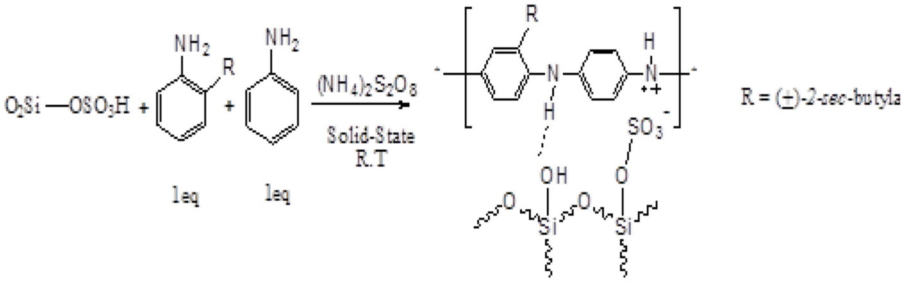
Conducting polymers and silica (SiO_2) are very important materials for a wide range of technological applications [1]. Enormous works on conducting polymers have been performed to enhance conductivity of conducting polymers by doping with inorganic and organic acids. Electrical properties of polymers are modified by adding inorganic particles within the polymer matrix. Among them, many PANI/inorganic polymer composites have been prepared recently. These composites based on polyaniline have been harvesting several intriguing properties within themselves due to the mutual influence of the individual constituents and synergism of their properties [1].

It has been found that ring-substituted (alkyl and alkoxy) and *N*-alkyl-substituted PANI are more soluble than unsubstituted PANI [2]. The most common method of chemical synthesis includes oxidation of the monomer with an oxidizing agent, e.g. ammonium peroxydisulfate, which is added to monomer solution [3].

In this work, a new chiral composite of poly(aniline-*co*-(±)-2-*sec*-butylaniline) with silica sulfuric acid has been synthesized at room temperature by chemical oxidation of monomers in presence of ammonium peroxydisulfate (APS) as oxidant [4]. In fact, copolymerization of mixture (1/1) of aniline and (±)-2-*sec*-butylaniline and doping of the obtained copolymer by silica sulfuric acid (SSA) has simultaneously been carried out in solid-state. The resulting composite was characterized by FT-IR and UV-vis spectroscopy. The morphology of composite was determined using scanning electron microscopy (SEM).



Scheme

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Cyanomethyl propane derivatives as pesticidal intermediates

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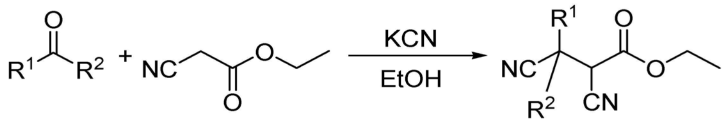
This research relates to a process for preparing certain cyanomethyl propane derivatives and the use of these compounds in the synthesis of pesticides and pesticide intermediates. Ethyl 2,3-dicyanopropionate was prepared and characterized by several methods.[1] However, many of these methods suffered from some drawbacks, that it is first necessary to isolate the intermediate formaldehyde cyanohydrins; These highly water soluble cyanohydrins are obtained by lengthy continuous extraction and have a limited stability, often decomposing violently upon attempted distillation. Furthermore, this reaction requires care given the risk of formation of dimeric side-products. In one aspect the present research seeks to provide a process for preparing cyanomethyl propane derivatives satisfying one or more of the following criteria:

- avoiding the use of formaldehyde cyanohydrins;
- avoiding the dimerisation side reaction;
- obtaining the required product directly in high yield and with high purity.



R^1, R^2 = Alkyl & Aryl

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How Analytical Chemistry Helps Organic Chemists to Understand Physical Chemistry?

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The massive use of analytical techniques, especially molecular spectroscopy, on the research methods of organic chemists has done much to condition universities to teach them a couple of modern physical (organic) chemistry courses. The commercial availability and widespread use of instrumentation for NMR, UV and IR spectroscopy has rendered an understanding of the theoretical bases of such techniques indispensable to the modern organic chemistry students and professors. On the other hand, all organic synthesis includes a separation (chromatography) step, which is primarily depends on physical chemistry theories.

In this article, it is described that there is a strong connection between (qualitative) organic analysis and physical chemistry. There will be an approach in this presentation between the theoretical concepts of physical chemistry and what are involved in the practical aspects of interpretation essential to the student who will be using chromatography and/or spectroscopy as an analytical tool in his undergraduate or graduate research.

Alumina Supported Acidic Ionic Liquid: Preparation, Characterization and Its Application as Catalyst in the Synthesis of 1,8-Dioxooctahydroxanthenes

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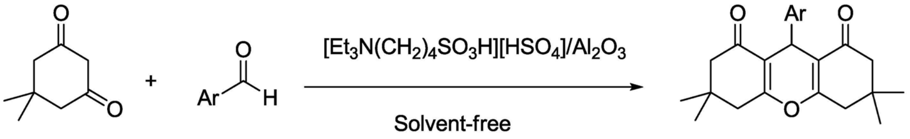
Xanthenes are important class of organic compounds with a large number of naturally occurring, as well as synthetic derivatives, and occupy a prominent position in medicinal chemistry.[1]A number of these compounds have been considered as dyes and fluorescent visualization materials for biomolecules and laser technologies.[2] Furthermore, these compounds have been investigated for their agricultural bactericide activity,[3] anti-inflammatory effect,[4] and antiviral activity.[5] Recently, many synthetic methods for preparing xanthenediones have been reported by the condensation of aromatic aldehydes and active methylene carbonyl compounds in the presence of various acid catalysts.[6-9] Many of these procedures suffer from lack of selectivity, unsatisfactory yields, being costly, toxicity of the reagents, or required special conditions.

Thus,we report herein an efficient synthesis of 1,8-dioxooctahydroxanthenes by the reaction of dimedone with aryl aldehydes using $[Et_3N(CH_2)_4SO_3H][HSO4]/Al_2O_3$ as a new solid acid supported catalyst. Reusability, easy work up, inexpensive, ready availability of the catalyst makes the procedure an attractive alternative to the existing methods for the synthesis of 1,8-dioxooctahydroxanthenes.



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Synthesis, lipophilicity studies and antibacterial properties of some novel indolecontaining pseudopeptides

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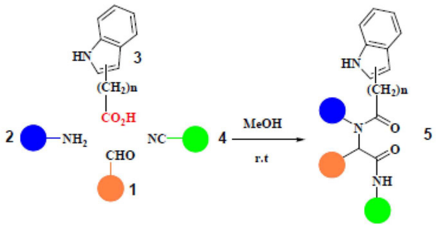

Indole nucleus is a substructure found in numerous natural products and pharmaceuticals possessing anti-inflammatory, antimalarial, antidepressant, antitumor and various other activities. Among the large family of indoles, indole carboxamides have recently attracted a great deal of attention of chemists and biologists due largely to their various pharmacological activities such as antioxidant, hypocholestrolemic, antihistaminic and Immunosuppressive.

Furthermore, in recent years, peptides and pseudopeptides especially those containing tryptophan have gained popularity as promising building blocks for design and development of novel materials with potential application areas ranging from drug design to biotechnology [1].

Considering all above, we`ve been greatly encouraged to synthesis novel indole-containing pseudopeptides via Ugi-4CR by the importance of indole carboxamides and the fact that although functionalized indole ring systems have been found frequently in biologically active compounds, indole derivatives as MCR partners are rather under-represented[2].

The compounds have been screened for their antimicrobial activity and they are found to exhibit moderate antimicrobial activities. The lipophilicity studies showed that most of the compounds possess optimum range for oral absorption and cell membrane permeation, as well as blood brain barrier permeation.

Keywords : Indole-containing pseudopptides, Antimicrobial activity, Lipophilicity

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The synthesis of 6-substituted-2-oxo-2H-chromene-3-carbohydrazides

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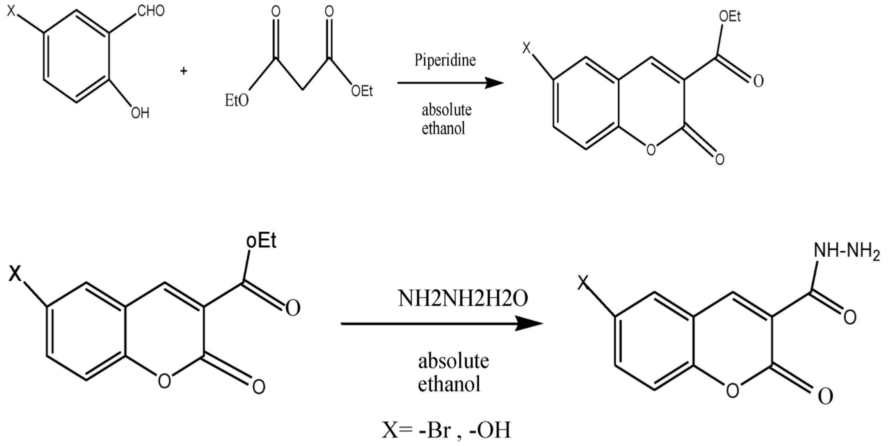
Abstract

Coumarins possess a variety of bioactivities including anticoagulant and antimicrobialeffects [1]. Some drug derivatives ofcoumarins are coumaromycin ,novobiocin and charteusin.[2-4]. 6-substituted-2-oxo-2H-chromene-3- carbohydrazides have been synthesized by the reaction of the 6-substituted-2-oxo-2H-chromen-3-carboxylate with hydrazine hydrate in the presence of ethanol under reflux condition after 5 hours.6-substituted-2-oxo-2H-chromen-3-carboxylate obtained from reaction of substituted 2-hydroxy benzaldehyde and diethylmalonate inabsolute ethanol usingpiperidine as base under reflux.The structures of novel synthesized compounds have been established by IR , H-NMR and Mass spectral data .

Keyword: chromene – hydrazine hydrate– diethylmalonate – carbohydrazid



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Palladium-Catalyzed intermolecular decarboxylation and Arylation of coumarin-3-carboxylic acids with Aryl bronic acid

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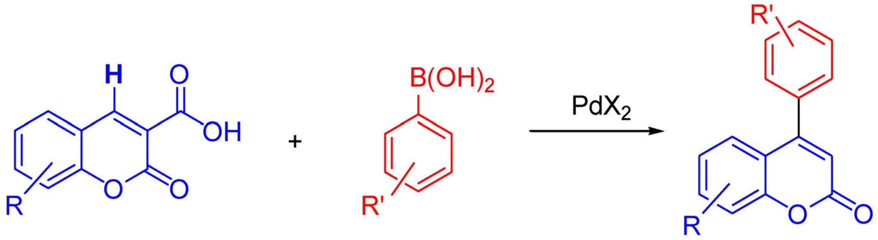
4-Arylcoumarins have attracted considerable attention as a result of their interesting biological and pharmacological activities and their presence in a variety of natural products. Depending on the substitution pattern, their antiprotozoal,[1] anticancer,[2] anti-HIV,[3] and cytotoxic properties[4] have been recognized. The transition-metal-catalyzed functionalization of C-H bonds is a powerful method for generating carbon-carbon bonds. Moreover palladium catalyzed cross-coupling reactions between organometallic and arene moieties are among the most employed methodologies for the synthesis of biaryls[5]. In this work a palladium catalyzed C-H activation of coumarin-3-carboxylic acids following decarboxylation with boronic acids is synergistically combined to synthesize coumarins arylated exclusively in the C-4 position (Scheme1).



Scheme1. Arylation of coumarin-3-carboxylic acids with aryl bronic acid derivatives

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Facile access to polysubstituted indoles via three component one – pot reactions in the presence of p-TSA

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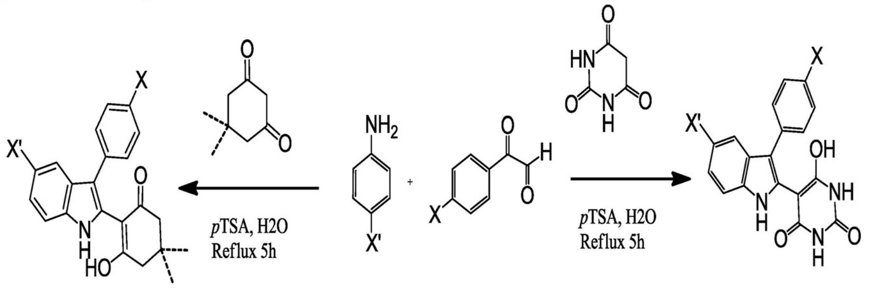
Multi-component reactions (MCRs) play an important role in organic chemistry. The significant contribution of MCRs is in the state of modern organic chemistry and their potential use in syntheses of complex organic [1]. Indole and its derivatives are known as important intermediates in organic synthesis and pharmaceutical chemistry [2]. Here, we report a new, simple and general synthetic method of substituted Indoles in high yields from three-component one-pot reaction of p-anilines, the phenylglyoxals and barbituric acid or dimedon in refluxing water in the presence of p-TSA for 5 h.



The simplicity of this experiment and work up are noteworthy. The structures of compounds were deduced from their ^{1}H NMR, ^{13}C NMR, mass and IR spectral data.

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An efficient method for synthesis two brominated derivatives of 4-nitroaniline without protection amine group

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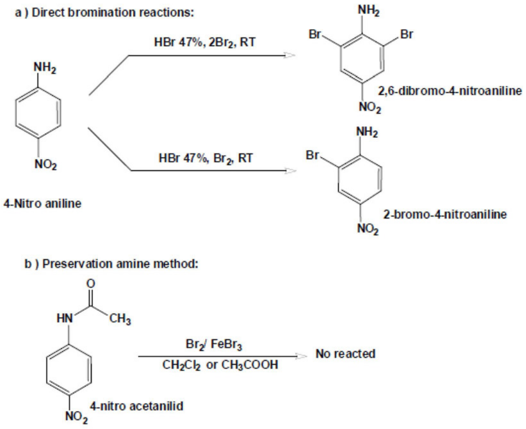
Organic molecules containing halogen atoms are found in many products. They are important intermadiets in reaction and in this type bromination and chlorination are straight forward processes . In aromatic molecules, electrophilic aromatic substitution reaction dependence to inductive and resonance effects that impressible from activator and deactivator groups. By protection of some functional group, slake these reactivity [1, 2]. In this research, 4-nitroaniline selected because it applied for very consumptions such as dyes and pigments synthesis, special antioxidant, corrosion inhibitor, pharmaceuticals, venom and gasoline intermediates [3, 4]. At present study in connection with our previous reports on the benign synthetic methods in organic chemistry, we wish to introduce an efficient protocol for the synthesis of new derivatives of brominated 4-nitroaniline by acid solvent. First, 4-nitroaniline powder was added in enough hydrobromic acid 47% in round-bottomed flask and warmed until completely dissolved, next solution cooled and wetted crystals formed the suspension. Then, cooled bromine was added dropwise to suspension and temperature is controlled for 4hr. Product powder extract from aqueous phase and recrystalized in ethanol [5]. These have been characterized with FT-IR and Melting point and solubility tests.



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Simple Synthesis of Amido coumarinyl furans Using A Multi–Component Reaction in Water

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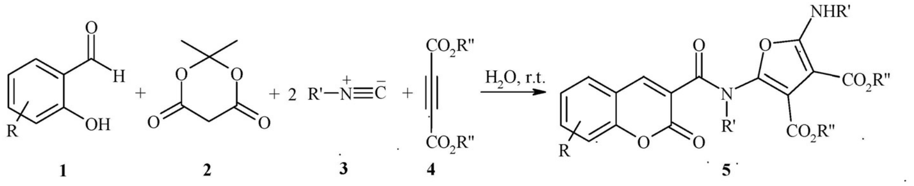
Furans, benzofurans, and their reduced forms are important core structures in functional materials and many biologically active natural products. Moreover, they are useful building blocks in total synthesis of natural products and pharmaceuticals.[1–4]

Coumarinyl compounds have been extensively used in medicinal chemistry. Some examples have been shown to be highly potent human β-secretase inhibitors and are used in the treatment of Alzheimer's disease. Most of the synthetic medicines containing coumarin, are prepared by the reaction between coumarin-3-carboxylic acids and amines.[5]

In recent decades green chemistry is a generally accepted term to describe the movement towards more environmentally acceptable chemical processes and products. Being nontoxic, readily available, nonflammable, inexpensive and environmental friendly, water has clear advantages as a solvent for use in green chemistry.[6,7]

Herein, we present a new synthetic method for the construction of potentially bioactive amido coumarinyl furan derivatives via a one–pot, isocyanide–based MCR involving commercially available starting materials. Thus a mixture of 2-hydroxy aromatic aldehydes **1**, meldums's acid **2**, dialkyl acetylenedicarboxylates **3** and isocyanides **4** afforded 2-(alkylamino)-5-{alkyl[(2-oxo-2H-chromen-3-yl)carbonyl]amino}-3,4-furandicarboxylates **5**.



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Pure and doped boron nitride nanotubes: A computational NMR study

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Abstract

Carbon and non-carbon nanotubes have been came into special focus of researches and received increasing attention during the past 10 years, due to their unique and fascinating properties, and wide potential applications [1] .

The electronic and structural properties of BNNTs have been investigated by either computational or experimental [2] studies.

We have investigated the properties of the electronic structure of the Disiline-doped boron nitride nanotubes (Disiline-BNNTs) by density functional theory (DFT) calculations. The structural forms are firstly optimized and then the calculated CS tensors in the optimized structures are converted to chemical-shielding isotropic (CS^I) and chemical shielding anisotropic (CS^A) parameters. The shielding values of B and N atoms are calculated by, continuous set of gauge transformations (CSGT) and individual gauges for atoms in molecules (IGAIM) methods, using B3LYP/6-311+G*. The B3LYP theory level with IGAIM method is the best choice to evaluate theoretical chemical shifts for compounds studied. The results reveal the significant effect of Disiline doping on the chemical shielding tensors at the sites of those 11B and 15N nuclei located in the nearest neighborhood of the Disiline -doped ring. Furthermore, in comparison to the pristine model, the values of dipole moments and LUMO–HOMO gap are changed in the Disiline -doped models.

Keywords: Disiline, DFT, Boron nitrid nanotube, Chemical shielding, Anisotropic, Isotropic.

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Synthesis and characterization of bis and tetrakis [tris(trimethylsilyl)silyl]borylferrocene

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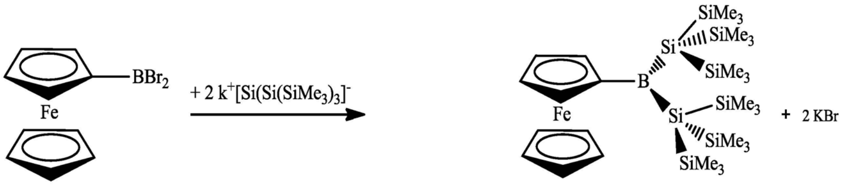
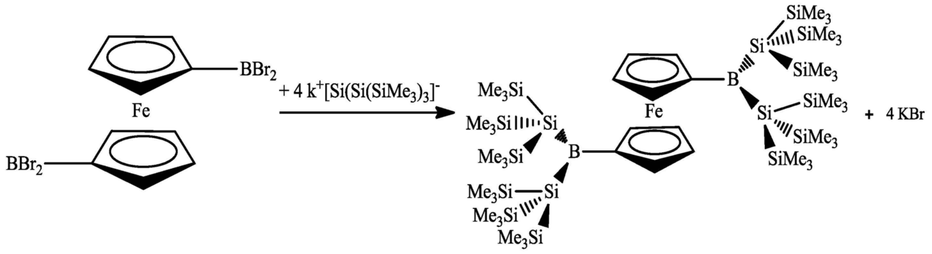
In the course of our studies of the synthesis of highly borylated aromatic systems, we report on the synthesis of bis and tetrakis [tris(trimethylsilyl)silyl]borylferrocene **2a** and **2b**.
The Compounds **(**dibromoboryl**)** ferrocene **1a**, and 1,1′- bis(dibromoboryl) ferrocene **1b** [1,2] were synthesized as the precursors for the synthesis of ferrocenylboran derivatives.
The first bis[tris(trimethylsilyl)silyl]borylferrocene (**2a**) and tetrakis [tris(trimethylsilyl)-silyl]borylferrocene **2b** were synthesized from the reaction of **1a** and **1b** with $K^+[Si(SiMe_3)_3]^-$ and characterized by ^{11}B-, ^{1}H- and ^{13}C-NMR spectroscopys. The Correctness of the proposed structures for the compounds **2a** and **2b** were discussed by the comparison of spectroscopic data of **2a** with the reported spectroscopic data and theoretical computations [1,3].



1a **2a**



1b **2b**

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Silica supported polyphosphoric acid (SiO_2 -PPA) Catalyzed three-component Synthesis of 1-(α-aminoalkyl) naphthols

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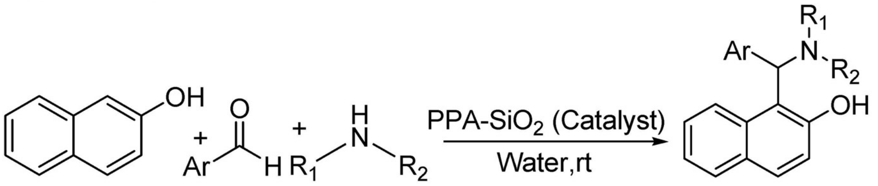
Multi-component reactions (MCRs) have been proven to be a very elegant and rapid way to access complex structures in a single synthetic operation from simple building blocks, and show high atom-economy, high selectivity and procedural simplicity due to the formation of carbon–carbon and carbon–heteroatom bonds in one pot procedure [1].

Compounds bearing 1,3-amino-oxygenated functional groups are ubiquitous to a variety of biologically important natural products and potent drugs including a number of nucleoside antibiotics and HIV protease inhibitors, such as ritonavir and lipinavir [2,3]. Thus, 1-(α-aminoalkyl) naphthols are important and the developing of new MCRs for their synthesis under mild reaction conditions is currently interest. In this research, we report a simple and environmentally benign methodology for the synthesis 1-(α-aminoalkyl) naphthols from the reaction of 2-naphthol, benzaldehydes, and amines in the presence PPA-SiO_2 was carried out in water as green solvent at room temperature (Scheme1).



Scheme1

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18th Iranian Seminar Of Organic
Chemistry
7-9 March 2012

Dual activation approach: $CaCl_2$ as a bifunctional and reusable catalyst for the one-pot three component synthesis of 4H-pyran derivatives

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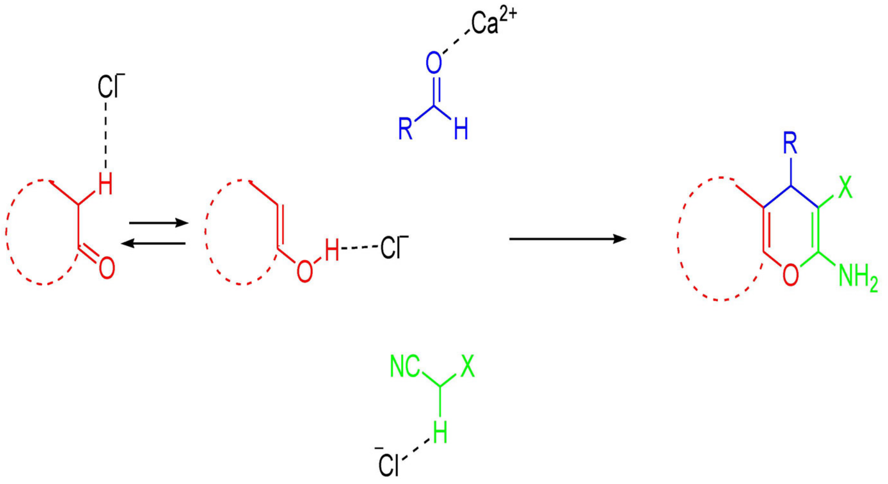
Reactions promoted by Lewis acids and Lewis bases are fundamental in organic synthesis; however, most such reactions are merely stoichiometric. Therefore, the development of catalytic reactions that use Lewis acid and Lewis base catalysts under neutral and mild conditions is particularly important; society needs forward-looking technology, which is based on environmental acceptability. The criteria include atom efficiency, formation of little inorganic waste, and selective synthesis of desired products. $CaCl_2$ is an inexpensive, water stable, environmentally benign and commercially available reagent that is able to act as a Lewis base [1] as well as Lewis acid [2] in organic transformations. A survey of literature shows that the one-pot three component synthesis of 4H-pyrans can be catalyzed successfully in the presence of acid as well as base catalysts. Based on the above facts and as a part of our research program to develop selective, efficient and green methods and catalysts in organic synthesis we report here the application of $CaCl_2$ as an efficient, inexpensive, water-tolerant and bifunctional catalyst for the synthesis of 4H-pyran derivatives. (Scheme 1)



Scheme 1. Bifunctionality of $CaCl_2$ in the synthesis of 4H-pyrans

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An efficient one-pot three-component synthesis of dihydropyrido[2,3-d]pyrimidines

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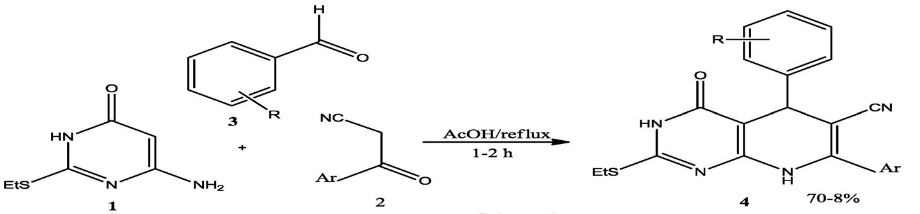
Multicomponent reactions (MCRs), in which several reactions are combined into one synthetic operation, have been used extensively to form carbon-carbon bonds in the synthetic chemistry. Such reactions offer a wide range of possibilities for the efficient construction of highly complex molecules in a single procedure step, thus avoiding the complicated purification operations and allowing savings of both solvents and reagents **[1].**

On the other hand pyridopyrimidines and their oxo and thioxo derivatives have been recognized as important organic materials in drug design and showing interesting biological activities [2]. In particular pyrido[2,3-d]pyrimidines represent a wide range of biological properties such as antipyretic, antibacterial, antitumoral, antihistaminic and calcium-channel-antagonist activities [2-4].

Based on our continued program in developing biologically important heterocycles [5], we report here a convenient and practical method for the synthesis of new derivatives of pyrido[2,3-d]pyrimidines by the reaction of 6-amino-2-thiouracil **(1)** (1mmol), acylacetonitrile **(2)** (1 mmol) and aromatic aldehydes **(3)** in glacial acetic acid under reflux condition. The reaction furnished the desired products in reasonable reaction times (1-2 h) and high yields (70-80%) (Scheme 1).



Scheme 1

The structures of all products were confirmed by spectroscopic (IR, H NMR, C NMR) methods.

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Micro extraction using hollow fibers for determination of drug in biological samples

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Recently, the new concept of three-phase liquid micro extraction was introduced based on applying two immiscible organic solvents in lumen and wall pores of hollow fiber[1]. In the present work, this novel micro extraction technique combined with high performance liquid chromatography has been developed for determination of Omeprazole. The effect of different parameters, such as effect of hollow fiber length, effect of extraction time , Two immiscible organic phases as organic membrane and acceptor phase¸the volume of acceptor phase at optimum conditions and interfering species were investigated. According to optimized conditions for HF-LLLME of Omeprazole was obtained by utilizing a 8cm porous hollow fiber impregnated with n-dodecane, an acceptor solvent of acetonitrile, 28mL donor aqueous solution and extraction time of 60min. The results demonstrated that three-phase hollow fiber micro extraction based on two immiscible solvents is a simple and accurate technique with very good pre concentration factor also served as a technique for sample clean-up[2].

Keywords:
Three -phase hollow fiber micro extraction¸ immiscible organic solvents¸ Omeprazole ¸ High performance liquid chromatography ¸detection.

References:

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Graphite Oxide: A Efficient Carbocatalyst for Oxidation Reactions

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The oxidation of organic substances has received significant attention as it represents an important functional group transformation, from both fundamental and practical perspectives.[1] Thus far, a wide range of homogeneous transition metal-based catalysts has been developed for this purpose.[2] Carbon-based materials catalyze a variety of reactions in solution.[3] Because of their low cost and wide variety of reasonably well-defined physicochemical properties and morphologies, carbon-based materials are desirable catalytic agents.

In continuation of our investigations herein we report the use of graphite oxide (GO),[4] a readily available and inexpensive material, as a mild and efficient carbon catalyst for the generation of aldehydes or ketones from various alcohols and alkenes under ultrasonic irradiation. GO was demonstrated to catalyze the oxidation of various alcohols and alkenes. These reactions were found to proceed under relatively mild conditions and afforded the desired product (aldehyde or ketone) in good to excellent yields. The present method has many obvious advantages as compared to many previous reports, including the simplicity and the generality of the methodology.

$$\mathrm{ROH} \xrightarrow{\mathrm{GO,\ )))}} \mathrm{RCHO}$$

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A novel and efficient one-pot method for synthesis of 3,4-dihydropyrimidin-2-(1H)-ones by carbon catalyst

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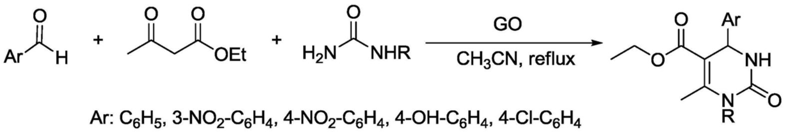
The multicomponent reaction (MCR) was considered as a powerful synthetic tool for preparing target molecules of biological relevance in an efficient manner.[1] The Biginelli reaction, one of the most useful multicomponent reactions, offers an efficient way to access multifunctionalized 3,4-dihydropyrimidin-2-(1H)-ones (DHPMs). Such heterocycles have proved to be efficient calcium channel modulators, mitotic kinesine inhibitors, adrenergic receptor antagonists, antibacterial and antiviral agents.[2]

Carbon-based materials catalyze a variety of reactions in solution.[3] Because of their low cost and wide variety of reasonably well-defined physicochemical properties and morphologies, carbon-based materials are desirable catalytic agents. However, little systematic attention has been given to their use and behavior as catalysts.

In continuation of our investigations on the synthesis of 3,4-dihydropyrimidin,[4] herein we describe a simple and efficient method for three-component cyclocondensation reactions of aldehydes, 1,3-diketones and urea derivative for the synthesis of 3,4-dihydropyrimidin-2-(1H)-ones derivatives using graphite oxide, a readily available and inexpensive material, as a mild and efficient catalyst under mild conditions. This new method has the advantage to give high yields, to be completed in short reaction times and simple product isolation procedure.



Ar: C_6H_5, 3-NO_2-C_6H_4, 4-NO_2-C_6H_4, 4-OH-C_6H_4, 4-Cl-C_6H_4
R: H, Me

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Aza-Michael reaction of 5–Aryl 1–H–tetrazole

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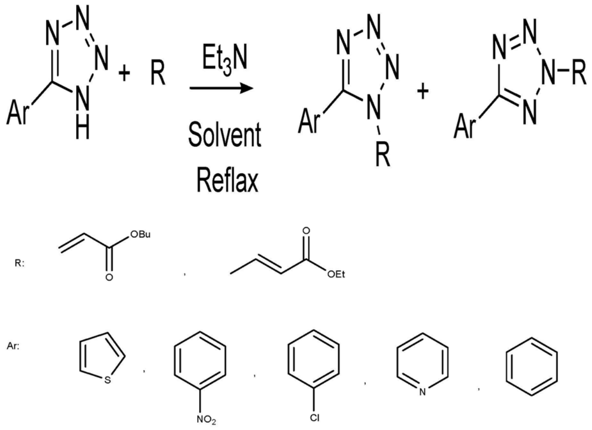
The Michael reaction is one of the most important reactions in organic chemistry. In general, conjugate addition reaction of nucleophiles to unsaturated carbonyl compounds requires basic conditions or acidic catalysts [1]. The Michael addition reaction proceeds even without a catalyst [2]. The addition of nitrogen nucleophilies to α,β-unsaturatedcarbonyl compounds or activated olefins, called aza-Michael reaction [3]. The aza-Michael reaction is an important step in the synthesis of bioactive natural compounds [4]. Most of the aza-Michael organocatalytic reactions are amine catalyzed and proceed via an enamine or iminium intermediate can avoid the possible competition between the nucleophile and the catalyst that can compromise the enantiomeric excess [5]. In the reaction of a series of 5-aryl 1-H--tetrazoles with α,β-unsaturated compounds, a series of alkylated tetrazoles obtained. Because of 1H-2H tautomerism of tetrazoles two alkylated isomers were identified. All prepared compounds characterized using IR, NMR, and MASS spectroscopy methods.



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One-pot multicomponent synthesis of piperidines using formic acide as catalyst

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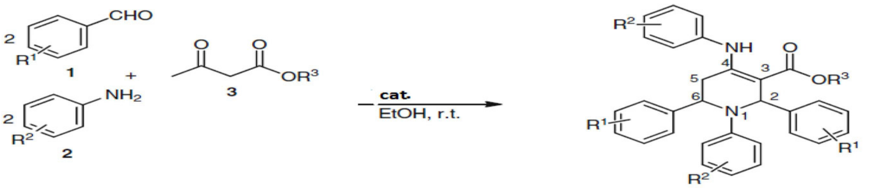
Multicomponent coupling reactions (MCRs) represent a highly valuable synthetic tool for the construction of novel and complex molecular structures with a minimum number of synthetic steps[1] and also offer potential advantages[2]. An essential tetrahydropyridine ring is building block for numerous natural products , synthetic pharmaceuticals and a wide variety of biologically active compounds [3].Among various method for synthesis of this compound MCR is the most efficient one.In this synthesis aromatic aldehydes, acetoacetic esters, and aromatic amines react in the presence of the catalyst . These reactions have improved recently by catalytical methodology [4],[5],[6],[7] and etc… .To extend methodology we use formic acide as catalyst of this reaction and get good result.the advantagouse of this reaction is easy work-up ,good yield ,mild condition and not expensive procedure.



cat=formic acide

Refrences :

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Hydrolysis chemistry of molybdocene dichloride: insights into the reaction mechanism

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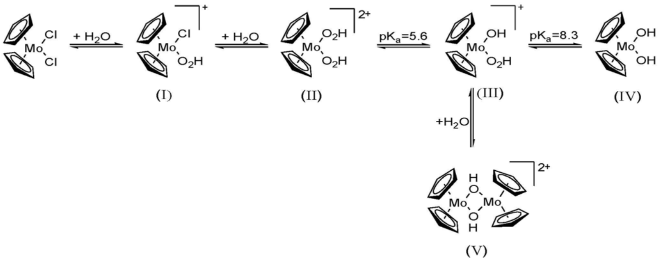
The interest in molybdocene dichloride and related metallocenes has dominated by their remarkable catalytic properties in organic synthesis and as anticancer agents [1]. Testing of a range of metallocene dichlorides identified Cp_2MCl_2 (M=Ti, V, Nb and Mo) as cytotoxic agents with potential as anticancer agents [3]. The hydrolysis chemistry of these compounds is complex, typically involving the formation of a number of dimeric and oligomeric species. The structure of the hydrolysis products is highly dependent on the pH and is often inferred only from titration studies. In most cases, hydrolysis of the coordinated halide or pseudo-halide ligands occurs first and affords aquated metallocene complexes, with OH or OH_2 ligands replacing X .The dissociation rate of the second X^- is dependent of X in Cp_2MoX_2. Taking into account the kinetic parameters and finding the most favorable reaction mechanism, has promoted us to investigate the hydrolysis chemistry of molybdocenes in a detailed theoretical calculation at B3LYP level of theory using aug-cc-pVDZ (cc-pVDZ-pp for Mo) and aug-cc-pVTZ (cc-pVTZ-pp for Mo) basis sets.



Three paths were found in the first and the second hydrolysis step in which, the water molecule attacks to the Mo atom and the chloride atom goes out spontaneously. In summary, the first hydrolysis step exhibits similar geometric features to the second hydrolysis step. Another plausible mechanism in the first and the second hydrolysis steps includes the cleavage of the Mo-Cl bond in the first time and adding of the water molecule to the structure in the next time. This process will repeat for adding of the second water molecules in the second hydrolysis step. The energetic properties, including the relevant thermodynamic quantities and the estimation of the rate constants, were obtained from the computations. Results indicate that S_N1 mechanism is the concerted mechanism of the hydrolysis processes. The computed values of free energy barriers and rate constants (k) in aqueous solution, for the first and second hydrolysis steps, are in excellent agreement with the experimental results under the same conditions.

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Hydrogen-bonding interactions between glycine and nitrosamine: A theoretical study

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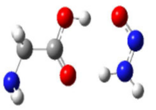
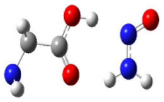
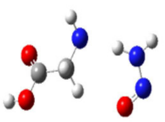
Amino acids are building blocks of proteins (polypeptides), which are the most important class of biological macromolecules. The primary attention has, however, been paid to glycine (Gly) which is the simplest amino acid. Since it represents a small and highly polar organic molecule containing several functional groups, its studies are of fundamental importance for understanding chemical bonding and evaluating links between modern theories and experimental observations [1,2]. Most of nitrosamines are carcinogenic compound and play an important role in the development of tumors and cancer in animals. N-nitrosamines are believed to require metabolic activation to exert their carcinogenic effect [3]. For the study of interactions between glycine and nitrosamine, computations were carried out using B3LYP, B3PW91 and MP2 methods with the 6-311++G (2d,2p) basis set. The counterpoise procedure (CP) was used to correct for basis set superposition error (BSSE) in the calculation of binding energy.



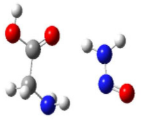
GN1



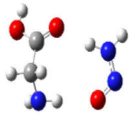
GN2



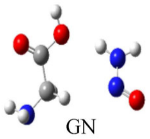
GN3



GN4



GN5



GN6

GN7

First of all, we considered all sites for interaction between glycine and nitrosamine. We found seven minima structures. All optimized complexes have cyclic structures with two H-bonds involved in the interaction. The GN5 structure is nine membered cyclic complex, GN2, GN3 and GN6 structures are seven membered cyclic complexes and GN1, GN4 and GN7 structures are eight one. The GN1,GN5 and GN7 structures contain two H…O hydrogen bond interactions, while GN2, GN3, GN4 and GN6 structures contains two H-bonds type interactions (O…H and N…H). The electronic binding energies (D_e) range from -50.99 to -12.76 kJ/mol. The relative stability order of the seven complexes is GN1> GN2> GN3> GN4> GN5> GN6> GN7. The structure GN1 is the most stable and cyclic structure GN7 is the less stable.

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Solvent-assisted catalysis mechanism on keto-enol tautomerism of trithiocyanuric acid

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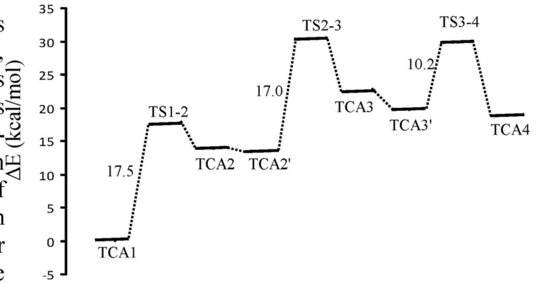
The first theoretical paper showing the catalysis of tautomeric processes by a water molecule published by Lledos and Bertran [1]. Tautomers are structural isomers that are conceptually related by the shift of hydrogen and one or more π bonds [2]. Many biomolecules may exist as a variety of tautomers. Since the energy difference between some of these tautomers is very small, their thermal energy may be easily transformed from one tautomer to another at room temperature. Moreover, for other tautomers with relatively high energy differences, solvent molecules which certainly act as catalysts are used to facilitate the tautomerization process.

In this present work, we will discuss the isomerization reaction process, in which, enthalpies, free energies and reaction rates in each step has been computed. B3LYP/6-311++g(2d,2p) method has been used to study the tautomerization of Trithiocyanuric acid (TCA) both in gas phase and water solution. For tautomerization in gas phase, the reaction path goes through three steps with three transition states. All these transition states contain an S-H-C-N 4-membered ring, in which the S-H-C-N torsion angles are all 0.00°. For tautomerism in H_2O solution, the reaction path also goes through three transition states. All the transition states contain 6-membered ring formed by C-N-H-O-H-S due to the forming of H-bonding complex between Trithiocyanuric acid and the solvent molecule. The presence of the solvent reduces considerably the energy barrier of the reaction. It is clear that methanole is a better catalyst than water. NBO analysis shows that there is a strong interaction between Trithiocyanuric and solvent molecules in transition states. AIM charge analysis indicates that the tautomerism shows a certain degree of proton transfer character. From the reaction enthalpy and reaction rate, tautomerism in water and methanole solvated system is easier than that in gas phase. Results indicate that the tautomerisms are endothermic both in gas phase and in solution.



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Synthesis and characterization of novel amide-benzothiazole copolymers

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Aromatic polyamides are one of the most important classes of high performance polymers, as they possess well mechanical properties, high thermal stability, chemical resistance, and low flammability [1]. Aromatic poly(benzothiazole)s (PBTs) also are a class of heterocyclic polymers that have been well-known for high thermal and thermoxidative stability and also are identified to have high-mechanical properties, and the high degree of molecular stiffness in the backbone [2-4]. Here in two aromatic monomers containing preformed bisbenzoheterocyclic groups connected by a meta and para-phenylene ring was synthesiszed. Then both bisbenzothiazoles were converted to dinitro by usual method using nitric acid and sulfuric acid and reduction of dinitro compounds with Tin(II)chloride in concentrated hydrochloric acid produced in bisaminobenzothiazoles. The structures were confirmed by ^{1}H-NMR, ^{13}C-NMR, FT-IR and also elemental analysis data. Then a series of new amide-benzthiazole copolymers containing meta and para-phenylene rings have been prepared from the reaction of simple terephthaloyl and isophthaloyl chloride, with both aromatic diamines at room temperature by low temperature solution condensation in high yield. Polymers structures were characterized by FT-IR, ^{1}H-NMR and elemental analysis. High molecular weight copolymers were obtained based on intrinsic viscosity and thermal stability of polymers investigated with thermogravimetry analysis (TGA) and diffraction scanning calorimetry (DSC) that showed high thermal stability.

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One-Pot Synthesis of 2,4-Diaminopyrimidine-5-carbonitrile Derivatives Using Sodium Acetate Supported on Alumina as Catalyst

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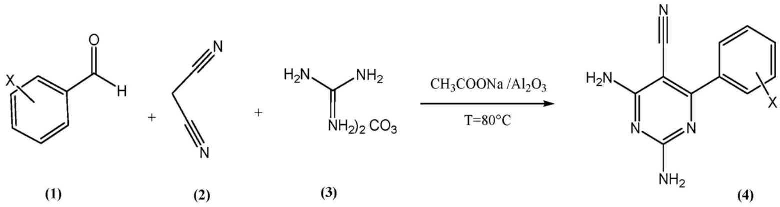
The one-pot condensation of aromatic aldehydes, malononitrile, and guanidine carbonate, in the presence of sodium acetate supported on basic alumina under solvent-free conditions, was reported. Looking for new efficient synthetic procedures toward heterocyclic compounds is one of the most widespread areas of research in organic chemistry. Pyrimidines, as the most important nitrogen-containing heterocyclic compounds, are of chemical and pharmacological interests that often play an essential role in medicinal chemistry. They are core constituents of analgesics, antihypertensives, antipyretics, and anti-inflammatory drugs [1]. They are also used in some pesticides, herbicides, and plant growth regulators [2]. Therefore we were prompted to find an ecofriendly procedure for the direct synthesis of 2,4-diamino pyrimidine-5-carbonitrile derivatives. In comparison to methods employing molecular solvents, the solvent-free approach proceeds more cleanly and provided better yields [3].

Herein, we reported the synthesis of 2,4-diamino-6-arylpyrimidine-5-carbonitrile derivatives **4,** through a one-pot cyclocondensation reaction of aromatic aldehydes **1**, malononitrile **2** and guanidine carbonate **3,** using simple and inexpensive sodium acetate supported on alumina as the catalyst under solvent-free condition (Scheme 1).



Scheme 1

Sodium acetate used in this process has important role in the reaction. First, it releases guanidine carbonate from its salt. Then, as an acidic catalyst, it activates the reactants to react with each other to form the diaminopyrimidine product. Excellent yields of products, simple work-up and performing the reaction under solvent-free conditions are the advantages of the present study.

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Synthesis of novel pyrimido[4,5-b]quinolines using ionic liquid as catalyst

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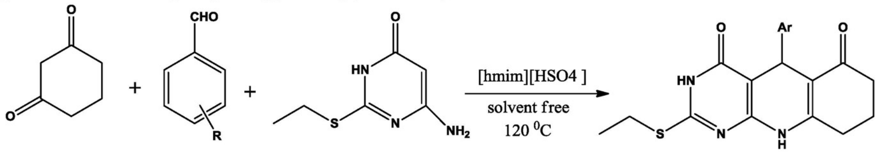
Multi-component reactions (MCRs) by virtue of their convergence, productivity, ease of execution and generally high yields of products have attracted considerable attention from the point of view of combinatorial chemistry [1]. On the other hand pyrimido[4,5-b]quinolines are important compounds because of their biological properties which are known to depend mainly on the nature and position of the substituent [2]. Quinoline derivatives display a broad range of biological activities such as anti-malarial [3], anti-tumor [4] and anti-bacterial [5]. Thus, considerable attention has been focused on the development of new methodologies to synthesize many kinds of pyridoquinoline systems.

Following our continued interests in the synthesis of biologically important heterocycles [6], in this research, we wish to report a very simple and highly efficient one-pot method for the synthesis of novel pyrimido[4,5-b]quinolines via a three-component cyclocondensation of equimolar amounts of 1,3-cyclohexadiene، aromatic aldehydes and 6-amino-2-(ethylthio)pyrimidin-4(3H)-one derivatives in the presence of ionic liquid [hmim][HSO4] (Scheme 1).



1 2 3

Scheme 1

4

This efficient method furnished the desired products (**4**) in high yields (75-95%) and short reaction times (10-30 min). High yields and ease of recovery and reusability of ionic liquid with consistent activity, makes this protocol efficient and environmentally benign.

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