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Third International Caucasian Symposium on Polymers & Advanced Materials

ICSP&AM

Organized by
Iv. Javakhishvili
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Science of Georgia

1-4 September 2013
Tbilisi, Georgia

Welcome

Dear Colleagues,

On behalf of the Organizing Committee I wish to extend cordial welcome to all participants of the 3rd International Caucasian Symposium on Polymers and Advanced Materials. Six years ago, 2007, this symposium took place in Tbilisi, Georgia. We are delighted to host you this year in the geographical centre of the "Caucasus", in Tbilisi.

The purpose of the conference is to encourage scientists working in polymer chemistry and advanced materials to present their investigations dedicated to problems and discoveries in above mentioned fields. Also “ICSP&AM 3” will help to introduce effectively innovative scientific researches of Georgian, Caucasus and neighboring scientific teams, which are less known for world scientific society.

We hope that this year meeting, gathering many participants, shall provide a good platform for academic and industrial scientists to discuss recent advances in the area of polymers and advanced materials.

Professor Omar Mukbaniani

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SYMPOSIUM SCHEDULE

1 September

12:00–17:00 Registration
17:30–19:30 Welcome reception

2 September

09:00–09:30 Opening ceremony (Prof. Omar Mukbaniani, Prof. Marc Abadie)

Co-chairmen: *Prof. Alain Perichaud and Prof. S. Davtyan*

09:00–09:20 *Marc J.M. Abadie* - ”Green Polymer Chemistry”.
09:20–9:40 *T. Agladze* - *“*The Size Dependent Phase Transformation of the Electrodeposited Transition Metals”.
9.40:10–10:00 *J.V. Grazulevicius* ”Polymeric and Low-molar-mass Glass-forming Semiconductors for Optoelectronic Applications”.
10:00–10:20 *M. Bratychak* - “Functional Derivatives of Polycondensated Resins”.
10.20:10.40 *Oleg L. Figovsky* - “Environment Friendly Nanotechnologies”.
10.40:11.00 *E. Erbay* - “RAFT Polymerization of Acrylic Esters by Using of New Chain Transfer Agents on the Basis of Thiocompounds”.

Coffee break 11.00-11.40

Co-chairmen: *Prof. Marc J.M. Abadie and Prof. B. Mamedov*

11:40–12:00 *S.P. Davtyan* - “Synthesis of the Super-Absorbents Hydrogels on a Basis of Polyacrylamide, Polyacrylamide/Bentonite, Polyacrylamide/Diatomite by Frontal Polymerization Mode”.
12:00–12:20 *Alain Perichaud* - *”*Self Healing of Protective Coatings*”*.
12:20–12:40 *E.B. Zeynalov.*- “ Thermooxidative Degradation of the Low-density Polyethylene in the Presence of Fullerenes C_{60}/C_{70}”.
12:40–13:00 *L. Nadareishvili* - *“*New Method of Obtaining of Gradually Oriented Polymeric Films”.

Lunch break 13.00-14.30

Co-chairmen: *Prof. E.B. Zeynalov_and Prof. G. Papava*

14:30–14:50 *V.M. Farzaliyev* - ”The Improvement of the Quality of Lubricating Oils by Polymeric Compounds”.
14:50–15:10 *Shahriar Ghammamy* - ”Synthesis and Characterization of New Nano composites and Study of their Biological Properties”.
15:10–15:30 *M. Obloj-Muzaj* - *“*Properties and Advantages of PVC Nanocomposites”.
15.30:15.50 *A.M. Guliyev* - ”Ring-opening Polymerization of Vinylcyclopropanes”.
15:50-16:10 *Sajjad Sedaghat* - *”*New Synthesis and Characterization of Nanoclay/Polyethy-

lene Terephthalate Nanocomposite".
16.10:16.30 *D. Neugebauer* - "Synthesis of amphiphilic graft copolymers via modification of hydroxy-functionalized copolymers".

***Coffee break* 16.30:16.40**

16:50–18:00 *Poster session p. 1-42* ("Polymers" and "Advanced Materials")

3 September

Co-chairmen: *Prof. M. Bratychak and Prof. A.O. Tonoyan*

09:00–09:20 *N.F. Janibayov* - "Synthesis of Metaldithiophosphates on HLaУ and HУ Zeolites and Polymerization of 1,3-Butadiene with these Heterogeneous Catalytic Dithiosystems".
09:20–9:40 *T.K. Jumadilov* - "Mutual Activation and High Selectivity of Polymeric Structures in Intergel Systems".
9:40–10:00 *B.A. Mamedov* - "Preparation of Nanopolyaniline and its Polymer-polymer Nanocompositions with High and Stable Electro-conductivity"
10:00–10:20 *N.A. Durgaryan,* - "Oxidative Polycondensation of p-Phenylenediamine in Organic Medium as a Method to Synthesise Poly(1.4-quinonodiimine-n,n'-diyl-1,4-phenylene)".
10.20:10.40 *G.G. Meskhi* - "Emission of Multi Charged Ions During N^+,O^+,N_2^+,O_2^+, Ar^+ Ions Bombardment of NaCl, Mg, Al, Si, S Surfaces".
10.40:11.00 *M. Motameni* - "Mathematical Model for Biopolymer Nanoparticles sorption in Whey".

Coffee break 11.00-11.40

Co-chairmen: *Prof. N. Durgaryan and Prof. M. Obloj-Muzaj*

11:40–12:00 *D. Chkhubianishvili* - "Investigation of the Reaction of Telomerization of Ethylene and Trichloracetic Ethyl Ester".
12:00–12:20 *A.O. Tonoyan,* - "Non-Stationary Modes of Frontal Polymerization".
12:20–12:40 *O. Mukbaniani* - "Synthesis and Investigation of Properties of Comb-type Organosilicon Polymers for Solid Polymer Electrolyte Membranes".
12:40–13:00 *Jimsher Aneli* - "Obtaining and Investigation of Polymer Electrolytes on the basis of Silicon-Organic Polymers".

Lunch break 13.00-14.30

Co-chairmen: *Prof. V. Syromyatnikov and L. Nadareishvili*

14:30–14:50 *K.G. Gusakova* - "Synthesis and Thermal Properties of Polycyanurate-based Thermosetting Nanocomposites".
14:50–15:10 *Mazyar Sharifzadeh baei* - "Composite polymer for adsorption of Nickle from colored wastewater".
15:10–15:30 *F.A. Nasirov* - "Cobalt Alkylxhanthogenate + Trialkylaluminum Catalytic Dithiosystems For Synthesis of Syndiotactic 1,2-Polybutadiene".
15:30-15:50 *S.S. Khutsishvili* - "Peculiarities of Nanoparticles Magnetism Dispersed in Polysaccharide Matrix".
16.00:16.20 *Tinatin Butkhuzi* - "Study of Influence of Ionic and Nonionic Additives on the

Structural Changes of Water Nanocages Confined in the AOT Reverse Micelles".
16.20:16.40 *A.Goletiani* **– "**Removal of Heavy Metal Ions from Wastewaters by Using of Renewable Bio Sources of Georgia**".**

Coffee break

16:40–18:00 *Poster session p. 42-84* ("Polymers" and "Advanced Materials").
18.00 *Closing lecture* (young scientists awards, raffle prizes).

4 September

9.00 Excursion in old capital of Georgia, Mtskheta (Lunch).
18.00 Gala Dinner in restaurant "Metekhis Chrdilshi".

Farewell

Abstract

Green Polymer Chemistry

*Marc J.M. Abadie**
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Green Polymer Chemistry is a crucial area of research and product development that continues to grow in its influence over industrial practices. Developments in these areas are driven by environmental concerns, interest in sustainability, desire to decrease our dependence on petroleum, and commercial opportunities to develop “green” products. Publications and patents in these fields are increasing as more academic, industrial, and government scientists become involved in research and commercial activities.

Green chemistry is the design of chemical products and processes that reduce or eliminate the use or generation of hazardous substances. Sustainability refers to the development that meets the needs of the present without compromising the ability of future generations to meet their own needs. In the past few years these concepts have caught on and have become popular topics for research.

In this presentation we provide an overview which briefly surveys the practice of green chemistry in Polymer Science with a particular emphasis on Green Processes, biodegradable polymers & Recycling. Examples are taken from our rexpertise, experience and research but also from recent litterature, and industrial reports. Other domains like Biocatalysis, Bio-based Materials are not considered.

In the polymer area, we will consider the following five related themes. :

. 1) Greener processes.
  - Benign solvents (e.g., water, ionic liquids, or reactions without solvents)
  - Improved syntheses and processes (e.g., atom economy, reaction ☐efficiency, toxicity reduction)

. 2) Biodegradable polymers and waste minimization
  - Diverse feedstock base (especially agricultural products and biobased ☐building blocks)

. 3) Recycling of polymer products

. 4) Energy generation or minimization of use

. 5) Optimal molecular design and activity

Abstract

IPN Based Hybrid Composites for Antifooling Properties

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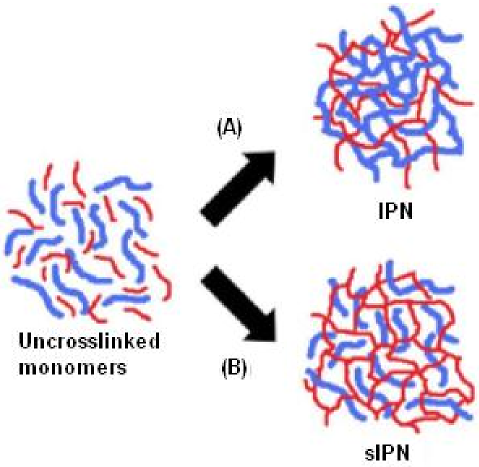
The first objective of our research is to study the curing kinetics and photoreactivity of monomers, trimethylolpropane triacrylate (TMPTA), trimethylolpropane tri(ethyleneoxide) acrylate (TMPT(EO)A), Poly(ethylene glycol) diacrylate, (PEGDA) Tripropylene glycol diacrylate (TPGDA), aliphatic urethane acrylate oligomer (CN8003) and difunctional bisphenol A based epoxy acrylate (CN104) and Bisphenol-F-epichlorhydrine (Epolam® 5015). UV curing analysis of each individual monomer will be conducted to find out each of their optimum curing conditions by varying concentration of photoinitiator and temperature of cure. The experiment was done by (DPC) and the rate coefficient, rate of polymerization and percentage conversion of the monomers will be reviewed.

To fabricate resistant thin film coatings, IPNs are formulated from these monomers and oligomers, each acrylates will be mixed with Epolam® 5015 at different ratio to form IPNs. The UV curing kinetics and the suitability of the coatings is determined by the surface energy, ultimate tensile strength (UTS) and hardness of these IPNs.



The last part of this paper is to improve the properties, mainly mechanical, magnetic and electrical, of the coatings by adding different nanofillers at different concentration, as well as with surfactant and to study their effect on the curing kinetics of TMPT(EO)A.

The Size Dependent Phase Transformation of the Electrodeposited Transition Metals

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Upon electrodeposition the transition metals frequently crystallized in a two basic forms: stable crystals with a body centered cubic cell (α−modification) and a metastable hexagonal structure ("γ −modification"). The indication of a driving force of a process stipulated formation of a metastable hexagonal phase at ambient temperatures while it is thermodynamically stable only at elevated temperatures is of fundamental and practical significance. Recently [1] it was shown that the hexagonal deposit which is formed at low cathodic overvoltages are not a γ-modification of a metallic manganese and chromium but represent a nonstechiometric metal hydrides. Metallic manganese and chromium predominantly deposited at higher overvoltages. The potential driven transformation of a metastable hexagonal hydride into a stable cubic phase is accompanied by release of hydrogen gas and change in morphology of deposits. In a Tafel region formation of large crystals with a simple face-centered tetragonal lattice takes place while at higher overvoltages a complex volume-centered cubic lattice is observed. At low overvoltages increase in an increase in grain size of the crystallites. From analysis of the Gibbs-Thomson equation and of the dependence of a sublimation pressure on crystal structure of solids [2,3] it was found that both free energy and vapor pressure over a hexagonal phase depend on a crystal size r. Owing to a considerably higher surface energy a metastable hexagonal phase exhibit lower free energy of formation at low values of r, while a cubic phase becomes more stable at higher cluster dimensions. The experimental data on variation of phase composition of deposits with the crystal dimensions correlate with the theoretically predicted trends.

References:

1. T.Agladze, M.Gabrichidze, Kinetics of manganese electrode in aqueous solutions, Electrochem. Acta, 2013. In Press.
2. I. Stranski, R. Kaishev, On crystal growth theory, Physics-Uspekhi (Russia), 1936.
3. W. Plieth, Electrochemical nanotechnology, W. Lorenz Ed., Wiley-VCH, Weinheim,1998.

Abstract

Obtaining and Investigation of Polymer Electrolytes on the basis of Silicon-Organic Polymers

Jimsher Aneli[1*], *Eliza Markarashvili*[1,2], *Tamar Tatrishvili*[1,2],
Maia Chigvinadze[1], *Omar Mukbaniani*[1,2]
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The electrolytes based on polymers consisted different salts of lithium attracts a wide interest of the scientists and engineers, while these materials present the bright subjects of the alternate energy sources. This interest is due to mainly lot of positive properties (low density, possibility of variation of the electric parameters in the wide range, durability, etc).

Presented work is devoted to investigation with use of impedance method of the electric physical properties of obtained by us polyelectrolyte membranes. It is studied the dependence of the electrolyte conductivity of electrolytes based on polysiloxanes containing with side groups of propylbutyrate, propyl acetoacetate and ethyltriethoxisilane on the concentration of included lithium salts. It is shown that this dependence is extreme and has maximum, the height and place of which in the corresponded diagram from the other side depend on the salt type and its concentration. The experimental data allow to provide the optimization of the polyelectrolyte composition for the selection of the material with maximal electric conductivity.

The curve obtained for temperature dependence of the ionic conductivity of electrolytes included two types of lithium salts has the Arrhenius type shape in the temperature range 25-90 °C and is a straight line, the inclination of which essentially is due to lithium salt type. For the all membranes the conductivity is increased, which connects with increasing of the ionic mobility. These dependences are reversible and are characterized with different hysteresis. It is established that electric conductivity of polymer electrolytes changed in the range $5x10^{-4}$ - $1x10^{-7}$ S/cm.

The voltamogrames of the polyelectrolytes at room temperature is characterized with saturation of electric current, the value and character of change of which depends on the content of the electrolyte. The analysis of experimental data is based on the polyelectrolytes structural peculiarities and phenomena, which stipulate the charge transfer in the polymer matrix.

Acknowledgement: This work has been fulfilled by financial support of Science & Technology center in Ukraine (Grant #5055).

Abstract

Composites Based on Epoxy Resin and Modified Filler

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It is known that physical and chemical properties of the composites essentially depend on interaction forces between ingredients. With the aim of enhancing of exploitation characteristics of the composite materials some substances amplifying these forces are used.

Presented work is devoted to investigation of the effect of filler modified with inorganic substance on some properties of composites on the basis of epoxy resin and dry wastes of the plant yucca (Yukka glorioza) as filler.

The samples were prepared by mechanical mixing of dian type of the epoxy resin and unmodified and/or modified by 5 mass% noted above modifier filler (average diameter of particles in the range 50-100 mcm) at concentrations of last in the interval 40-70 mass% at room temperature. The samples were obtained at using the known standards for measuring of mechanical strength, softening temperature (by method Vica) and water absorption. The chemical structure of the composites was studied with using of method FTIR.

It was established that good results correspond to composites containing about 50 mass% of unmodified filler and best ones to composites containing modified this filler with same concentration. The obtained results are described in terms of formation of the buffer zone between ingredients conducing to enhancing of their compatibility and interaction forces.

Abstract

Peculiarities of Frontal Polymerization of Acrylamide-Bentonite Mix Depending on Concentration and Type of the Initiator

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Peculiarities of frontal polymerization of the mixes of acrylamide-bentonite depending on concentration and type of the initiator are investigated. The temperature profiles with different amounts of filler are measured. Frontal polymerization of thermal wave propagation downward and upward is investigated. The dependence of the initiator's order on the type and nature of the initiator is shown. The study of hydrogels synthesis with bentonite receiving intercalated nanocomposites and investigation of its properties (their response to external environment) is of special interest because of their potential applications as drug delivery systems, in agriculture, and many of human existence situation.

Therefore, to generate uniform hydrogels, small samples are usually produced in frontal mode charged with the knowledge that the rapid polymerization in a localized reaction zone could negate phase separation and lead to a homogeneous product. Moreover, large hydrogel samples with similar equilibrium swelling ratio can be readily produced without the effect of microaggregation and phase separation.

Abstract

Cross-linking of Epoxy-Oligoesteric Mixtures in the Presence of ED-24 Modified Epoxy Resin

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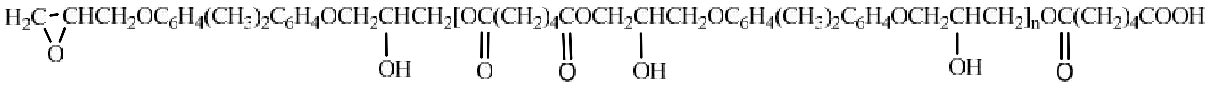
Epoxy resins are mixed with other oligomers to reduce the price of wares based on epoxies on the one hand, and to improve the operational characteristics of the materials on their basis – on the other. Among all epoxy-oligomeric mixtures the mixtures containing dianic epoxy resin, as well as oligomers with unsaturated double bonds are of special attention. In most cases the unsaturated oligomers are plasticizers of epoxy mixtures and are not chemically bound with polymeric network of cross-linked epoxy resin.

This work deals with the investigations of epoxy-oligomeric mixtures cross-linking based on industrial ED-20 dianic epoxy resin and TGM-3 oligoesteracrylate in the presence of carboxy-containing derivative of ED-24 epoxy resin of the general formula:



$$H_2C{-}CHCH_2OC_6H_4(CH_3)_2C_6H_4OCH_2CH(OH)CH_2[OC(=O)(CH_2)_4C(=O)OCH_2CH(OH)CH_2OC_6H_4(CH_3)_2C_6H_4OCH_2CH(OH)CH_2]_nOC(=O)(CH_2)_4COOH$$

Where n = 2–3.

The industrial dianic epoxy resin ED-20 was used as epoxy component. TGM-3 oligoesteracrylate was used as oligoesteric component. Polyethylenepolyamine (PEPA) was the hardener.

Cross-linking of epoxy-oligomeric mixtures was carried out stepwise: first at room temperature for 24 h and then at heating to 383, 403 or 423 K for 15, 30, 45, 60 and 75 min. The structural changes were controlled by the determination of gel-fraction content and films hardness.

The effect of epoxy-oligoesteric mixtures, temperature and process time on the formation of cross-linked products has been studied.

The role of functional groups during cross-linking was examined by means of IR-spectroscopy. The chemism of epoxy-oligoesteric mixtures cross-linking was suggested in the presence of ED-24 modified epoxy resin.

Thus we may ascertain that at room temperature the cross-linking of epoxy-oligoesteric mixtures takes place due to the interaction between molecules of ED-20 and carboxy-containing derivative of ED-24 epoxy resin with PEPA. Under mentioned conditions the partial cooligomerization of TGM-3 molecules takes place as well. The mixtures heating leads to the further formation of three-dimensional molecules due to the interaction between free carboxy groups of carboxy-containing derivative molecule which is a part of the main matrix with hydroxy groups. Moreover, at heating three-dimensional cooligomerization of TGM-3 molecules takes place.

Abstract

Optical Measurements of the Electrophoretic Suspension Kinetics

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D. Mladenova[1, 4], *M. Weiter*[1] *and I. Zhivkov*[1, 4]
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Electrophoretic deposition (EPD) is used for formation of coatings, e.g. in the automotive industry. Recently EPD is successfully utilized for thin film preparation with an application in the optics and electronics. One of the most remarkable features of the EPD process is the separation of the particle formation (in the suspension) from the deposition (on the substrate). Therefore the key point to control of the film structure and morphology is the control of the suspension properties. The suspension could be formed by a precipitation of the solution prepared by a precipitator (non-solvent). It is known that after the precipitation starts the formed suspension particles trend to aggregate, i. e. the deposition of the films from suspensions with different aggregates will leads to different film structure and morphology.

This paper aims to investigate the process of the suspension formation and aggregation by Dynamic Light Scattering (DLS) method.

The suspensions were formed by a precipitation of solution of poly[2-methoxy-5-(3′,7′-dimethyloctyloxy)-1,4-phenylenevinylene] (MDMO-PPV) in toluene using acetonitrile as a precipitator.

The kinetics of the DLS measurement of suspensions shows that within the first 15-1000 s from the suspension formation the particle size is relatively stable. After that a progressive increase of the suspension particle size is observed. These results are discussed within pointing out the possibility for the EPD film structure and morphology control by performing the deposition at different stages of the suspension particle formation and aggregation process.

Abstract

Functional Derivatives of Polycondensated Resins

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Polycondensated resins are widely used for the wares formed via molding technology and as protective or decorative coatings, glues, caulking compounds, etc. In order the formed wares have high performance attributes the polycondensated resins should contain functional groups different by their nature capable to form three-dimensional structures during wares formation. The increase of such groups number improves the ware properties.

Epoxy (ER), phenol-formaldehyde (PhFR) and polyglycidylphenol-formaldehyde (PGPhFR) resins were used as the initial compounds to synthesize new functional derivatives of polycondensated resins.

The initial ER used for the synthesis of functional oligomers were:

- ER based on Bisphenol A;
- ER based on glycols;
- ER based on diamines;
- ER based on cianuric acid;
- alicyclic epoxy resins;
- nitrogen-containing epoxy resins.

The functional derivatives of PhFR have been obtained using the following:

- modification of PhFR of novolac type with 1,2-epoxy-3-tert-butylperoxypropane;
- modification of PhFR of resol type with tert-butylperoxymethanol;
- modification of PhFR of novolac type with glycidylmethacrylate;
- modification of PhFR of novolac type with furfurolglycide ether;
- modification of PGPhFR with tert-butylhydroxyperoxide.

The kinetic regularities of the mentioned functional derivatives of polycondensated resins synthesis were studied. The synthesis procedure was suggested and new functional oligomers were synthesized. The structure of synthesized oligomers was confirmed by the chemical and spectral investigations. The areas of functional derivatives of polycondensated resins application were proposed.

Abstract

Chemical Modification of Epoxy Resins by Diatomic Alcohols

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It is well-known that the products based on epoxy resins are characterized by a series of positive properties and used in different branches of industry for the production of variable wares. To improve the operational properties of such wares the epoxy resins are modified by various low- and high-molecular compounds. Among low-molecular compounds used for the chemical modification of epoxy resins are acids, anhydrides, hydroperoxides, phenols, monohydric alcohols and others.

In this work we studied the possibility to modify dianic epoxy resins by diatomic alcohols.

Benzyltriammonium chloride, potassium hydroxide and the catalytic system consist of quaternary ammonium salt plus potassium hydroxides were examined as the catalysts of the reaction between dianic epoxy resin and diatomic alcohol. The effective rate constants for the reaction between ED-24 epoxy resin and 1,4-butandiol were calculated. We suggested the procedure of oligomer synthesis via chemical modification of ED-24 and 1,4-butandiol. The structure of the synthesized oligomer was confirmed by chemical and spectroscopic analyses. The ways of synthesized products application were proposed.

Abstract

Study of Influence of Ionic and Nonionic Additives on the Structural Changes of Water Nanocages Confined in the AOT Reverse Micelles

*Tinatin Butkhuzi, Manoni Kurtanidze and Marina Rukhadze**
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Similarity between micelles of surfactants and living systems is mainly determined by resemblance of aggregation processes in living organisms to phenomenon of micelle formation in solutions of surfactants. The microemulsion systems represent a good artificial model of biological membranes due to the likeness of their structure. The analogous picture of normal membrane structure in cell is created by reverse micelles, besides water dissolved in the core of micelle represents the best model of the confined water in biosystems. Therefore investigations devoted to the study of properties of water presented in the core of reverse micelle are especially topical. Introducing of kosmotropic and chaotropic additives into the water pockets of reverse micelles is also important because of their influence on the structure of water pockets [1,2]. The goal of the proposed work was to study the influence of different ionic and nonionic additives (kosmotropes sodium acetate and glucose, chaotropes potassium perchlorate and urea) introduced in the water nanodroplets of reverse micelles on both structural changes of water pools of reverse micelles and association degree of a molecular probe to sodium bis(2-ethylhexyl) sulfosuccinate (AOT) reverse micelles by using infrared and ultraviolet-visible spectroscopy.

To study the microstructure of the water solubilized in AOT reverse micelles, the O-H stretching vibrational absorption spectra in the region of 3000-3800 cm^{-1} were fitted into three subpeaks with the help of a Gaussian curve fitting program. IR investigations of water-Brij-30-hexane reverse micellar systems show that three types of water are presented in the water pockets of the reverse micelle. Addition of ionic and nonionic additives into the water core results in the changes of ratio of the bound, free and trapped water fractions. The microenvironment of AOT reverse micelles was investigated by UV-visible spectroscopy on the basis of o-nitroaniline as molecular probe. Different influence of kosmotropic and chaotropic additives on the changes in electronic absorption spectra of o-nitroaniline was observed. Therefore binding constants of a molecular probe to AOT reverse micelles under the influence of kosmotropic and chaotropic additives are different.

Results may be useful in the investigations of water structure, when it is confined to nanometer-scale cavities.

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2. B. Hribar, N.T. Southall, V. Vlachy and K.A. Dill. How Ions Affect the Structure of Water. Journal of American Chemical Society, 124, 12302-12311, 2002.

Abstract

Zeolite Based Hybrid Cationites

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It is known that ionites on the basis of natural inorganic sorbents are obtained by their impregnation with monomers which contain ionogenic groups, at their further polymerization. Lattice of inorganic sorbent, in our case is used as a matrix for organic ionite.

There are ionites and particularly anionites, in which zeolite acts as a lattice of synthetic polymer.

Imperfection of organic ionites with organic lattice (polymer lattice) is in complexity of technology of their obtaining and high price. The process of obtaining of ionite lattice on the basis of organic polymer is connected with multistage organic synthesis both of original monomers and polymers on their base. Alongside with it, lattice of natural origin contributes to the increase of thermal stability of ionites. Such ionites are able to function at high temperatures, which is very urgent at their exploitation in extreme conditions.

For the synthesis of cationites with inorganic lattice we used natural zeolite, clinoptilolite of the composition: $(Na_2K_2)O \cdot Al_2O_3 \cdot 10SiO_2 \cdot 8H_2O$, as one of the initial components. With this in view clinoptilolite was modified in advance for its transformation into hydrogen (H-form) one, and was treated further with chloropropionic acid.

In the modified clinoptilolite, at its treatment with acid, Na and K can be removed from the lattice, which form water soluble chlorides and at the washing of the formed H-form clinoptilolite, they are removed, as a result of which silanol groups are formed. At the interaction of these groups with chloropropionic acid the chemical bonds are created among them according to the following scheme:

$$\equiv Si–OH + ClCH_2CH_2COOH \rightarrow \equiv Si–O–CH_2CH_2\text{-}COOH + HCl$$

Spectroscopic studies showed that in IR specter of the cationite the absorption band is observed in the region of 1090–1050 $см^{-1}$, that is characteristic to the Si–O–C bond, which refers to the formation of ether bond.

Cationite obtained by interaction of chloropropionic acid with H-form zeolite, is characterized by the following properties: grain size 1-2 mm, apparent density 0,6–0,8 g\ml, static exchange capacity with respect to 0,1 N NaOH solution - 5-6 mg-equiv/g.

If we compare the exchange capacity of the obtained cationite with that of natural zeolite, we'll see that its exchange capacity 0.2- 0.3 increases 4-5 times. At the same time, introduction of easily dissociated ionogenic carboxyl groups into zeolite composition contributes to the improvement of kinetics of exchange of a series of ions.

Cationite is stable to the impact of acids and alkali, possesses high mechanical resistance.

Thermal stability of cationite was estimated through its heating in water, for 24 hrs, at various temperatures. Studies showed that at 60-200 ^0C interval the exchange capacity of cationite with respect to 0,1 N NaOH solution practically doesn't change. At the increase of temperature from 60 to 200 ^0C it decreases from 5 to 2 mg-equiv/g.

Thermal stability of ionites was determined in dynamic heating conditions. It turned out that thermal stability remains at the level of results obtained at the terms of their testing under static conditions. Thus, cationite obtained on the basis of modified natural zeolite – clinoptilolite (H-form) is characterized by high thermal stability and mechanical strength, high static exchange capacity and can be used for water treatment at high temperature.

Abstract

Unsaturated Biodegradable Poly(ester-amide)s and Their Chemical Transformations

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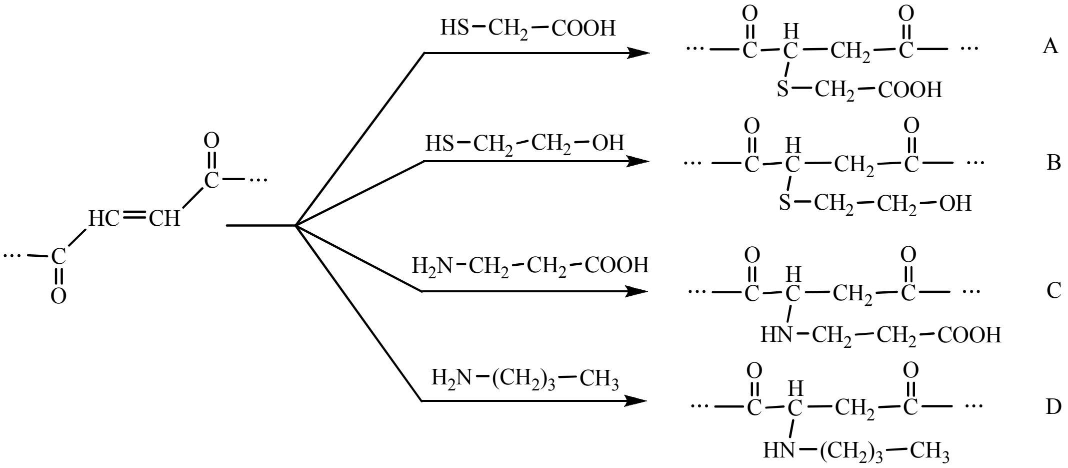
α-Amino Acid Based (AAB) Poly(Ester Amide)s (PEAs) are relatively new class of biodegradable biomaterials [1,2]. Besides the diversity in material properties, they have shown good biocompatibility [3,4] that makes PEAs highly attractive for biomedical applications. One of the most convenient and universal ways to render biodegradable polymer functional is the incorporation of unsaturated double bonds in the polymeric backbones [5].

Unsaturations in new unsaturated PEA polymers are activated due to the presence of two adjacent carbonyl groups, and these active >C=C< group can undergo various chemical transformations when interacting with nucleophiles (Sch. 1). We used a thiol (thioglycolic acid and mercaptoethanol) and amine (β-alanine and n-butylamine) reagents to study the reactivity of such unsaturated groups in USPEA $FA_{0.40}/8_{0.60}$-Leu-6.



Scheme 1. Chemical transformations of unsaturated PEA polymers.

These polymers can be processed into different shapes and subjected various chemical and photo-chemical transformations that substantially expand the scopes of their application as absorbable surgical devices and sustained, controlled drug eluting systems.

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Abstract

Investigation of the Reaction of Telomerization of Ethylene and Trichloracetic Ethyl Ester

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Interest in radical telomerization has been aroused by the fact that, with its help, it is possible to obtain relatively low-molecular long-chain organic compounds containing different functional groups, which is hardly feasible with common methods. Such compounds are of wide practical application.

The reaction of telomerization of ethylene and trichloracetic ethyl ester under study is of particular interest. The reaction proceeds by the following scheme:

$$nCH_2{=}CH_2{+}CCl_3CCOEt \xrightarrow{initiator} Cl(CH_2CH_2)_n\, CCl_3CCOEt,\ n{=}1\text{-}4$$

Telomers derived from ethylene and trichloracetic esters are used for the synthesis of psychotropic drugs Gamalon and ε-Capron (ε-capronic acid), and biologically active substances lysine and metonin.

For the purpose of studying the above reaction, we carried out a series of autoclave tests. We studied the effect of the reaction conditions, the ratio of reagents, the initiator composition and the reaction temperature on the yield and composition of obtained telomers.

Based on the obtained data, we investigated the phase state of the system ethylene- trichloracetic ethyl ester, the reaction kinetics according to ethylene consumption, private constants of the transmission of the chain over a wide temperature range and the optimal conditions of production of individual telomers.

We determined the entropy of the thermodynamic characteristics of the above-described reaction, such as the standard thermal effect of the reaction, the factor of the heat capacity equation $C_p=\varphi(T)$, and the initial and final efficiency of the reaction, according to the molecular structure by the method of group correction.

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Abstract

Adsorbtion of Bacteriophages on Ca / Mg Insoluble Salts and Some New Routes to Bactericidal Surgical Materials

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The interaction of serial bacteriophage preparations of Biochimpharm, LLC “Bacteriophagum Staphylococcicum” (Liquidum) and complex “Phagyo” (Pyobacteriophagum liquidum) with water insoluble Ca and Mg fine-dispersed salts was studied. It was found that bacteriophages were adsorbed on the said salts at room temperature within 30 min. After the filtration of the obtained suspensions the basic portion (up to 97%) of admixtures (ballast proteins and fragments of nucleic acids) were moved off with filtrate that was assessed by UV study. The bacteriophages titer in filtrate showed that *ca*. 100% of the bugs are adsorbed on the solid salts. The adsorbed bacteriophages retained a high activity that was established by the study of bactericidal activity of the obtained solids using bacterial loan (lysis zone +4) as well as by their desorption from the water insoluble salts and subsequent titration. Using the salts with adsorbed phages as antibacterial agents, and amino acid based polymers originally developed in our laboratory as biodegradable matrices, we obtained new composite materials showing a high bactericidal activity. These new biocomposites have a high potential to be used as dressings for treatment of infected wounds and cavities, as coatings for surgical devices to prevent biofilm formation, to name a few.

Abstract

Synthesis of the Super-Absorbents Hydrogels on a Basis of Polyacrylamide, Polyacrylamide/Bentonite, Polyacrylamide/Diatomite by Frontal Polymerization Mode

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The Frontal Polymerization is a nonconventional, ecologically safe, high-efficiency method of polymers, polymer composites and nanocomposites synthesis. In the past 20 years it was shown both advantages of the frontal polymerization method - the easiness of technological realization as well as the very properties of received products.

In the frontal mode it was carried out the synthesis of the super-absorbents hydrogels on a basis of polyacrylamide, polyacrylamide/bentonite, polyacrylamide/diatomite.

It is shown, that the obtained materials have a very wide range of applications in a different areas of human existence.

The investigation show that frontal polymerization contributes to deagglomeration of disperse nanoparticles. The intercalation of linear polyacrylamide macromolecule into the layer structure of bentonite is also shown.

Abstract

Phenol-Formaldehyde Composites

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Phenol-formaldehyde type plastic masses, thanks to their practical significance occupy special place among heat- and thermo-resistant polymers of spatial structure.

The present work pursued to study polymer composites obtained on the basis of natural inorganic mineral material – diatomite and novolac type oligomers and plastic materials obtained through their treatment.

Application of diatomite as one of the main components enables us to decrease markedly share of a polymer in polymer composite and to decrease the price of plastic materials. Novolac oligimer is obtained through interaction of formaldehyde and phenol [1, 2].

Polymer composites contain 30-80 mass% of natural diatomite. Major technological characteristics have been defined for their thermal treatment. These are: temperature, 180^{0}C, specific pressure 69 mPa, time of standing/hardening - 40 sec at 1 mm thickness of the bject.

Physical-mechanical and dielectric characteristics of the obtained plastic materials were studied. Properties of plastic materials depend on diatomite concentration in the composite. Composite that contains 30 mass % diatomite has relatively low characteristics at shock strength and its dielectric indices are relatively low.

When diatomite concentration in polymer composite is up to 80 mass%, its mechanical and dielectric properties improve, but fluidity decreases markedly, which complicates processing of polymer composites.

It was proved that the composites are of optimal composition when diatomite content is up to 40-60 mass%. Objects made of such polymer composites, in some cases are characterized by far better characteristics than the objects made of currently known analogous industrial designnation polymer composites.

It became possible to substitute completely the costly and deficient fillers in polymer composites with cheaper and more accessible local natural material – diatomite.

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Abstract

The Comparative Study of Thermostable Protein Macromolecular Complexes (Cell Proteomics) From Different Organisms

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Achievements in proteomics have significantly expanded our imaginations not only about of specific proteins involved in biological processes, but about their function as macromolecular complexes. The role of polyfunctional macromolecular protein complexes in the biosynthesis of fatty acids, erythrocyte membrane proteins macromolecular complexes that are involved in exchange of CO2/O2 was found (1, 2). No less important is the comparative study of cell proteomics of various organisms (3). From various organs of white rats we have identified thermostabile tissue-specific protein complex that regulates cell proliferation and is not characterized by species specificity (4).

The Goal. Extraction and comparative characterization of thermostable protein complexes from phylogenetic distance organisms.

Material and Methods. The thermostabile protein complexes obtained by alcohol extraction from normal and tranformed cells of various organisms (bacteria, snail, lizard, newts, frogs, etc, also human postsurgical material and cell culture) were used for research. For comparative analysis hydrophobic interation chromatography and gel electrophoresis assay were used (4).

Results and discution. We have determined that different cells of phylogenetic distance organisms contain protein complexes with hydrophilic and hydrophobic parts (molecular weight from 12 to 45kD) and with similar electrophoretic movement. Low molecular weight component (Hydrophilic) of the complex is revealed with relatively minor amount in transformed cells and was not observed at all in human renal cancer cells. The determination of the identity of mentioned components by the Mass Spectrometry is the aim of our future research.

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Abstract

RAFT Polymerization of Acrylic Esters by Using of New Chain Transfer Agents on the Basis of Thiocompounds

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Narrow polydispersity Polyalkylacrylates were synthesized with RAFT polymerization of butylacrylate or 2-ethylhexylacrylate by using new S-alkylarylthiophosphate type chain transfer agents. A well-defined polyalkylarylacrylates with a wide range of controlled molecular weights and narrow polydispersity ($1.22 < Mw/Mn < 1.42$) were obtained. The results indicate that the new S-alkylarylthiophosphate type chain transfer agents are effective for the controlled/"living" RAFT polymerization of acrylates with different alkyl groups and polymerization process is well-controlled: a linear increase of molecular weights occurs with respect to conversion and the polydispersity is relatively low.

Synthesized narrow polydispersity Polyalkylacrylates were successfully tested as a viscosity additives to base motor oils.

Abstract

Hyperbranched 1,4-cis+1,2-Polybutadiene Synthesis by Using New Catalytic Dithiosystems

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Branches in polydiene structure strongly reduce solution viscosity by improving its processability, increasing operating ability of vulcanization and other such preferences. On the other hand, branching polydienes easily decompose via light and biological affecting, that solves elimination problem of waste polymers from the environment.

Homogeneous Cobalt-Dithiocarbamate bifunctional catalytic dithiosystems – Dialkyldithiocarbamate Cobalt+Alkylaluminumdichloride (or Alkylaluminumsesquichloride) were developed for the synthesis of hyperbranched, low viscosity high molecular weight 1,4-cis-polybutadiene with the 20.0-40.0 % content of 1,2-vinyl bonds. The effect of type of ligand in cobalt compound, used solvent, cobalt and monomer concentration, AI:Co ratio, temperature, polymerization time on conversion, stereoselectivity and molecular mass in the butadiene polymerization were studied. Productivity of these catalysts is 20.0-55.0 kg PBD/g Co•hour with the yield of polybutadiene - 86.0-99.0 %. The obtained hyper branched polybutadienes has branching index of 0.22÷0.70 against of branching degree 0.94÷0.98 in linear polybutadienes.

Synthesized hyper branched 1,4-sis+1,2-polybutadiene can be used in the production of tiers, technological rubbers and impact resistant polystyrenes.

Abstract

The Improvement of the Quality of Lubricating Oils by Polymeric Compounds

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In this article are given the results of the investigations conducted at the institute of chemistry of additives of the academy of sciences of Azerbaijan Republic in the direction of preparation of polymeric compounds which are carried out different functions in the composition of lubricating oils in dependence on the meaning of their molecular mass and chemical composition.

The results of the conducted investigations have shown that for the purposes of the improvement of thermal stability of viscous additives, initial monomers used for their analysis are underwent to copolymerization with vinyl aromatic and carboxylic compounds.

With the purpose of the development of poly functional polymeric compounds is conducted functionalization of oligomers of the high α-olefins. This way gives the possibility to develop lubricating compositions of the more simple structure which leads to economic effect.

Between the additives to motor oils are detergent dispersant additives and about 50 – 60 % of all additives comes on their portion.

On the base of oligomers of high α-olefins sulfonated, succinimide and thiophosphate additives were synthesized.

Introduction of synthesized additives into the structure of lubricating compositions will give the possibility to develop lubricating compositions of various purposes.

Abstract

Environment Friendly Nanotechnologies

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In this presentation we will present the following new industrial nanotechnologies:

- Nanostructured composites based on Interpenetrated Polymer Network;
- Epoxy-rubber composites with nanoteterogenic structure;
- Nanocomposites based on hybrid organo-silicate matrix;
- Polymer nanocomposites with very low permeability and high resistance to aggressive environments;
- Polymer matrix nanocomposites and nanomembranes produced by SDP method;
- Biodegradable materials based on Nanocellulose;
- Polymer nanocomposites contained carbon nanotubes and fullerenes with terminated hydroxyurethane groups;
- Nanocomposites based on liquid polybutadienes.

These industrial nanotechnologies are environment friendly and are mainly “green chemistry” product with using, for example, nonisocyanate polyurethanes based on modified soya been oil contained reactionable cyclocarbonates groups.

Abstract

Novel Surface-active Monomers Containing Phosphate Group: Synthesis, Properties and Application

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The application of various polymeric materials for medical purposes is growing very fast. Nowadays polymers have been applied in tissue engineering, bone repair and many other biomedical fields. Various functional groups incorporated into a polymer structure impact on biocompatibility, cell and protein binding reactions and growth. On the other hand the utilization of such functional polymers with distinct surface active properties can significantly expend the ways of their application. One approach of obtaining such materials consists of utilizing of surface active monomers with functional groups located in hydrophilic part or in hydrophobic part. Nowadays materials containing phosphate groups are widely used in various fields of biomedicine. For this purpose novel surface active maleate and methacrylate monomers with terminated phosphate group located in hydrophilic part have been synthesized. Poly(ethylene glycols) with different molecular weights have been used for formation of hydrophilic blocks. The synthesized monomers exhibit surfactant properties and reduce the surface tension at the aqueous solution – air interface. The polimerizable properties of resulted monomers have been studied. Synthesized surface active monomers have been shown to be capable of copolymerization with various commercial monomers with formation of reactive copolymers. The kinetic of polymerization and surface active properties of obtained copolymers have been investigated. Synthesized polymers have been shown to be promisingly applied as drug delivery vehicles and in tissue engineering.

Abstract

Synthesis and Characterization of New Nano composites and Study of their Biological Properties

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Nano structured materials have been extensively explored for the fundamental scientific and technological interests in accessing new classes of functional materials with unprecedented properties and applications. This is based on positively perceived characteristics of them.
Characteristics specially properties include mechanical performance, electric behavior, thermal properties, biodegradability, optical properties, bactericidal effects, magnetic characteristics, permeation and separation properties are from more important groups. Two building strategies are currently used in Nanotechnology: a ‘‘top-down” approach and the ‘‘bottom-up” approach. The commercial scale production of Nano materials currently involves basically the ‘‘top-down” approach, in which Nano metric structures are obtained by size reduction of bulk materials, by using milling, Nanolithography, or precision packing engineering. Smaller sizes meaning to have bigger surface area, desirable for several purposes. The newer ‘‘bottom-up” approach, on the other hand, allows Nano structures to be built from individual atoms or molecules capable of self-assembling. In this research the preparation of new Nano composites reported that characterized by the FT- IR, X-ray diffraction analysis (XRD) and Scanning Electron Microscope (SEM)**.** (Figure)

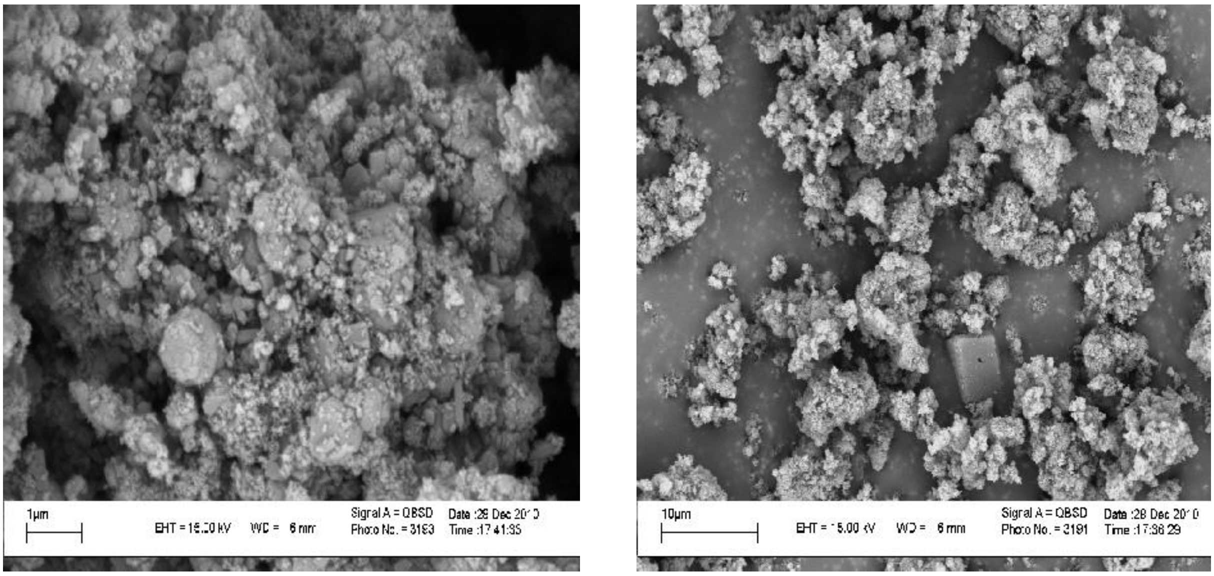

Figure. Al_2O_3/TiO_2 Nano-composite morphology with Magnification A) 10000 times, B) 30000 times.

Abstract

Polymeric and Low-molar-mass Glass-forming Semiconductors for Optoelectronic Applications

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Charge-transporting polymers and molecular glasses are widely used in optoelectronic devices, such as electrophotographic photoreceptors, light-emitting diodes, solar cells. In this presentation the resent results of the work on the synthesis and properties of charge-transporting polymers and molecular glasses performed in the author's laboratories are reviewed. We prepared soluble charge-transporting polymers and oligomers by chain growth (photo)polymerization of oxiranes, oxetanes, thiiranes, vinyl ethers bearing different electroactive groups also by polycondensation and polyaddition of bifunctional electroactive monomers. We use cationic and radical photocross-linking of bifunctional monomers bearing electroactive moieties for the preparation of insoluble charge-transporting layers. Such layers are useful in the fabrication of multi-layer optoelectronic devices when they are prepared by the solution processing.

We also synthesized hole-transporting molecular glasses belonging to the families of condensed aromatic amines, hydrazones, enamines, ethynylenes, stilbenes and electron-transporting materials belonging to the families of aromatic imides. The ionization potentials of hole-transporting materials range from 4.80 to 5.80 eV. Time-of-flight hole drift mobilities in the amorphous films of 2,7-substituted derivatives of carbazole and carbazole-based enamines exceed 10^{-2} cm^2/V. Electron mobilities in the layers of the newly synthesized perylene diimide derivatives exceed 10^{-3} cm2 V^{-1} s^{-1} at high electric fields. Well defined carbazole oligomers have appeared to be effective host materials for blue organic electrophosphorescent devices. The triplet energies of these materials approach 3.0 eV. Using these host materials, blue phosphorescent OLEDs having efficiencies of up to 15 %, 31 cdA^{-1}, and 28 lmW^{-1} were demonstrated. Some of the recently synthesized high-triplet-energy glass-forming hosts have appeared to be effective ambipolar semiconductors. They were successfully used for the development of single layer organic light emitting diodes.

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Abstract

Ring-opening Polymerization of Vinylcyclopropanes

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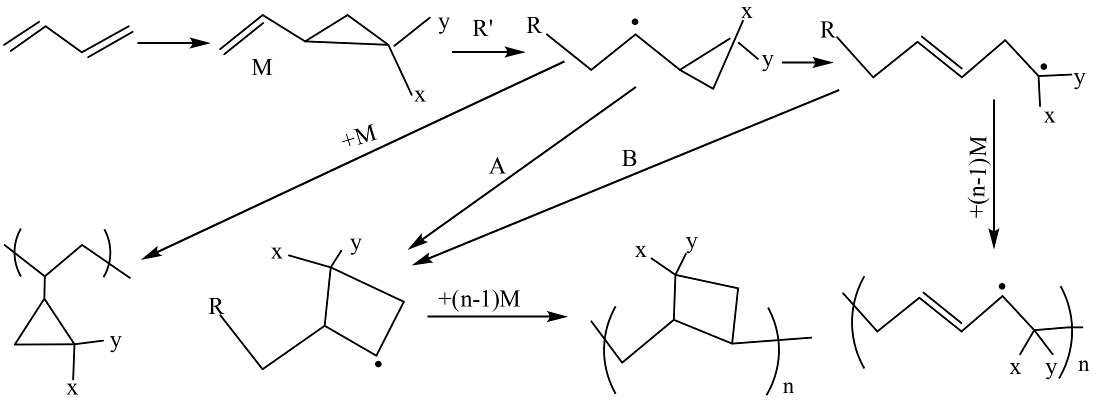
The functionally substituted cyclopropanes are characterized by high cycle intensity and that's why are easily subjected to the polymerization with cycle opening.

In this work the results prepared at radical polymerization of a number of industrial vinylcyclopropane (VCP) having substituents both in double bond and in three-membered cycle have been presented. VCPs containing polar and non-polar, cyclic and non-cyclic, vicinal and geminal substituents in cyclopropane ring have been synthesized. The syntheses have been carried out by cyclopropanation of one of two double bonds of diene hydrocarbons by various carbenes generated in catalytic conditions in the presence of copper salts and in interphase conditions in the presence of catalyst Makoshi. The polymerization was carried out in the presence of the corresponding radical initiators both in solution and in mass.

The results of kinetic and structural investigations and also model reactions prepared by spectral and chemical methods of analyses showed that the vinylcyclopropanes are subjected to the polymerization in the presence of radical initiators with formation of pentenamer links. In a case of polymerization of VCP with the substituted CH_2OR along with pentenamer links there are formed the unidentified products in structures in which olefin protons are absent.



It follows from a scheme that it is firstly formed a cyclopropylcarbinyl radical which as a result of opening of high-stress cyclopropane ring is converted into thermodynamically more stable allylcarbinyl radical. The selective opening of cyclopropane ring has been stipulated by stabilizing action of functional substituent on growing radical.

Thus, a high intensity of cyclopropane ring and stabilizing action of functional substituent is the moving force leading to the proceeding of polymerization of VCP with ring opening.

Abstract

Study of Modification Process of Simple Aromatic Ethers

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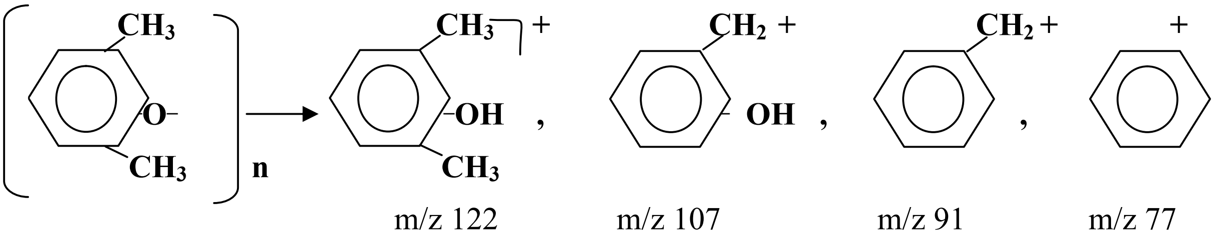
In antifriction plastics aromatic simple polyether – polyphenylene oxide (PPO) has been used as a binder. But the insufficient stability of PPO in the process of friction conditions needs the necessity of its modification.

Modification of PPO has been carried out by fluorine containing oligomers - fluorine alkanes: $Cl(CF_2)_nH$, where n = 7 – 12 and by $Cl(CF_2)_nOSO_2F$ where a privilege of n=7-12. The privilege of fluorine alkanes in comparison to other modificators is expressed in organic solvents by good solubility, high temperature of decomposition and possibility of receiving low disperse product during crushing.

In polyphenyleneoxide modified by fluorine alkane after pressing at 300°C there is observed formation of insoluble fraction in chloroform by 70%. Content of insoluble part lesser depends on the number of fluorine alkanes (up to 1 – 7 %) and the nature of extreme groups.

By the method os mass-spectrometry it has been studied a process of thermal decomposition of modified PPO at temperature 300°C together with the products of thermal decomposition characteristic for PPO, there have been observed in great quantity the destruction products of flurine-alkans: CF_2 – m/z 50, HCF_2 – m/z 51, $(CF_2)_2$ – m/z 100, $H(CF_2)_2$ - m/z 101.



Modification of PPO by fluorine alkane improves the friction properties of polymer: the wear – resistance is increased twice; friction coefficient is reduced from 0.35 to 0.25. The modified polymer has low and stable friction coefficient within the wide range of temperature – up to 50 – 225°C.

Abstract

Ionites on the Basis of Zeolites

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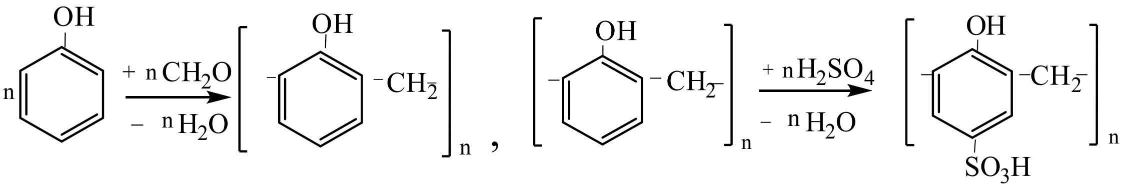
One of the actual problems is purification of liquids, drainage and drinking waters from salts. On the basis of natural sorbent – clinoptilolite, cationite of high and low ion exchange capacity, compirising of strong and weak ionogen groups has been synthesized. The natural zeolite - clinoptilolite, the oxide formula of which is – $(Na_2K_2Ca)O \cdot Al_2O_3 \cdot 10SiO_2 \cdot 8H_2O$, is characterized by high thermal stability, porosity and plays a role of a matrix.

In pores of clinoptilolite in presence of catalysis, on the first stage there was implemented a phenol molecule, further at 125 – 135°C, during polycondensation with aldehyde there was created a growing oligomer of phenol-formaldehyde resol type. The methylol group react with groups of silanol available in zeolite, as well with each other and there is created a polymer having a spatial structure in which on the further stage through the sulphures there is performed introduction of active sulphur groups: $(Na_2K_2Ca)O \cdot Al_2O_3 \cdot 10\ SiO_2 \cdot 8H_2O$;



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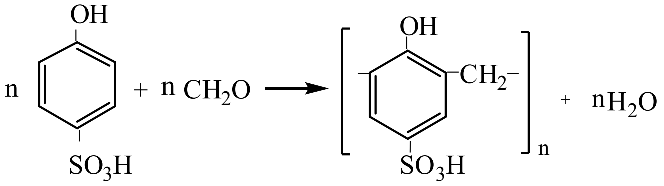

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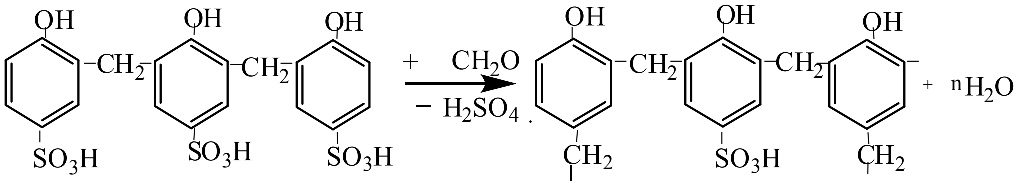

By studying the effect of various factors which influence on the value of statistic exchane capacity of cationite the optimal conditions of receiving the cationite, the relation between the zeolite and phenol, mas %: 85:15 have been established. The temperature of polycondensation reaction is 125 – 135°C, duration of the process of sulphuration is 2- 3 hours.

The statistic exchange capacity of cationite received by this method equals to 5.5 – 8.0 mgekwg $^{-1}$ (relative to 0.1 N HCI)

Abstract

Organo-mineral Ionites

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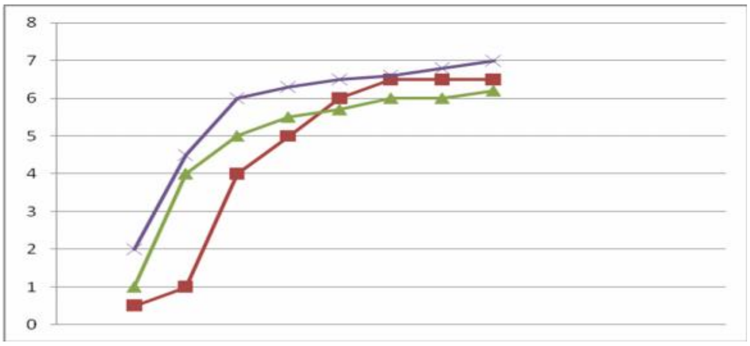
The goal of the present work was to synthesize ionites, to synthesize organo-mineral ionites in which the natural mineral sorbent would be chemically bound with organic part of the ionite, Ionogenic group of such ionites is capable to participate efficiently in the process of exchange in water solutions. To resolve this problem we used natural ionite – clinoptilolite of the following composition expressed in oxides: $(Na_2K_2)0 \cdot AI_20_3 \cdot 10\ Si0_2 \cdot\ 8\ H_20$.
The other component is bromine-acetic acid ($BrCH_2COOH$), which because of activity of bromine atom easily comes into reaction with hydrogen atom of hydrogen form (H-form) zeolite.
At the interaction of bromine-acetic acid with hydrogen form zeolite, in organic solvent, at the temperature 60–80^{0}C, ionite is formed which possesses carboxyl ionegenic groups.
IR-spectral studies of the ionite showed absorption bands in the region of 1090–1050 cm^{-1}, which are characteristic to Si-O-C chemical bond.
Effect of various factors on static exchange capacity of clinoptilolite was studied with respect to the conditions of condensation reaction of bromine- Zeolite easily sorbs bromine-acetic acid, but molecules of bromine-acetic acid are likewise easily washed out from the pores of zeolite. Preliminary studies proved that at its treatment with water, bromine-acetic acid is completely washed out from the zeolite.
Study of effect of various factors on the process of interaction, showed that optimal conditions for the process to achieve maximum value of static exchange capacity of cationite are: zeolite/bromine-acetic acid (mass share) ratio 7:1, correspondingly, reaction temperature: 60-65 ^{0}C, and reaction duration 8 hours.
Dependence of cationite static exchange capacity (SEC) on the basis of chemically modified clinoptilolite on conditions of synthesis.



Static exchange capacity of low-acid cationite with carboxyl ionogenic groups, at 0.1 N NaOH water solution, increases from 0,1 – 0,9 (for chemically modified zeolite) to 5-6 mg-equiv\g.

Abstract

Synthesis and Thermal Properties of Polycyanurate-based Thermosetting Nanocomposites

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Layered silicates, particularly montmorillonites (MMT) posessing unique morphology, are widely used in generation of polymer/clay nanocomposites. High performance polycyanurates (PCNs) offer a combination of excellent thermal and dimensional stability, high glass transition temperatures, high purity and adhesion to conductor metals at high temperatures etc. However, due to their highly cross-linked structure, these polymers are inherently brittle. Thus, reinforcement of PCNs with MMT through generation of clay-filled PCN nanocomposites is one of perspective ways of improvement in mechanical properties of the PCNs without any loss in thermal properties. The main problem revealing while clay dispersing appears in incompatiblity of hydrophilic layered silicates and hybrophobic polymer matrix. Therefore, surface modified nanoclays have to be used.

The present work is focused on synthesis and characterization of PCN/MMT nanocomposites synthesized using different amino-functionalised nanoclays. The effect of type of MMT modification and of clay amount on kinetics of PCN formation and also on chemical stucture, morphology and thermal chacteristics of the nanocomposites produced are discussed.

Acknowledgement: The authors are grateful to the CCUE IMC of the NAS of Ukraine for thermal, optical and infrared spectroscopy measurements.

Abstract

Degradation of Polyhydoxybutyrate in Vivo Environment of Ukraine: Structure and Morphology Studies

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Over the last decades, much attention has been paid to the disastrous pollution of the Earth with millions tones of polymer wastes. Recently a lot of countries restricted to the usage of polymer bags etc. and transferred to biocompatible environmentally friendly materials able to complete degradation in vivo environment after utilization without any undesirable consequences. Among the known biopolymers one can distinguish polyhydroxyalkanoates, possessing similar material properties to polypropylene and also high biocompatibility with living organisms, good resistance to moisture and aroma barrier properties etc.

The present research was devoted to the study of the influence of environmental conditions of Ukraine on degradation process of polyhyroxybutyrate (PHB) and PHB-based compositions. Gradual changes in chemical structure and morphological peculiarities of the films after partial degradation in vivo environment are presented. The influence of soil type and its characteristics on decomposition rate will is shown.

Acknowledgement: The work was fillfilled under the Grant of the President of Ukraine for the gifted youth (President order No.72/2012-rp). The authors also are grateful to the CCUE IMC of the NAS of Ukraine for thermal, optical and infrared spectroscopy measurements.

Abstract

Heat-resistant Hybrid Polymer Nanocomposites Filled with Fusible Metals

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Hybrid polymer nanocomposites (HPN) were synthesized by joint polymerization process of organic and inorganic components. Organic component was a mixture of polyisocyanate (PIC) and macrodiisocianate (MDI). Heat-resistant composites with 80%wt. of PIC and 20% wt. of MDI were taken as the basic for further processing and filling. Inorganic component was water solution of sodium silicate (SS). Aerosil A175 and powdered glass were used for SS modification. Tin and lead powders were dispersed in the reactive mixtures of organic and inorganic components during HPN synthesis. Polymerization of pure HPN, modified HPN and filled HPN passed at $T = 20\pm2\ ^0C$ during 24 hours.

The structure of the modified HPN obtained was found in the form of membrane with regularly shaped interconnecting pores with ~ 90 µm in diameter. The formation of such structure was due to the emission of carbon dioxide in the set of reactions, which run during OIS polymerization. The introduction of metallic fillers in the modified porous structure of HPN increases rates of transport, dissipation and uniform distribution of thermal energy in HPN bulk. That leads to higher values of thermal stability, precise structural transitions and broad operating temperature range of the filled HPN. However, the level of electrical conductivity of the filled HPN ($\sigma_{DC} \approx 10^{-12}$ S/cm) changed insufficient comparing to the pure HPN ($\sigma_{DC} \approx 10^{-14}$ S/cm). Heating of the filled HPN to the temperatures higher than structural transitions temperatures of HPN and melting temperatures of metallic particles leads to electron conducting phase formation in the porous HPN bulk. Further cooling of the filled HPN to the temperature lower than structural transitions temperatures of HPN and crystallization temperatures of metallic particles leads to formation of continuous electron-conducting metal cluster in HPN volume with level of conductivity $\sigma_{DC} \approx 10^{-3}$ S/cm.

Abstract

RP-HPLC Packing Materials on the Base of Silica-polymer Sorbents

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Recently hybrid packings have become available stable within wider pH range (up to pH 12) but with retention characteristics identical to classical silica-based packings.

Problems of the silica gel surface modification with polymer layers and the influence of deposited polymer quantity on chromatographic properties of the resulting sorbents have been considered. The surface polymer modification of wide-porous micro-spherical silica (MS) obtained by means of hydro-thermal treatment of meso-porous silica gel under autoclave conditions has been described. The polymer layer itself was formed by octadecylmethacrylate-methylmethacrylate co-polymer (ODMA-BA). As a result efficient packings for reversed-phase high performance liquid chromatography (RP-HPLC) have been obtained.

Tailor-made polymer coatings can serve as an alternative to classical bonded stationary phases. Polymer modification is one of the methods to eliminate disadvantages of the silica packings' (narrow working pH range and "silanol" interactions). Another advantage of polymer modification is the possi-bility to assert the presence of several functional groups on the surface simultaneously. The number of functional groups may be changed inserting new monomers during co-polymerization process. On the other hand, one can graft different required functional groups to the surface of already coated polymer by means of "grafting polymerization".

ODMA-BA-MA Symmetry 300 hybrid sorbent with polar groups on the polymer phase surface conditioned by the presence of maleic anhydride (MA) in co-polymer has been synthesized.

It has been shown that polymer-containing packing materials for RP-HPLC possess some properties different from that for convenient C_{18} packing materials. Uracyl may not serve as dead volume marker for columns packed by ODMA-BA and ODMA-BA-MA polymer phases inasmuch definite retention of it takes place by these phases, namely interaction of uracyl molecules with stationary phase surface take place. It is expedient to use butylparabene retention time as dead volume marker for such columns. Chromatographic characteristics of propranolol on columns containing polymer-coated MS also sharply differ from its chromatographic parameters on convenient C_{18} columns.

Abstract

Reactive Oligomers Based on Epoxidized Sunflower-Seed Oil

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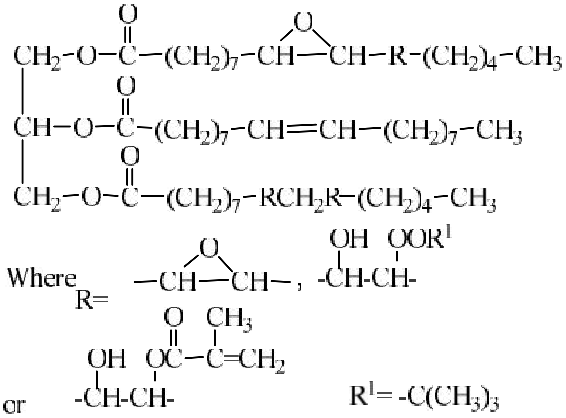
Epoxidized sunflower-seed oil (ESO) is used as a reactive component of different polymeric mixtures allowing to improve the elasticity of wares based on polymers.

In this work we proposed to modify ESO by different low-molecular compounds. The ESO derivative synthesized by us may be represented by the following formula:



Methacrylic acid, tert-butyl hydroperoxide and the mixture composed of methacrylic acid and tert-butyl hydroperoxide were used as low-molecular compounds. Benzyltriethylammonium chloride, $ZnCl_2$, 18-Crown-6 and the mixture 18-Crown-6 + $ZnCl_2$ were used as the catalysts for the reaction between ESO and low-molecular compounds.

The effect of catalyst nature and amount, as well as ratio between the initial compounds, reaction medium, process temperature and time on the synthesis of reactive oligomers was studied. The procedure of reactive oligomers synthesis was proposed. The oligomers characteristic was confirmed by chemical and spectral methods of investigations. The possible application of the synthesized compounds was examined.

.

Abstract

Siloxane Matrix with Methyl Propionate Side Groups and Polymer Electrolyte Membranes on their Basis

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Hydrosilylation reaction of cis- and trans-isomer mixture of 2.4.6.8-tetrahydro-2.4.6.8-tetramethylcyclotetrasiloxane with methylacrylate and vinylthiethoxsilane at 1:3:1 molar ratios of initial compounds in the presence of Karstedt's catalyst have been studied and $D_4^{R,R'}$ type organocyclotetrasiloxane with methyl propionate side groups have ben obtained.

Copolymerization reaction of $D_4^{R,R'}$ with hexamethyldisiloxane as a terminating agent in the presence of potassium hydroxide in inert atmosphere at 50-110^0 C temperature have been studied and comb-type polymers with regular arrangement of methyl propionate groups in the side chain have been synthesized. It was shown that by varying of terminated agents it's possible to regulate molecular masses of polymers.

The structure and composition of synthesized organocyclosiloxanes $D_4^{R,R'}$ and polymers were studied by FTR,^{1}H, ^{13}C and ^{29}Si NMR spectroscopa data.

Via sol-gel processes of polymers with various amount of lithium trifluromethylsulfonate (triflate) and 1-2 drop of 0.1 M HCl alcohol solution the solid polymer electrolyte membranes have been obtained.

Electrophysical properties of synthesized solid polymer electrolyte membranes have been studied and electro conductivity of membranes has been determined.

Acknowledgement: This work has been fulfilled by financial support of Science & Technology center in Ukraine (Grant #5055).

Abstract

Synthesis of Metaldithiophosphates on HLaУ and HУ Zeolites and Polymerization of 1,3-Butadiene with these Heterogeneous Catalytic Dithiosystems

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Metal dithiophosphates are widely investigated as various chemicals-additives such as stabilizers for polymeric materials and additives for engine oils, corrosion inhibitors, etc. In the recent years these metal complexes are also investigated as a component of homogeneous bifunctional catalysts-stabilizers for oligomerization and polymerization reactions of dienes, in particular 1,3-butadiene, with simultaneous stabilization of the end products.

Homogeneous catalysis has a number of advantages such as higher catalyst activity and selectivity. But, most important obstacle, which blocks their large scale applications in Industry, are the problem of separating homogeneous catalysts from the reaction medium, inefficient removal and recovery of the solvents and monomers after polymerization, which often requires more process steps and energy than the actual polymerization. Consequently that puts once a problem for researchers to create such catalytic systems which would work as heterogeneous systems, but possess advantages of homogeneous catalysis.

As is known process of phosphorsulfurization of alcohols and phenols with phosphorus pentasulfide occurs with the hydroxyl groups present in their molecules. Zeolites also have hydroxyl groups in the structure and it is possible to carry out reaction of phosphor sulfurization and to syntheses of O,O-disubstitued dithiophosphoric acids on zeolite matrix and then to obtain metal complexes on their basis. In this article the problems appear synthesis of dithiophosphates of HУ and HLaУ zeolites by the reaction of their surface hydroxyl groups with phosphorus pentasulfide and synthesis of Ni-, Co-, Fe-, Cr-containing dithiophosphates on their basis are considered. Synthesized nickel- and cobalt-containing zeolite dithiophosphates in combination with aluminum organic compound (diethylaluminumchloride) are highly active and selective catalysts for preparing of low and high molecular weights of 1,4-cis polybutadienes. Their productivities reach 1900-2500 kg polymer/g Me•hour (for cobalt catalysts) and 800.0-1110.0 kg polymer/g Me•hour (for nickel catalysts) that are much more than that in homogeneous nickel- or cobalt-containing catalytic dithiosystems 27-40 kg polymer/g Me•hour.

Abstract

Photochromic Liquid-Crystal Multifunctional Nanomaterials

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Photochromic liquid crystal (LC) polymers represent a perspective materials, which under the influence of light change their structure and properties. Retaining properties of LC and photochromic molecules in one system, interaction between them gives special properties and enables the creation of new multifunctional nanomaterials. This "smart materials"are present unique for photonics, optoelectronics, information record and storage.

The work describes a new method of creating polymer multifunctional smart nanomaterials based on composition consisting of nemato-chiral LC, doped with photochromic spiropyrans.Choice as a dopant spiropyran with long alkyl chain at the nitrogen atom, increases effective photosensitivity compared with the system, containing spiropyran with a short chain. Merocyanine form, photoinduced by ultraviolet (UV) light from spiropyran with long alkyl chain, is amphiphilic molecule with zwitterionic lyophilic head and lyophobic tail, is self-organized as micelles in the nematic-chiral LC. The formation of micelles disturbes the thermodynamic equilibrium. The new formed merocyanine molecules are added to already existed photoexposed molecules for restoration the equilibrium. It increases the absorbing centres ultimately. The phenomenon of increase effective photosensitivity was observed as in composition either in encapsulated polymer films, produced by the improved method of microcapsulation. The increase of photosensitivity, along with the radical length, is well defined upon information recording in the polymer films. The contrast strengthening between UV- irradiated and non-irradiated areas of the films, shows the increase of photosensitivity.

Photochromic LC polymer films with improved photosensitivity prodused by us would perspectiv multyfunctional nanomaterials for the applications in various fields of nanotechnology.

This work was supported by the Shota Rustaveli National Science Foundation (SRNSF), project number No.11/12

Abstract

Mutual Activation and High Selectivity of Polymeric Structures in Intergel Systems

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Upon contact with internal functional groups of the hydrogels can not participate in intermolecular interactions. For such systems, optimal is research of remote interaction of two or more hydrogel in aqueous or nonaqueous media.

In connection with this study was given properties of aqueous and saline solutions of several intergel systems consisting of acidic hydrogels such as polyacrylic and polymethacrylic acid and basic hydrogels – polyethylenimine, poly-4-vinylpyridine and poly-2-methyl-5-vinylpyridine. Intergel systems – systems consisting of two or more hydrogels and common solvent.

pH dependence, conductivity systems in aqueous media and supernatant, and swelling of hydrogels of the initial molar ratio of the acidic and basic hydrogel in the presence and absence of low molecular weight salts of mono and polyvalent metals was studied. An important element of this study is the absence of direct contact between the hydrogel.

The results showed that at certain ratios gel polyacid : gel polybase a sharp decrease in electrical conductivity of the medium and the growth rate of swelling is seen. These processes are associated with activation of mutual crosslinked polymeric structures of intergel systems due to binding of the cleaved from hydroxyl group proton amine groups as in the case of polyacrylic acid gel – gel polyethyleneimine (gPAK-gPEI) the following processes are:

$$\sim COOH \leftrightarrow - COO^- + H^+ \ (1),$$
$$\geq N + H^+ \leftrightarrow \geq NH^+ \ (2)$$

The result of these processes is the formation of high charge density in the internodal links of both hydrogels. These charges are electrically uncompensated because of lack in an aqueous medium of low molecular weight electrolytes. Thus, in the result of remote interaction of hydrogels included in intergel system a new highly active, highly ionized state of hydrogels is formed, i.e. a mutual activation of polymeric structures included in the intergel system is occurred.

The obtained experimental data suggests that the interaction distance is a new way to control the reactivity of hydrogels of intergel systems, which allows you to create highly selective sorbents for different ions and new materials based on the composition of polymer networks.

Sorption capacity and selectivity of interegel systems have been studied with respect to sodium ions, calcium, copper, iron and nickel. The above system showed a high sorption capacity and selectivity for certain ratios of hydrogels and conditions for all studied metal ions.

References:

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2. T.K. Jumadilov. The effect of remote interaction of polymer hydrogels in innovative technology. Industry of Kazakhstan. 2, 70-72, 2011.
3. Scientific discovery № 368 "The phenomenon of change in the degree of swelling of hydrogels in their remote interaction," The priority of the discovery March 20, 2008 Authors: Jumadilov Talkybek Kozhataevich, Suleimenov Ibrahim Esenovich, Mun Grigoriy A.

Abstract

The New Type Of Hybrid Composition Material

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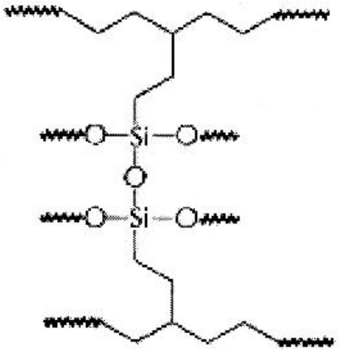
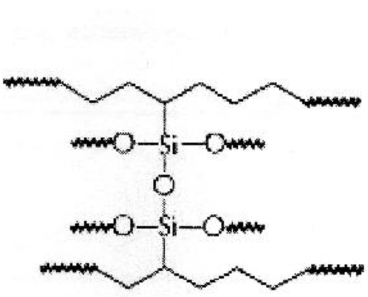
Discussed cross-linked polyethylene with siliceous methods. It has been studied cross-linked polyethylene of siliceous technology (PEX) and presumptive mechanism with this chemical reaction. This method is chemically cross-linking polyethylene with organosilane (vinyl trimethoxysilane). Silane cross-linking can be done in two ways: method - Sioplast and method-Monosil. In both methods, the chemical reaction principle remains the same. Active molecules vinylsilane replace hydrogen atoms in the macromolecules of polyethylene, using a weak C=C double bond. Then the organic radicals attached water molecule forming a stable hydroxyl and the neighboring polymer radicals are closed through a connection Si-O, forming a space lattice. Cross-linking polyethylene occurs without the involvement of organic radicals. To complete the process of stitching on this method, the product must be processed within a few hours in a water bath. The maximum proportion of cross-linking quantifies vinylsilane and holding time in the steam bath. Displaces water from PEX accelerated by the presence of tin catalyst.

It is established structure polyethylene of that cross-linked with siliceous by technology:





On the basis cross-linked polyethylene, new type- metallic plastic pipe hybrid composition material was received. By testing methods was determined the basic physical-mechanical and technically characteristic of metallic-plastics pipes.

Abstract

Composition for Polyurethane Foam

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Today polyurethane foam is one of the most common building materials. The polyurethane foam are lightweight but strong enough material has the lowest coefficient of thermal conductivity, is environmentally friendly, is ecologically safe durable, and able to provide acoustic insulation and corrosion protection. Universal features allow us to create polyurethane foam insulation pipes, roofs, walls, and ceilings, basements, industrial and residential buildings.

There are two main methods of production of flexible polyurethane foam-adjective and periodic. We have used the periodic method, which is a non-waste technology.

A composition for the production of polyurethane foam contains YORANOL, TDI, water, SILICONE, TEDA (A-33), TD, MCL. The optimal quantity of various components in composites has been established. The dependence of the viscosity of the polyol component, parameters of making foam and mechanical indexes, has been investigated.

Typical physical properties: the apparent density of 20-25 kg; compressive stress at 40% deformation; relative compression set no more than 6%; tensile stress at least 90 KPa; the elongation at break of not less than 100%;

Abstract

Peculiarities of Nanoparticles Magnetism Dispersed in Polysaccharide Matrix

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Magnetic properties, distinctly reflecting differences between bulky and nano-sized materials, take a special place among the unique physical characteristics of nanoparticles. Such effects are most pronounced in iron nanocomposites. The water-soluble iron nanocomposites, synthesized using the natural polysaccharide arabinogalactan as a matrix ensuring the self-organization of the system, are investigated by the EPR technique.

It is shown the aggregative stable iron-containing nanocomposites, Fe_3O_4 nanoparticles, dispersed in arabinogalactan, possess ferromagnetic properties. This is confirmed by the corresponding values of their magnetization and character of the spectra temperature dependence. The FMR spectra of the nanocomposites studied show asymmetric broad absorption bands (500-700 G) that testify the small changes in the sizes and shapes of the nanoparticles formed under variation of iron content in the nanocomposite from 3.5 to 6.4%.

The dramatic changes of in the spectra are observed when iron content increases up to 9.2-12.5 %. The appearance of several absorption bands in the spectra, the position and intensity of which vary at different levels of microwave power, the characteristic angular dependence of the spectrum shape at the sample orientation change in magnetic field indicates a significant anisotropy of the nanoparticles distribution that is supported by TEM data. The changes observed in the spectra can evidence a possible alteration of the nanoparticles domain state when their sizes rise and iron content in the nanocomposites increases. This assumption is confirmed by the appearance of the inflection point (6.4% iron content) on dependencies of g_{eff}-factor and width of EPR signal, magnetization parameters and nanoparticle sizes upon iron content in the nanocomposite.

Thus, the design of the objects having relationship of magnetic activity with the sizes and shapes of the nanoparticles and, consequently, controlled set of physical and chemical properties, is of interest for the development of biocompatible magnetic multifunctional materials for both engineering and medicine.

Abstract

New ABA Triblock Copolymeric Micelles for Delivery Poorly Soluble Drugs

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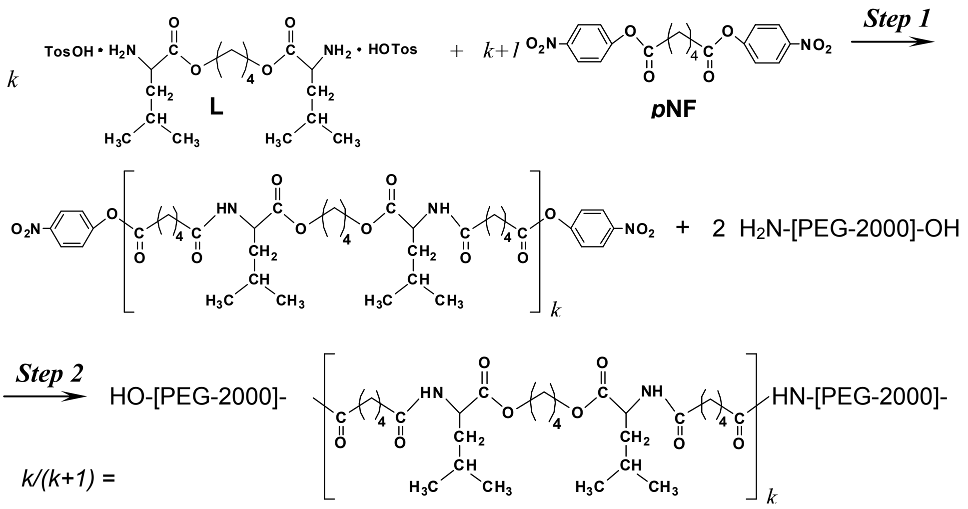
The present work deals with the preliminary successful synthesis of a new class of biodegradable micelle-forming block-copolymer, namely ABA triblock-copolymer, composed of PEG, amino acids and other nontoxic building blocks like fatty diols and dicarboxylic acids. For constructing this new class of biodegradable block-copolymers, we decided to use amino acid-based biodegradable poly(ester amide)s (PEAs) as hydrophobic blocks since these polymers showed reasonable biodegradation rates and excellent biocompatibility [2,3]. In the present study, the hydrophobic PEA block composed of adipic acid, L-leucine and 1,4-butanediol was exploited. Among various schemes, we have examined for the synthesis of micelle-forming triblock-copolymer, the best was found to be the two-step method depicted in Scheme (1) below:



Scheme 1. The synthesis of micelle-forming biodegradable ABA triblock-copolymer.

The ABA triblock-copolymer obtained was tested for the micelle-forming property using dynamic light scattering (Malvern zetasizer Nano ZS ZEN3600). According to this study the triblock-copolymer formed micelles with a neutral zeta-potential and of 50±2 nm in size within the concentration range 0.25-10 mg/mL that means the micells are rather stable. According to the literature data the most suitable size of pharmaceutical micelles is between 10 and 80 nm [4]. This allows to conclude that the ABA triblock-copolymer we have obtained is promising for constructing biodegradable micellar nanocarriers suitable for delivering poorly water-soluble drugs.

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Abstract

Composite Materials Based on Modified Coal Tar Pitch

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Structural compositional polymeric materials are one of the most common materials of present time. The basis of polymeric matrix of these materials is different polymers. Production of polymers is a compound process that determines their high cost. Having regard to the high demand for polymeric composites the search of cheaper ones is very actual today.

Coal tar pitch is a unique product with a rich set of properties, among which are polymeric ones. Coal tar pitch is cheaper than classical polymers and it characterized by resistance to acids, alkalis, water, does not put on biodestruction under the influence of various microorganisms, has low thermal conductivity.

Modification of coal tar pitches provides a wide opportunity to adjust and change their properties. This opens a new direction - the use of coal tar pitch chemical potential for creating the disperse-filled compositional polymeric materials.

Past studies have shown the possibility of active influence on polymeric properties of coal tar pitch by modifying with chemical additives such as polyvinyl chloride and polymer of polyolefin line with intergrafted functional groups. The results of thermochemical and structural changes indicate that between coal tar pitch and modifiers the chemical and physicochemical interaction takes place. Reactions of polymerization and polycondensation leads to the structuring of coal tar pitch, increasing the strength of structure, thermal stability.

The obtained pitch composite has relatively high mechanical properties and thermal stability. The obtained material for all parameters can be attributed to the hard-burning polymer composite what gives it a cogent advantage comparably to thermoplastic polymers.

Tests of modified coal tar pitch as a polymer matrix showed that it can successfully compete with classical polymers in order to create compositional materials.

Abstract

Obtaining of Ultrafine α-Alumina for Corundum Ceramics

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α-alumina nanopowders have great potential for a variety of applications: high performance engineering, obtaining elecric, electric-technical, bio-compatable, ceramic materials, catalists, adsorbents, membrane, filters, synthesised jewellery stones and singlecrystals. It was found that ceramic materials physico-mechanical propoerties basically depend on α-alumina nanopowders obtaining and their consolidation methods. Currently great attention is paid to the fabrication of special-purpose items. Many methods are used to obtain ultra-disperse Al_2O_3 among them are sol-gel process, deposition, chemical decomposition, plasmachemical, electrochemical, micro-emulsion, hydrothermal, airzol, corrosion, polymer-precoursor, high temperature oxidation, etc. Operating characteristics of the Corundum ceramic samples are conditioned by presence of micromixtures, particles structural-morphological structure nad also sintering technologies. We have obtained α-alumina accounted for modified polymer-precoursor and self-distributed oxidation-reduction reaction. Aluminum nitrate, aluminum alkoxides, oxidants and bio-functional compounds (glycols, amine-oxides, biopolymers, etc.), which form organic-inorganic gels have been used as initial precursors. Organic-inorganic gels are obtained from aluminum and organic compounds homogenization at 80-200^{0}C and from carbonization of the resulted mass within different temperature ranges 300-800^{0}C. In addtion carbonization results in black powder, which basically consist of γ-alumina. Its transition into α-alumina has been performed in the air 1180-1200^{0}C during 2 houres. We demonstrate that transition temperature in $\gamma \rightarrow \alpha$ phase decreases (1200^{0}C) by 120-150^{0}C as resulted by adding α-modification aluminum oxide in the initial reaction mixture. According to literature sources it is recognized obtaining α-alumina by sol-gel method with presence of ammonium nitrate in the reaction is allowed at 800-1100^{0}C temperature range. γ- and α-alumina modification aluminum oxides characterised by lamellar structure are obtained by partially hydrolyzed aluminum isopropoxide gel and aluminum nitrate interaction at 400-500^{0}C. Thikness of the layer is 50-80 nm, length is 8-15mkm. The layers are easily granulated in nanosize powders. Bulk densitiy of the aluminum powders obtained by self-distributed oxidation-reduction reaction is 30-70mg/ml. The microstructure of powders and Corundum samples obtained from them has been studied by optical and electrical scanning microscopes (Nikon ECLIPSE LV 150, NMM-800TRF, Nanolab-7). Micro hardness has ben measured on the device (DUH – 211S). The grain size of the synthesized powder has been determined by means of Analysette 12 Dyna sizer. Phase analysis of the samples has been performed on X-ray difractometer (DRON-3M). Thermal analysis (TG-DTG-DSC) has been carried out on Setsys Evolution device (Setaram Tag 24).

Abstract

Sol–gel Methods and Polymerization for Synthesized Hg-based Polycrystalline Superconductors

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Among all of the known high-T_c superconductors the Hg-based cuprate superconductors $HgBa_2Ca_2Cu_3O_y$ have the highest critical temperature $T_c \approx 135K$. This peculiar property makes the Hg-1223 phase as an invaluable material for its practical utilization. Preparation of Hg-based cuprate superconductors by the solid state reaction method are labor-consuming (expensive, multi-stage) also needed high temperature and long times for observation chemical homogeneity and chemical reactivity. We report the sol-gel methods for preparation Hg-based polycrystalline superconductors. The basic idea of sol–gel is to start from a solution of cations and to jellify it by polymerization.

The synthesis of $Ba_2Ca_2Cu_3O_y$ is carried out by dissolving separately $CaCO_3$, CuO in nitric acid and $BaCO_3$ in acetic acid. The solutions are mixed afterward in the stoichiometric ratio. The cations Cu^{2+} in the solution are complex with addition of acid-EDTA:
$(H_4Y)=[CH_2N(CH_2\text{-}COOH)_2]_2$ and the pH was adjusted ≈3 just to dissolve completely the elements into a clear solution. To this solution were added acryl amide monomers, i.e., $H_2C=CHCONH_2$ and N,N'-methylenebisacrylamide. A few milligrams of a chemical initiator *a*,*a*'-azoisobutyronitrile, i.e., $C_8H_{12}N_4$, was added to initiate the polymerization. The gel is then dried at 120 ^oC temperature for 12 h. The obtained precursor $Ba_2Ca_2Cu_3O_y$ is then mixed with HgO in nominal stoichiometric quantity. The resulting powder is pelletized and inserted in a quartz tube that is closed under vacuum. These pellets were sintered in furnace at 850 °C for 10 hours. The structure of the obtained materials was determined by XRD. Transition temperature was measured by ac susceptibility and high harmonic methods.

Finally, we observed that, the sol–gel processing is efficient and very shortening the superconducting phase formation times.

This work has been fulfilled by financial support of the Shota Rustaveli National Science Foundation, Grant No. FR/423/6-260/12, number of contract 31/36.

Abstract

The Method of Calculation of Stability Constants of Fulvic Complexes

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In spite of researches, experimental datas on stability constants of complex compounds of fulvic acids are heterogeneous. One of the reasons to this is application of various average molecular weights of fulvic acids associates. In its turn, this puts the correctness of calculation of stability constants of fulvic complexes under question.

Therefore, it's difficult to investigate complex formation processes taking place in natural waters, identify migration forms of heavy metals and evaluate and assess chemical-ecological condition of natural waters. In diluted water solutions the dominant form of heavy metals is represented by dyhidroxocomplexes - $Me(OH)_2$. If considering fulvic acids as two-base acids, the reaction between dihydroxocomplex and the anions of fulvic acids may be written in the following way:

$$Me(OH)_2^0 + mFA^{2-} \leftrightarrows Mei(OH)_2\, FA^{2m-} \qquad (1)$$

$$\beta = \{ [Me(OH)_2\, FA^{2m-}] \} / \{ [Me(OH)_2^0] [mFA^{2-}] \} \; (2)$$

In solution, the concentration of hydroxofulvic complex equals to the difference between initial (C_{Me}) and final (C'_{Me}) concentrations of metal received after formation of complex

$$[Me(OH)_2\, FAm^{2m-}] = C_{Me} - C'_{Me} \qquad (3)$$

$$[Me(OH)_2^0] = [C'_{Me}] \qquad (4)$$

$$\beta = (C_{Me} - C'_{Me}) / \{ [C'_{Me}] [FA^{2-}]^m \} \qquad (5)$$

From - (5)

$$\beta \cdot [C'_{Me}] = (C_{Me} - C'_{Me}) / [FA^{2-}]^m \qquad (6)$$

At the fixed pH, the left part of the equation is a permanent value and we mark it as K'.

$$K' = (C_{Me} - C'_{Me}) / [FA^{2-}]^m \qquad (7)$$

The logarithm of this equation is

$$\lg K' = \lg(C_{Me} - C'_{Me}) - m\lg [[FA^{2-}] \qquad (8)$$

The numeral meaning (m) of the stoichiometral coefficient or the ligands number in the inner coordination sphere of complex equals to tangent of tilt angle of straight line built in coordinates $\lg(C_{Me} - C'_{Me})$——$m\lg [[FA^{2-}]$.

During making the diagram, to challenge the systematic mistake for this purpose was used the least square method to calculate the exact value of tangent of tilt angle.

$$m = tg\alpha = (n\Sigma x_i y_i - \Sigma x_i \Sigma y_i) / (n\Sigma x_i^2 - (\Sigma x_i)^2) \qquad (9)$$

$x_i = \lg [[FA^{2-}]$ და $Y_i = \lg(C_{Me} - C'_{Me})$

Abstract

Investigation of Fulvic Acids Isolated From Natural Waters by Thermal Analysis

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The aim of this work was to study the humin acids isolated from the bottom sediments and from the water sample by the methods of thermogravimetric and thermal analysis. The thermal analysis was carried out on the derivatograph Q-1500; in the air, standard sample - Al_2O_3, temperature range 20-800 ^{0}C. Differential thermal analysis (DTA), thermogravimetric (TG) and differential thermogravimetric (DTG) curves were recorded simultaneously.

The thermograms of both samples were characterized by one endothermal effect, which was mainly caused by dehydration of the fulvic acids. The effect was registered at 110 ^{0}C .The loss of mass equals to 8%. Both in low (190-350 ^{0}C) and in high temperature range (350-650 ^{0}C) the thermograms are characterized by two exothermal effects (210, 330, 480, 630 ^{0}C). Thus the loss of mass in the low temperature range makes 28 %, but in the high temperature range it equals to 64%.

Exothermal effects and the variation of their corresponding masses in the low temperature range must be conditioned by the splitting chain, liberation of the functional groups and partial oxidation of the formed products or because of the destruction of the structural components of peripheral parts of FA molecules accompanied by dehydrogenation and decarboxylation.

Exothermal effects and their corresponding changes in the high temperature range must be conditioned both by the splitting of aliphatic chain and liberating of more stable functional groups, releasing of cycles and aromatic nuclear

Quantitative estimation of the correlation between the central and peripheral parts in the molecule of FA is possible by the value z=m/M, were m denotes the loss of mass in the low temperature range and M in the loss of mass in the high temperature range. The less the ration, the more aromatized is the substance. The degree of aromatization of FA is quite high: z=0,43.

Abstract

Fulvic and Humin Acids in Surface Waters of Georgia

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Geopolymers (fulvic and humin acids) actively participate in complex formation and sorption processes taking place in natural waters. The datas about their concentration are very few. Our objective was to study the concentration of humin and fulvic acids in surface waters of Georgia.

We concentrated waters By the Frozen method. Concentrates were acidified to pH2 for coagulation of humin acids. Than the solution was centrifuged. To isolate fulvic acid from centrifugate the adsorption-chromatographic method was used. The charcoal was used as a sorbent

Humin and Fulvic acids (mg/l) in surface waters of Georgia

Table 1

The object	Humin acids		Fulvic acids	
	Min	Max	Min	Max
Rivers				
Mtkvari	0.11	0.58	0.31	4.23
Farvani	0.11	0.31	0.60	2.58
Aragvi	0.00	0.04	0.08	0.40
Xrami	0.00	0.03	0.33	0.43
Rioni	0.00	0.07	0.18	0.78
Tskhenisckali	0.00	0.04	0.20	0.58
Lakes	Min	Max	Min	Max
Lisi	0.00	0.00	0.56	0.70
Bazaleti	0.00	0.02	0.19	0.48
Tmogvi	0.00	0.03	0.12	0.33
Faravani	0.18	0.38	0.65	1.90
Sagamo	0.10	0.60	0.66	1.98

The elemental composition ranges of humin and fulvic acids are C: 50,4-52,8%; H: 3,8-5,9%; N:2,8-5,5%; O:37,0-42,7% and C:48,7-54,2%; H:4,3-5,2%; N:1,7-2,4%; O:38,8-45,1% respectively.

Abstract

Preparation of Nanopolyaniline and its Polymer-polymer Nanocompositions with High and Stable Electro-conductivity

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Polyaniline (PANI) in nanosizes and its nanocompositions with copolystyrene maleic acid (PSMA) treated by isopropylamine (IPA) and polyethylene glycol (PEG) of PSMA and product of interaction of copolystyrene maleic anhydride (PSMAn) with p-aminobenzene sulfoacid (PSMAn-AS) have been prepared by the oxidative polycondensation of aniline in the presence of ammonium persulfate and hydrochloric acid under action of ultrasound in a medium of nitrogen. The polymer matrices have been synthesized in the following way: PSMAn – radical copolymerization of styrene and maleic anhydride, PSMA – hydrolysis of PSMAn, PSMA-IPA – by treatment of PSMA with IPA, PSMA-PEG – treatment of PSMA with PEG and PSMAn-AS – reaction of PSMAn with p-aminobenzene sulfoacid. The compositions and structures of the prepared polymer matrix systems have been established by the methods of elemental, chemical, IR- and PMR-spectroscopic analyses. The values of electrical conductivity of nanopolyaniline and its polymer-polymer nanocompositions determined by the method of four points are high and stable (for nano-PANI 8.3-27.8 $Om^{-1}\cdot cm^{-1}$, and for nanocompositions 0.2-2.4 $Om^{-1}\cdot cm^{-1}$). The sizes of particles synthesized in various conditions of PANI and distribution of components in nanocomposition have been determined from SEM picture and XRD diagram. The results showed that in above-mentioned conditions the particles of PANI in sizes 50-100 nm are formed. The character of influence of the conditions of synthesis (concentration, nature and ratio of components, temperature and reaction duration, type of polymer matrix, etc) on values of electro-conductivity of PANI and its nanocompositions has been revealed.

The template oxidative polycondensation of aniline in the presence of above-mentioned matrix polymer systems under action of ultrasound in the presence of nitrogen has been carried out and the soluble and meltable nanocompositions of PANI with high dispersity and homogeneous distribution of its particle in polymer matrix have been prepared. The similar compositions have been made by a method of displacement of solutions of PANI and matrix polymers. The electro-conductivities of these compositions are stable and are in the field close to metallic conductivity.

Abstract

Polymer Electrolyte Membranes on the Basis of Methylsiloxane Polymers with Cyanoacetate Side Groups

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Hydrosilylation reaction of 2.4.6.8-tetrahydro-2.4.6.8-tetramethylcyclotetrasiloxane with allyl cyanoacetate 1:4.2 molar ratios of initial compounds in the presence of Karstedt's catalyst have been studied and D_4^R type organocyclotetrasiloxane with propyl cyanoacetate side groups have been obtained.

Copolymerization reaction of D_4^R in the presence of potassium hydroxide in inert atmosphere at 50-110 ^{0}C temperature have been studied and comb-type polymers with regular arrangement of methyl propionate groups in the side chain have been synthesized.

The structure and composition of synthesized organocyclosiloxanes D_4^R and polymers were studied by FTR,^{1}H, ^{13}C and ^{29}Si NMR spectroscopy data.

Via sol-gel processes of polymers with lithium trifluromethylsufonate (triflate) or lithium bis-(trifluoromethylsulfonyl)imide and 1-2 drop of 0.1 M HCl alcohol solution the solid polymer electrolyte membranes have been obtained.

Electrophysical properties of synthesized solid polymer electrolyte membranes have been studied and electro conductivity of membranes has been determined.

Abstract

Oxidative Polycondensation of p-Phenylenediamine in Organic Medium as a Method to Synthesise Poly(1.4-quinonodiimine-n,n'-diyl-1,4-phenylene)

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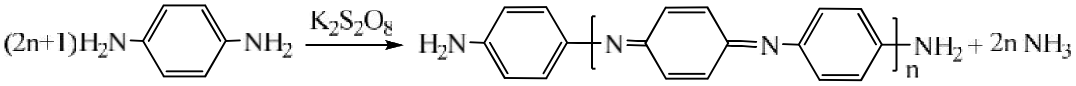
Polyaniline is one of the most important industrial polymers due to its environmental stability and low synthetic cost, but its structure is very complicated and depends upon different synthesis conditions and post-synthesis treatments [1-3].

This work had been focused on the syntheses of electroactive polymers with well defined structures. We have developed new method of N,N'-disubstituted quinonediimines synthesis by oxidative condensation of 1.4-aromatic diamines [4,5]. The N,N'-bis(4-aminophenyl)1,4-benzoquinonediimine has been synthesized through this method[6]. In continuation of these work, poly(1.4-quinonediimine-N,N'-diil-1,4-phenylene) was synthesized by the oxidative condensation of 1.4-phenylendiamine with potassium peroxydisulfate in a molar ratio 1,2:1 and the electrical properties of obtained both virgin and doped with iodine and hydrochloric acid polymers were investigated.



It has been found, that when 1 N hydrochloric acid as a doping agent was used in molar ratio 1 : 6, two processes were occurred simultaneously – addition reaction of HCl to 1,4-benzoquinonodiimino-N,N′-diyl-1,4-phenylene units (83 %) and salification (17%):

It was found that condensation by 1,4-coupling of amino groups of N,N'-bis(4-aminophenyl)1,4-benzoquinonediimine with quinonediimine groups occurred during heating in ethanol. To prevent this reaction, acetylation of end amino groups of both N,N'-bis(4-aminophenyl)1,4-benzoquinonediimine and poly(1.4-quinonediimine-N,N'-diil-1,4-phenylene) were carried out and corresponding acetylated more stable compounds were synthesized. Obtained compounds were characterized with ^{1}H NMR, UV, IR spectroscopic methods.

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Abstract

Fluorescent Macrocycles

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Nowadays azomethines are used as substrates to prepare a large number of industrial and biologically active compounds via ring closure, cycloaddition and replacement. Moreover azomethines are also known to have antimicrobial, antifungal, antitumor biological activities and are used as herbicides. They are also applied in industry as dyes and pigments with luminescent properties. Azomethines are used as ligands for complexation of metal ions giving the complex compounds of rich physical, chemical and biological properties. For that reason a huge number of mono- and bisazomethines are described in the literature. Moreover, while abundant information on the reactivity and physical-chemical properties of 5-member cyclic azomethines (oxazoles) exists, macrocyclic azomethines have not been the subject of any investigations. In addition, macrocyclic compounds like crown ethers and cryptand have received great attention in the last few years both in chemistry and in biology.

Based on all these observations we undertake the synthesis of macrocyclic azomethines, bearing properties of both azomethines and macrocyclic compounds highly interesting and beneficial for the field development. We have reported the method of synthesis of 20-membered cyclic polyazomethine compounds [1]. Some chemical and physical properties of these macrocycles have been also investigated [2]. They are excellent azo partners and have ability to give tetrakis azo dayes via one-pot azo coupling reaction.

There is a need to design stable dyes that possess desirable photophysical properties, stability, and targeting ability. In the proposed project we are going to undertake a synthesis of novel substituted macrocyclic azomethines and perform a detailed study of their chemical and physical properties as a biomarkers and dioxygen containers.

On the base of preliminarily performed investigations, we are able to declare that offered compounds are characterizing with interesting properties, namely:

- Easy and inexpensive preparation method
- Flexible technology, giving opportunity of further purposeful modification of the properties with easy transformations (to carry out electrophilic substitution reactions, to form stable complex compounds, etc)
- Good/excellent physical, chemical and technical properties (fastness against physical, chemical and biological treatment)
- Special optical properties of biomarkers (absorption - in the near-UV region, emission – in the visible region; blue-violet luminescence in the solid state, low excitation energy, etc).

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Abstract

Polymers Containing Aniline Tetramers Connected with 1,4-Phenylenebistriazenyl Groups: Synthesis and Investigation

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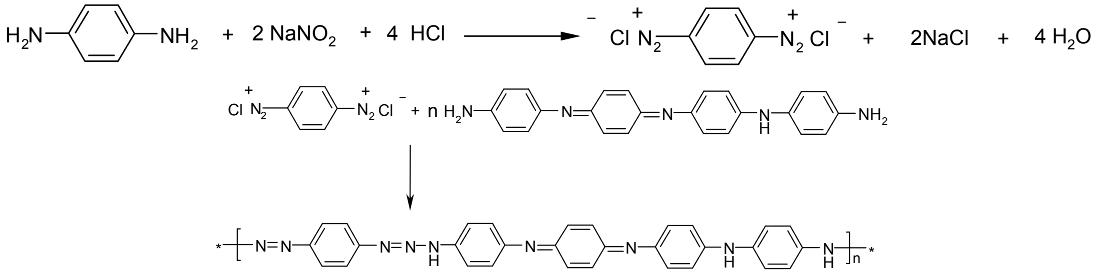
Polyaniline in its emeraldine base form contains benzoquinonediimine and two phenylenimino groups and is one of promising electroconductive polymers due to its unique structure and redox behavior and its oligomers of controlled chain length demonstrate conductivity on the same order of magnitude as that of the bulk polymer [1-3]. Incorporation of conjugated oligomers into polymer structures combines the properties of the specific oligomer and desired polymer properties such as mechanical strength and film forming properties. The functionalized oligomers undergo further polycondensation to afford a variety of electroactive materials. Previously we have synthesized and studied the properties of different types of triazenephenylenes and triazenediphenylenes [4,5]. They were shown to have an interesting electrical and intensive photoluminescent properties and good solubility. Oligoanilines can be incorporated into polymer main chains as well as side chains [6-8] Now we report the result on the synthesis and investigation of the polymer containing triazene-1,3-diyl-1,4-phenylene-1,3-triazene- and emeraldine base model tetramer segments in the repeat units, i.e. polymer in which tetramer units are in the main polymer chain and connected with p-phenylenebistriazenyl groups. For this purpose, firstly, 4,4'(bis-p-aminoanilino)diphenylamine had been oxidized by potassium persulphate in acidic medium and amino/amino capped emeraldine base model compound was synthesized. Then obtained oligomer was used as a monomer for the synthesis of polymer with well defined structure. Polymer was obtained by the diazotation of p-phenylenediamine and azo coupling with obtained oligomer.



Comparative study of conductivities between obtained and some previously synthesized triazene-p-phenylene group containing polymers doped with iodine, hydrochloric and perchloric acids, has been explored. It has been found, that introducing of tetramer in polymer chain influence on conductivity and the conductivities of the samples with the same doping level was on tree order higher for the polymer containing tetramer segments when doped by iodine and hydrochloric acid and is primarily of the same order when doped by perchloric acide.

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Abstract

Emission of Multi Charged Ions During N^+,O^+,N_2^+,O_2^+, Ar^+ Ions Bombardment of NaCl, Mg, Al, Si, S Surfaces

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The interaction of energetic ions with surfaces plays an important role in the field of surface science. Relevant topics are the ionization of atomic particles at surfaces, the modification of surfaces and surface analysis. During ion sputtering of solid surfaces the mass spectra of emitted secondary ions contains the multicharged ions as well, its research is obviously important for determining the mechanism of their formation. In this work production of multicharged (double and triple) escaping ions at ion-surface interactions are experimentally investigated. During ion-surface bombardment some different manners of multicharged ions formation and neutralization at emission are also discussed. Quasimolecular approach of atomic particles interaction is also used in our research and the numerous experimental results depended on the various factors on formation and emission of multicharged ions is presented. The emission of multicharged ions at bombarding of the NaCl, Mg, Al, Si, S surfaces by N^+,O^+,N_2^+,O_2^+,Ar^+ primary ions with energies Eo=0,5-50 keV at different experimental conditions are investigated by using the SIMS method. The measurements of secondary ions yields depending on an angle of bombardment of primary ions, counted from normal to a researched surface and depending on pressure of oxygen in the chamber of interaction are also measured. At ion - surface interaction inner shell vacancies can be formed and multicharged ions can be produced as a result of Auger-transitions either during Auger decays in solids or after ion emission in vacuum. Present experimental investigations of double and triple charged ion yields shows that Auger processes can take place either in solids or after emission in vacuum. The neutralization processes of the double and triple charged ions emitted from Al and Si surfaces were studied. The processes of formation and emission of multicharged ions are rather sensitive to atomic and electronic structure of surfaces.

In our case the processes of Auger neutralization are more probable: with the participation of surface plasmons and the neutralization of ions as a result of resonance-tunnel capture of electrons from the semiconductor of metallic surface. Consequently, neutralization processes of multicharged ions at emission from solids are more probable in Al (metal) than in Si (semiconductor). Number of multiplecharged ions shows difference between probability of neutralization ions at emission either during Auger decay in solids or after ion emission in vacuum. In case of our experimental investigation neutralization is more probable for triple than for double multicharged ions.

The numerous experimental results confirm that during ions bombardment of surfaces inner shell vacancies can be formed in atoms and as a result Auger-transitions emit Auger- electrons and multicharged ions. The experimental data shows, that the Auger-transitions take place both in solids, and in vacuum - after emission as well. The processes of formation and emission of multicharged ions are rather sensitive to atomic and electronic structure of surfaces.

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Abstract

Physical-mechanical Properties of B_4C-TiB_2 and B_4C-ZrB_2 Composites

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Experimental works have been conducted the objective of which was to improve mechanical properties of boron carbide by introduction of doping elements into the system. Titanium and zirconium were selected as doping elements, which were introduced into the system in the form of TiB_2 and ZrB_2. Six types of boron carbide – titanium and zirconium diboride mixture with various titanium and zirconium diboride content were used in experiments. Optimal process parameters, as well as doping elements concentration, necessary to provide required high mechanical parameters in the composite were defined. The physical and mechanical properties of the composite had studied. Scanning electron microscopic study and ceramography had carried out.

High hardness-high toughness Composites B_4C-TiB_2 and B_4C-ZrB_2 with improved mechanical properties had produced by hot pressing at 2000° C temperature.

The above composites can be used when measuring refractory material hardness at temperatures up to 2000^0C. Besides, possibility of its application in nuclear engineering, in abrasive materials, etc. also extends.

Simultaneous increase of impact elasticity and hardness parameters provides important possibility to use this material as construction ceramics.

Abstract

Mathematical Model for Biopolymer Nanoparticles Sorption in Whey

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Hydrophilic nanoparticles prepared in this study were based on maleic acid in chitosan solution. In this experiment 0.02, 0.03 and 0.05 g of chitosan nanoparticles in 10 ml whey and pH 4, 5 and 6 were compared to capture particles. Results from spectroscopy (UV) observed, 6=pH and concentration of 0/05 g of chitosan nanoparticles has the highest sorption, so the testing process and the concentration was adjusted according to the pH. these experiments were performed in a continuous infinite system and experimental parameters of pH, time Contact and temperature on adsorption has been studied. Mathematical model developed in order to investigation of sorption kinetics base on experimental data.

Abstract

Synthesis and Investigation of Properties of Comb-type Organosilicon Polymers for Solid Polymer Electrolyte Membranes

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The potential applications of solid polymer electrolytes in high energy density solid state batteries, gas sensors and electrochromic windows has stimulated considerable investigation of the fundamental factors governing the ion-transport behavior of these materials.

Polysiloxanes are the excellent candidates for usage in solid polymer electrolytes because of their high chain flexibility, chemical stability, high thermal/oxidative stability, low toxicity, easy processability and low cost. The polysiloxanes, with very low glass transition temperatures, extremely high free volumes, are expected to be good hosts for Li^+ transport, when electron donor units are introduced into the polymer backbone.

In this presented work we report the synthesis of new comb-type polysiloxanes with various side fragments containing electro donor groups. Comb-type polyorganosiloxanes may be synthesized by two ways: Via hydrosilylation reaction of polymethylhydrosiloxane with allyl or vinyl containing compounds in the presence of platinum catalysts or using dehydrocoupling reactions of polymethylhydrosiloxane with hydroxyl containing compounds in the presence of catalysts. It must denote that the reaction at this time proceeds with obtaining of various linking systems and often cross linking, and branching processes take place, which is undesirable technologically. In spite of this the modification reactions of polymethylhydrosiloxane via hydrosilylation reaction still remains as an interesting way for obtaining of new siliconorganic polymers, but the main disadvantage of this method is that not all active ≡Si-H groups participated in the hydrosilylation reaction, which causes branching process through the formation of silsesquioxane bonds and explains the increase in the molecular weights.

The second way for synthesis of comb-type oligomers is the hydride addition of methylhydrocyclosiloxanes to allyl or vinyl containing compounds with ether, ester and trialkoxysilyl fragments, in the presence of platinum catalysts; obtaining of cyclotri(tetra, penta)siloxanes with various attached fragments and polymerization of methylorganocyclosiloxanes with terminated agent and without it.

Via sol-gel processes of some comb-type oligomers with lithium triflate and bis(trifluoromethylsulfonyl)imide (5-20%) solid polymer electrolyte membranes have been obtained. The dependence of ionic conductivity as a function of temperature and salt concentration has been studied.

Acknowledgement: This work has been fulfilled by financial support of Science & Technology center in Ukraine (Grant #5055).

Abstract

Gradually Oriented State of Linear Polymers

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Widespread method of the structural modification of the linear polymers is the uniaxial oriented stretching – action of the homogenous mechanical field on the polymer sample. The relative elongation in the entire volume of the obtained oriented polymer is identical.

Uniaxial oriented stretching can be carried out in another mode. Previously we have developed the landmark decision of uniaxial oriented stretching and established the conception about new structural state of the thermoplastic polymers – about gradually oriented state (GOS).

Transition of the isotropic polymers in the GOS is produced by the action of inhomogeneous mechanical field on the polymer sample. Quantitative parameters of the obtained gradually oriented polymers are: range of change of relative elongation/orientation degree, extent and profile (linear, hyperbolic, parabolic, logarithmic, etc.).

In this report mathematical model of controlled uniaxial graded oriented stretching of linear polymer films is discussed. Based on this model the configuration of the inhomogeneous mechanical field (profile of clumps, geometry of the sample, positional relationship of the clamps and the sample) is defined, which provides transition of the isotropic polymer films into GOS with pre-determined values of parameters.

For experimental confirmation of the theoretical material two types of PVAL - films having a trapezoid shape with hyperbola and linear sides were studied. The films were stretched at 358K with rate 1,5 mm/min on 100-500 % with respect the small base of the trapezoid. The topographic pattern clearly indicates the existence of the elongation gradient. The distribution of relative elongation in the gradually stretched PVAL - films was calculated. Fairly good agreement between the theoretical calculations and experiment is set.

Uniaxial graded oriented stretching method can be considered as a scientific and technological innovation for the creation of a new type FGMs/elements on the base of linear polymers/copolymers and its composites with gradient of all properties which are depended on the elongation/orientation degree.

Abstract

New Method of Obtaining of Gradually Oriented Polymeric Films

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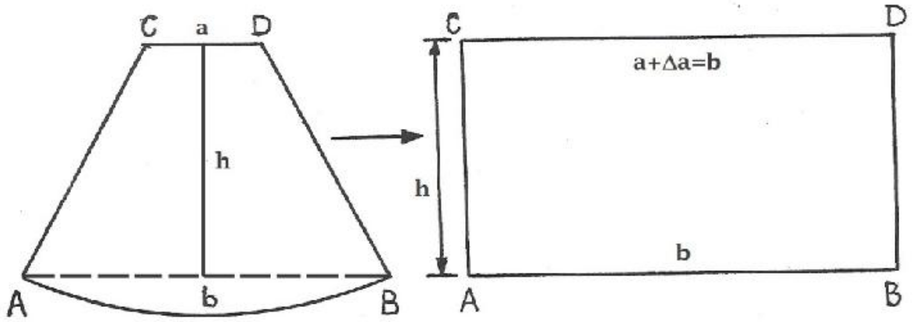
The simplest and most common kind of orientation of polymers is the uniaxial orientation - action of a uniform mechanical field on the polymer sample. Uniaxial oriented stretching can be carried out in another mode. Scientific basis of this innovations is a concept about new structural state of the thermoplastic polymers – about gradually oriented state (GOS) proposed by us for the first time. This state quantitatively is described by three parameters: range of the relative elongation change, its extent and distribution profile (linear, hyperbolic, parabolic, logarithmic, sinusoidal, etc).

On the basis of this conception a fundamentally technical solution of the uniaxial oriented stretching is developed. This is the orientation of thermoplastic polymers in the gradient mode, which is done by action of the inhomogeneous mechanical field on the izotropic polymer films. There are elaborated some guided graded orientation methods.

In this paper a new method of preparation of the gradually oriented polymeric films with rectangular shape and the given parameters (see above) is discussed. The selected parametrs are: range of relative elongation change $\Delta L/L = 0 - n$ (b/a=n); extent of relative elongation change – h; profile of distribution of relative elongation change - hyperbola. The film with these parameters can be obtained by uniaxial stretching of *ACDB* curvilinear trapezoid.



To calculate the geometric dimensions of the curvilinear trapezoid a mathematical model is proposed. By uniaxial stretching of the trapezoid-film in parallel clamps of the stretching device the desired pattern is obtained.

Uniaxial graded oriented stretching methods can be considered as a scientific and technological innovation for the creation of a new type FGMs on the base of linear polymers/copolymers and its composites with gradient of all properties which are depended on the elongation/orientation degree.

Abstract

Side Chains Azobenzene Moieties in Polymethacrylates for LC Alignment

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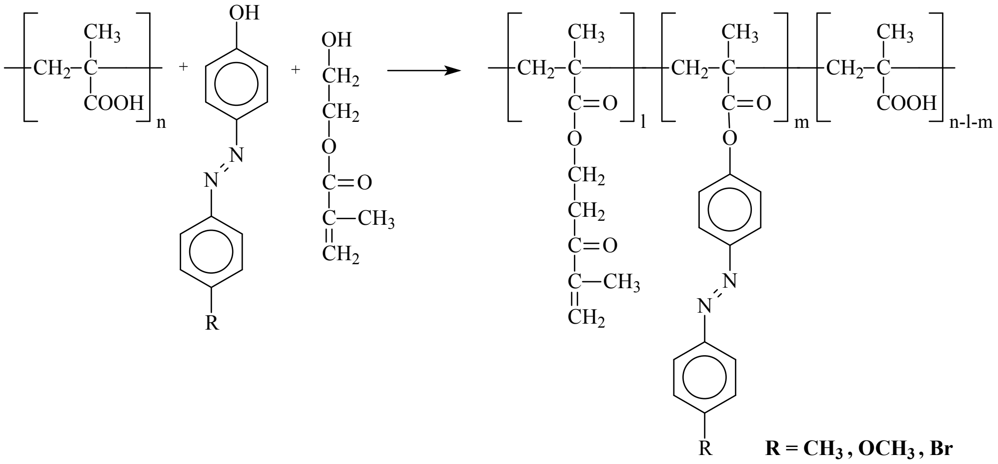
One of the most common classes of photoalignment materials consists of azopolymers. The design of such photoaligning systems is based on the incorporation of photoactive azochromophore into side or main polymer chain. Illumination of these materials with exciting light stimulates reversible or irreversible trans-cis isomerization of azochromophores. When the exciting light is polarized, initially isotropic orientation distribution of photosensitive fragments transforms into anisotropic one characterized by some degree of orientational order [1]. The LC molecules, adjacent to the orientationally ordered photoaligning film, reproduce to certain extend this order due to anisotropic interaction with the molecules or anisotropic fragments from the surface of this film.

In our work we make an attempt to improve photoalignment stability of methacrylic azopolymers by including of crosslinkable unsaturated hydrocarbon groups in side chain of polymer along with azobenzene fragments. The photoinduced orientation of azofragments was fixed with accompanying crosslinking reaction to enhance thermal stability of the induced order. The polymer analogues reaction method for synthesis of structural dyed polymers based on polymethacrylic acid and hydroxyazobenzenes of different structures were used.



For photooptical investigations the polymers of approximately equal composition were chosen. For testing of LC alignment we used symmetric LC cells made of two equally treated photoaligning layers withy parallel easy axis. The cell thickness was defined by spacers of 20 µm in diameter. The cells were filled with nematic LC E7 purchased from Merck.

LC alignment quality in the cells was observed with the naked eye and polarizing microscope. Alignment thermostability was investigated by keeping cells with LC at high temperature (80°C) for 30 min, subsequent cooling and testing with polarizing microscope.

It was shown that polymer films have ability to orientation under polarized light. Oriented films have important properties to orient liquid crystal (LC), covered them. Insertion of methacrylic groups with free double bonds leads to slight deterioration LC alignment but make a contribution to its stability due to cross-linking reaction. This peculiarity can be used for creation of photosensitive layers for LC displays and other devices.

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Abstract

New Heterogenized Cobalt Containing Catalytic Dithiosystems For Gas Phase Polymerization Of Butadiene

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Cobalt-containing bifunctional catalytic dithiosystems has been heterogenized on various supports (such as silica gels, aluminum oxides, zeolites, etc.) by the methods of direct deposition or pre-alumination. The received data demonstrate that the pre-alumination method show a very high activity in gas phase polymerization of butadiene. These catalysts productivity reaches 650.0-2200.0 kg PBD/g. Co•h., which is much higher than the output of solution process using the same homogenous catalysts (57.0 kg PBD/g Co•h.) and the known gas phase process using the heterogenized neodymium-catalysts (500.0 kg PBD/g Nd•h.).

Synthesized Polybutadienes can be used in the production of tires, technological rubbers and impact resistant polystyrenes.

Abstract

Cobalt Alkylxhanthogenate + Trialkylaluminum Catalytic Dithiosystems For Synthesis of Syndiotactic 1,2-Polybutadiene

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A new highly activity and stereoregularity Cobalt alkylxhantogenate + Trialkylaluminum catalytic dithiosystems have been developed for obtaining of photodegradable highly crystalline syndiotactic 1,2-polybutadiene. Activity and stereo regularity of these catalysts were studied in comparison with known cobalt-containing catalytic dithiosystems of butadiene polymerization dependence of process outcomes on the nature of ligands on cobalt-compounds, catalyst components concentration and ratio, as well as the influence of temperature on catalyst activity and selectivity. These catalysts in toluene solution has showed very high activity and stereo regularity in butadiene polymerization: butadiene conversion – 90.0-99.0 %, 1,2-content- 94.0-99.0 %, intrinsic viscosity - 1.3-3.5 dL/g; crystallinity – 63.0-98.0 %, syndiotacticity – 93.0-98.5 %, melting point – 175-212°C. Was established the optimal parameters of synthesis of high-molecular mass and highly crystalline syndiotactic 1,2-polybutadiene: [Co]=(1.0-2.0)•10^{-4} moL/L; [M]=3.0 mol/L; Al:Co=(50-100): 1; T=40-80°C.

The basic application areas of syndiotactic 1,2-polybutadiene - the thermoplastic resin, allowing to obtain the whole spectrum of the products possessing of elastomeric and thermoplastic properties, are: preparation of rubber mixes, in particular, for manufacture of tires, packing polymer-film materials; the various compositions, used in such scopes as a microcapsule for the medical purposes, ceramics, semi permeability membranes, adhesives, synthetic leather, oil resistant tubes, coatings for semi-conductor devices, no woven materials, etc.; carbon fibers, possessing increased durability at a stretching.

Synthesis of Amphiphilic Graft Copolymers via Modification of Hydroxy-functionalized Copolymers

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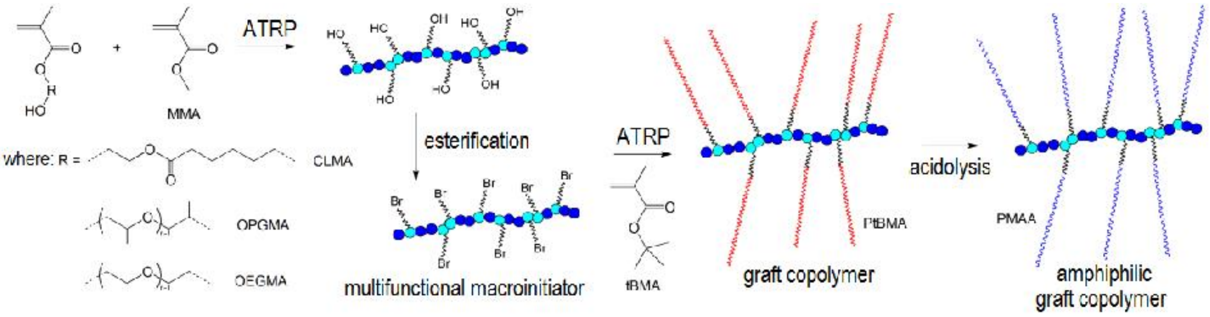
Earlier, the hydroxy-functionalized polymers based on 2-hydroxyethyl (meth)acrylate were applied for synthesis of graft copolymers [1,2], which present interesting topology, where backbone and side chains are distinguished. The combination of segments with various physicochemical properties let to design structures with unusual hard-soft (difference in glass transition temperatures), amorphous-crystalline (difference in morphologies) or hydrophilic-hydrophobic/ amphiphilic (difference in solubilities) behavior, which is strongly depended on environment and/or other stimuli [3].

In our studies, we focused on other hydroxyl-functionalized methacrylic monomers, which were used for the synthesis of new well-defined amphiphilic graft copolymers via four-step procedure (Scheme 1). First, metyl methacrylate (MMA) was copolymerized by atom transfer radical polymerization (ATRP) with methacrylate containing hydroxyl groups, that is 6-hydroxyhexanoic acid 2-(2-methacryloyloxy)ethyl ester (CLMA), oligo(ethylene glycol) monomethacrylate (OEGMA, M_n=400 g/mol) or oligo(propylene glycol) monomethacrylate (OPGMA, M_n=375 g/mol). The copolymers with various content of hydroxyl groups (1 - 33 mol. %) were modified by esterification with α-bromoisobutyryl bromide to prepare multifunctional macroinitiators, which next were used for ATRP of *tert*-butyl methacrylate (tBMA). The graft copolymers with various numbers (DG = 1-33) and lengths (DP_{sc} = 7-113) of hydrophobic PtBMA side chains were transformed by acidolysis with trifluoroacetic acid into hydrophilic poli(methacrylic acid) (PMAA) segments. The amphiphilic character of graft copolymers give opportunity to form self-assembly micelles, which can be applied as nanocarriers in drug delivery.



Scheme 1

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Abstract

Amphiphilic Star-shaped Copolymers Bearing Fluorogenic Groups

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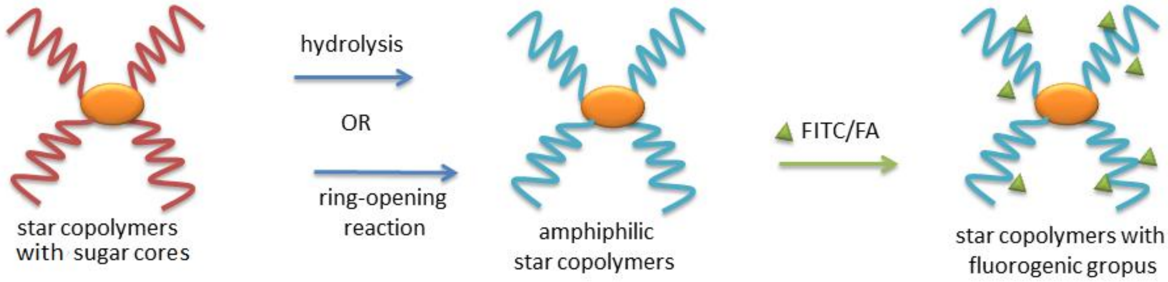
Star shaped polymers have been attracted considerable interest in the recent years [1]. They are the subject of different investigations because of their wide employment in manifold industrial areas (e.g. as viscosity modifiers, surfactants, motor oil additives, coating and paint additives) [2]. Since some of the star polymers with non-toxic and biocompatible properties, have great perspectives in controlled release applications [3]. The synthesis of regular star polymers can lead to monodispersity in both, the number of arms (*f*) and their degree of polymerization, due to instantaneous development of controlled polymerization methods, including the atom transfer radical polymerization (ATRP).

Herein, we present the synthesis and post-polymerization modification of star copolymers (Scheme 1). These polymers were prepared by ATRP initiated by acetal derivatives of D-glucopyranosides cores bearing 3, 4 or 6 tertiary bromide functionalities. The comonomers, methyl methacrylate (MMA) and *tert*-butyl methacrylate (*t*BMA) or MMA and glycidyl methacrylate (GMA) have been applied to obtain polymethacrylate arms varying the contribution of pendant *tert*-butyl or glycidyl groups, respectively. Subsequently, the acydolysis of P(MMA-*co*-*t*BMA)$_f$ and in the case of P(MMA-*co*-GMA)$_f$ ring-opening reaction with nucleophile (ethylenediamine, sodium azide) were performed to get water-soluble copolymers, with except of azide-functionalized polymers soluble in polar DMF.

Chemical conjugation of fluorescein derivatives (fluorescein isothiocyanate - FITC or fluoresceinamine - FA) to the amino groups present in the modified units of GMA or to the carboxylate groups in the deprotected methacrylic acid units, respectively, has been attempted to generate fluorescent properties of star copolymers. This effect let to monitor the cell uptake and tracking localization of copolymers in cell cultures, what will be important in further experiments of drug delivery.



Scheme 1

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Abstract

Method of Producing Microcapsules

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Microencapsulation of substances opens new opportunities for decision of technological and industrial problems. Modern methods of microencapsulation allow enclosing in a sheath the substance practically in any aggregative state. It allows keeping properties of encapsulated substances till the moment of its direct use. Today there are lots of ways for producing microcapsules which can be carried out by various methods: chemical, physical and physico-chemical. In a number of technologies combined methods of sheath formation are used, and the choice of optimum methods or their combinations are defined by properties of encapsulated product, requirements to produced microcapsules and purchase of technological process.

In the present work the method of producing gelatinous microcapsules was advanced by us.

At the first stage modification of gelatin was carried out by means of addition of sodium palmitate $C_{16}H_{31}NaO$ to gelatin aqueous solution. At the second stage emulsification of encapsulated liquid (tetrachloromethane) into the modified gelatin solution was carried out by intensive mixing up to the necessary size fractions. Then the additive (20 %-solution of sodium sulfate) was injected into produced emulsion as the result of which gelatin sedimentation on a surface of emulsion of micro drops took place. Further sheath formation of microcapsules occurred by two ways:

1) by slow decrease of solution temperature up to 150°C with the subsequent addition of 37 %-solution of formaldehyde for solidification of microcapsules.

2) by pouring out produced emulsion into a great volume of cooled 7 %-solution of sodium sulfate Na_2SO_4. Solidification of microcapsules was carried out by addition of 37 %-solution of formaldehyde.

Microcapsules produced by this way have got the size 30-50 micrometers.

This work was carried out within the framework of the project 063 “Development of the methods of obtaining of self-healing composition coatings” under the program of Groups of junior researchers of the project “Commercialization of technologies” of Ministry of Education and Science of Republic of Kazakhstan and the World Bank.

Abstract

Properties and Advantages of PVC Nanocomposites

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Two types of spherical nanofillers: silicone/methacrylic core/shell filler and silica (from sol-gel process) were prepared and used in suspension vinyl chloride polymerization in pilot scale - 1 m^3 reactor, according to our new technology [1-3]. Methods of nanofillers preparation are also technologies of our Institute.

Sol-gel silica nanospheres from experimental production of "Silikony Polskie" company made according to our technology [4] of grain diameter about 60 nm was used in a sol form. The core/shell filler [5] made in co-production of "Silikony Polskie" (core) and the Institute of Engineering of Polymer Materials & Dyes in Poland (shell) was of about 100 nm diameter and used in VC polymerisation in aqueous dispersion. The grain size distributions of both fillers were very narrow. Both fillers were used in small concentration (0.5 wt. %/VC).

Nanosilica in PVC composites improved polymer bulk density while core/shell filler gave higher plasticizer absorption *i.e.* better polymer porosity.

The properties of PVC nanocomposites obtained were compared with virgin PVC by 4 companies: Deceuninck (Belgium; profiles), Ergis-Eurofilms (Poland; films), Anwil SA (Poland; rigid blend) and our Institute (rigid and plasticized blends).

The results showed the significant improvement in impact strength and stiffness of rigid goods as well as slight increase in tear resistance of the films.

It appeared impact modifiers content in profile blends could be reduced about ~50 % and more (at 50 % impact strength is still better than of virgin PVC). Reduction of impact strength modifiers content gives not only cost effect but the same time improves tensile properties. The production of PVC nanocomposites *in-situ,* i.e. in the polymerization step is possible at the existing polymerization production equipment.

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2. Polish Patent Applications P-388960, P-397404, P-397405.
3. European Patent Application PCT/PL2009/000087.
4. Polish Patent PL-198 188.
5. Polish Patent PL 210 583.

Abstract

Self Healing of Protective Coatings

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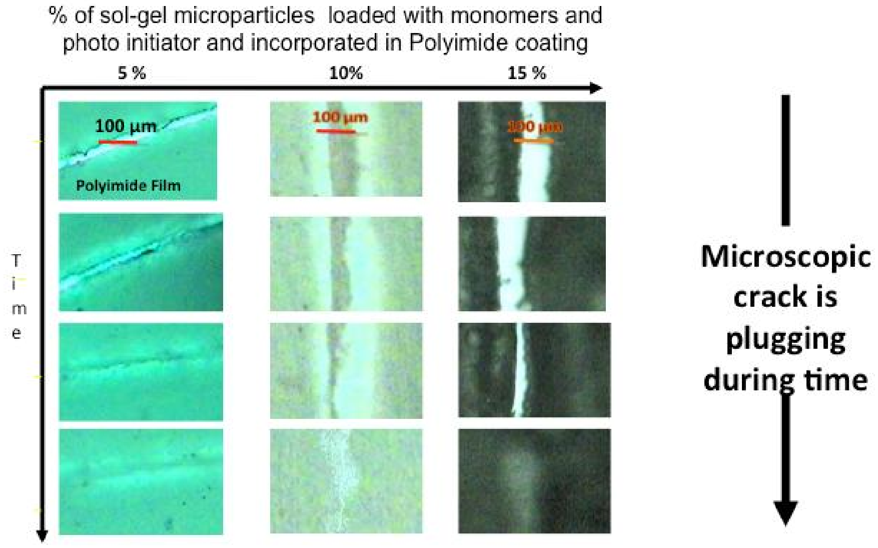
The repair is achieved through microencapsulated polymerizable agents incorporated into the coating matrix.

In this experience, for solar panels of satellites and by photopolymerization, we have incurporated 5, 10 and 15 % of our microcapsules obtained by sol-gel process in a polyimide coating. We make a crack of 100 microns on each sample and then we turn on UV light. Cracks are gradually plugging.



A general implementation of this principle had been developed to accommodate other environmental factors like exposure to air or humidity to trigger the polymerization of encapsulated monomers and repair cracks.

Using autoxypolymerization of encapsulated siccative oil we can fill cracks thanks to oxygen if the capsule is broken.

Exposure to humidity can also be used to repair materials damages, in this case using Isophorodiisocyan, Isocyanurat or Toluendiisocyanat monomers.

By way of summary, the original approach to self-healing we have developed is to use environmental factors like: light (UV and visible), exposure to air, or humidity to trigger the polymerization of encapsulated monomers and repair cracks in the materials they have been applied to.

Abstract

Antibacterial Determination, Synthesis, Characterization and Properties of Silver Nanocomposites

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Silver-Polyaniline (Ag-PANI) nanocomposites were prepared by in-situ oxidative polymerization of aniline monomer in the AOT solution as an emulsifier. The synthesis of Silver-Polyaniline nanocomposites was investigated as a function of several parameters such as aniline concentration, concentration of emulsifier (AOT), concentration of oxidation agent and concentration of silver nitrate. The formation of Ag-PANI nanocomposite was characterized by scanning electron microscopy (SEM) in each stage of controlled parameters. In vitro antibacterial tests were performed using Escherichia coli (E. coli) to determine the antibacterial capability of the Ag-Polyaniline nanocomposites.

Abstract

New Synthesis and Characterization of Nanoclay/Polyethylene Terephthalate Nanocomposite

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Nanocomposite of montmorillonite KSF (MMT)/Hexametylenediamine (HMDA) is synthesized by using HMDA as an organic moiety and MMT in acidic medium at 80 ^{0}C.
Preparation of nanocomposite with nanoparticles of TiO_2 and polyethylene terephthalate (PET) was prepared in this work. The modified nanoclay/ nanocomposite were prepared in presence of ethylene glycol, terephthalic acid and modified nanoclay by polycondensation process. The Structure of the nanocomposites were evaluated by using X–Ray diffraction (XRD) and fourier transform infrared spectroscopy (FTIR). XRD spectrum showed that distance between layers of modified nanoclay was increased and these were suitable for preparation of nanocomposites by polymerization technique. Also FTIR and spectrums were confirmed existence of ammonium in the nanoclay. The morphology of this nanocomposite was also determined by scanning electron microscopy (SEM). These findings were showed that PET was polymerized into layers of modified nanoclay.

Abstract

Synthesis of Atenolol on Functionalized Multiwall Carbon Nonotube Surface and Study Its Properties

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Atenolol is a drug belonging to the group of beta (β) blockers. In this work, carboxylated-multiwalled carbon nanotubes (MWNT-COOH)/Atenolol was synthesized by in-situ synthesis method. The synthesis was performed using MWNT-COOH and 4-hydroxy phenyl acetamide as raw materials. Then atenolol was synthesized on the MWNT surface. The structure of product was characterized by Hydrogen nuclear magnetic resonance (H-NMR) and fourier transform infrared spectroscopy (FTIR). Also, the morphology was determined by scanning electron microscopy (SEM) and transmission electron microscopy (TEM) which showed that atenolol was synthesized in the nanometer dimension

Abstract

Novel Lanthanide Polycomplexes for Electroluminescent Devices

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Organic light emitting diodes (OLEDs) are considered the next generation of technology for flexible flat panel displays and low cost solid state lighting. In particular, organic light emitting diodes that have the potential to achieve an internal quantum efficiency close to 100% have attracted considerable research interest. Lanthanide β-diketones have attracted much attention because of their spectroscopic properties. Investigation of luminescence and optical absorption properties of lanthanide β-diketones is of great importance since these complexes are widely used as light-converting optical materials, light-emitting diodes, luminescent probes, polymer sol–gel derived glasses, electroluminescent devices [1-4]. Light emitting devices are usually made of solid state materials that emit lights of various wavelengths upon the stress with an electric field.

Lanthanide complexes that contain polymerizable groups can be polymerized or copolymerized together with another monomer. This results in a polymer or copolymer in which the lanthanide complex is part of the polymer backbone or of the side chain.

We synthesised monomer – 2 methyl-5-phenylpentene-1-dione-3,5, their complexes with Yb(III), Ho(III), Tb(III), metallopolymers based of them.

The monomers, polymers and their complexes were analysed by NMR-, electronic, diffusion and infrared spectroscopes, elemental and termogravimetric analysis. Polymers were synthesized by free-radical polymerization in DMF.

The luminescent spectrum of obtained metallocomplexes and polymers in solutions, films and solid state are investigated and analyzed.

The obtained results allowed to determine the composition, structure and symmetry of synthesized compounds.

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Abstract

Composite polymer for adsorption of Nickle from colored wastewater

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Recent project deals to study the adsorption of Ni ions from colored wastewater using adsorbents composite polypyrrol based on polyvinyl alcohol. These experiments were conducted in a batch system. Identification of the synthesized adsorbents was performed by SEM (Scanning Electron Microscope) & FTIR (Fourier transform infrared). Effect of the experimental parameters pH, contact time and dose of adsorbent base on the surface adsorption of colored wastewater has been studied. According to results, optimum pH for absorption of Ni by mentioned absorbent was 3. Absorption increased with increasing contact time and after 14 min reached to equilibrium state. Optimum dose of adsorbents has been reported 0.4 grams. The obtained equilibrium data in the initial concentration of Ni in the studied temperature range has a good adaptation with Freundlich isotherm. Evaluation of experimental data Indicated that the surface adsorption of Ni follows the pseudo-second order equation.

Abstract

Phenol-Formaldehyde Oligomers with Unsaturated Double Bonds

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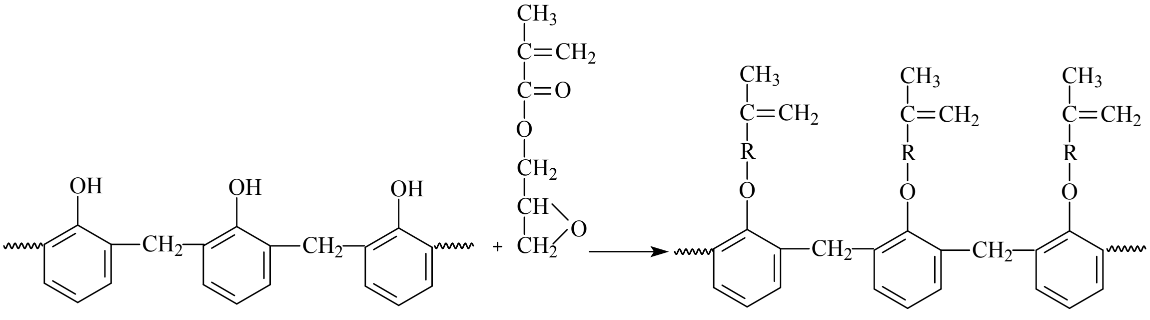
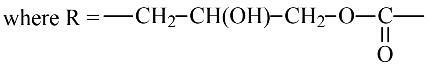
Well-known phenol-formaldehyde resins (PhFR) are used while the production of press-materials, glues, protective coatings, mastics, casting blends, etc. The wide application is conditioned by their high thermal stability and physico-mechanical properties, as well as resistance to aggressive media and organic solvents. The defects of the mentioned resins are their low adhesion and elasticity. To improve the properties of the wares based on PhFR they are modified by both low- and high-molecular compounds.

In the present paper we study the possibility of novolac PhFR chemical modification by glycidylmethacrylate (GMA) in accordance with the equation:



(PhFR) (GMA) (MGMAPhFR)



$$\text{where } R = -CH_2-CH(OH)-CH_2-O-\underset{\underset{O}{\|}}{C}-$$

The modified PhFR (MGMAPhFR) may be obtained due to the interaction between PhFr hydroxy groups and GMA epoxy groups.

In order to develop MGMAPhFR synthesis procedure it was necessary to study the effect of the catalyst (KOH) amount, reagents ratio, reaction temperature and time of the process proceeding.

The lowest reaction rate was observed in the case of 0.2 and 0.4 KOH moles per PhFR phenol group. On the other hand, taking into account that at the catalyst amount of 0.6 and 0.8 moles the reaction rate is the same and further increase in the catalyst amount does not increase the reaction rate, KOH amount of 0.6 moles was chosen to be the optimum one.

The increase in GMA amount increases the reaction rate. The effective activation energy is 40.30 ± 1.05 kJ/mol.

MGMAPhFR was studied as an additive to epoxy-olifomeric mixtures based on ED-20 industrial epoxy resin, peroxy derivative of ED-20 resin and TGM-3 oligoesteracrylate. MGMAPhFR amount was 8.3–26.7 wt %. The physico-mechanical and protective properties were examined for the films based on epoxy-oligoesteric mixtures. The advantages of polymeric coatings with MGMAPhFR were shown compared with those containing non-modified PhFR.

Abstract

Reaction Mechanism and Quantum-Chemical Computation of Hydrosilylation Reaction of Allyl Glycosides

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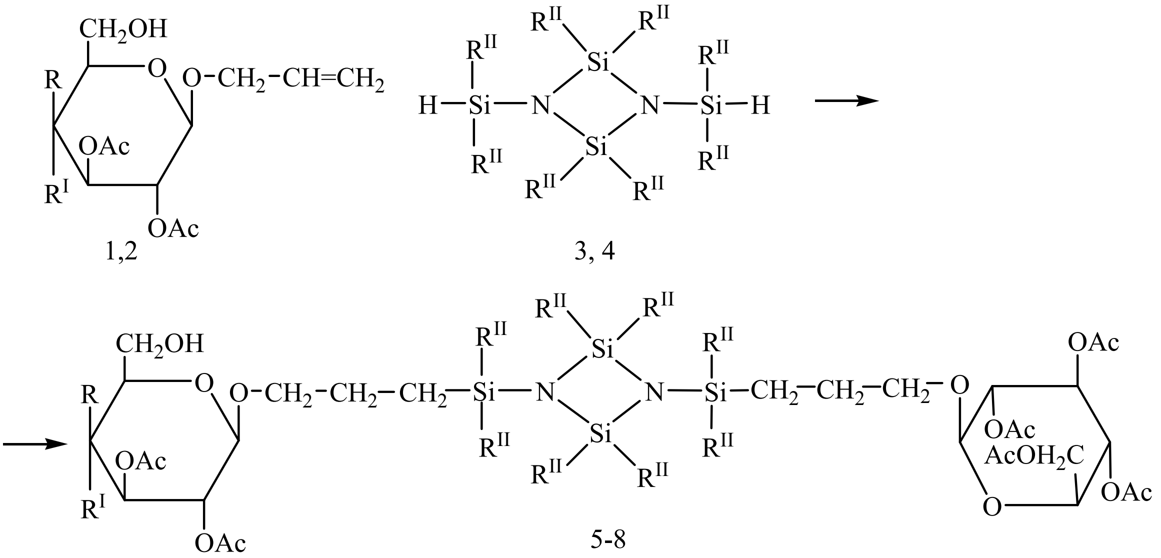
Synthesis of low-toxicity compounds has become important in biological and pharmacological studies, and so there is interest in using carbohydrates to modify linear and cyclolinear siloxanes, which may lead to a substantial change in the nature of the drug action.

We have studied the reaction of hydrosilylation of 1-O-allyl-2,3,4,6-tetra-O-acetyl-β-*D*-glucopyranoses (1) and 1-O-allyl-2,3,4,6-tetra-O-acetyl-β-*D*-galactopyranoses (**2**) with 1,3-bis(dimethylsilyl)-2,2,4,4-tetramethylcyclodisilazane (3) and 1,3-bis(diphenylsilyl)-2,2,4,4-tetraphenylcyclodisilazane (4) in the presence of catalyst – $Co_2(CO)_8$.The reactions mainly occurs according to Farmer's rule, although a small amount of the Markovnikov addition product is also formed.



R=H, R^I =OAc (1);   R=H, R^I =OAc, R^{II}=Me (3,5), Ph (4,7)
R=OAc, R^I =H (2);   R=OAc, R^I =H, R^{II}=Me (3,6), Ph (4,8)

The course of the reaction was monitored from the decrease in active hydrogen on the silicon over time. We have established that in 1.5 h, the hydrogen in the ≡Si–H group is completely removed, which is supported by the IR spectrum.

Addition of 1.3-bis(dimethylsilyl)-2.2.4.4-tetramethylcyclodisilazane (3) to allyl glucoside (1) was selected to study the pathway and mechanism of the model reaction.

Quantum-chemical computation was performed using CS MOPAC (Chem 3D Ultra version 8.03). Each computation by the AM1 method was preceded by optimization of the compounds, i. e. minimization of the energy by molecular mechanics (MM) and the quantum-chemical method. This reaction was examined in two directions, according to the Farmer and Markovnikov rules. The calculated heats of formations of products and reactions showed that production of 5 was highly probable.

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Abstract

Catalytic Effect of Ionic Liquids on Polycyclotrimerization of High Performance Cyanate Ester Resins

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Polycyanurates (PCNs) represent a family of thermosetting polymers possessing such attractive intrinsic features as excellent dimensional stability, high glass transition temperatures (T_g > 250°C), low dielectric constants (2.5-3.2), inherent flame-retardancy, and high adhesion to conductor metals and composites. Therefore, they are promising materials for airspace and electronic application, especially as polymer matrixes for structural composites, adhesives, compounds, coatings, working under severe conditions (high temperatures, corrosive media, …). Ionic liquids have attracted attention due to their significant role in controlling the reaction as a catalyst in a variety of green chemistry processes, and for use in polymer synthesis as solvents.

The purpose of this work is to study a possible catalytic effect of different ionic liquids (ILs) on conversion of cyanate groups at synthesis of PCN/ILs systems.

Kinetic peculiarities of polycyclotrimerization process of dicyanate ester of bisphenol E (DCBE) in the presence of different ILs (such as 1-methyl-3-octylimidazolium tetrafluoroborate, 2-(hydroxy-ethylamino)imidazolinium chloride, triethylamine-2-trifluoromethanesulfonate) have been investigated using Fourier Transform Infrared Spectroscopy (FTIR) technique. It has been found that even a small amount of ILs (1 wt.%) accelerates significantly the reaction of polycyclotrimerization of DCBE leading to formation of polycyanurate network.

Abstract

Solar Cells Based on Polymer Semiconductor - Dye Nanocomposites

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Organic solar cells are nowadays ones of the most attractive and applicable topics for investtigations. Such photovoltaics are very suitable for the green energetics. As a rule polymeric photovoltaics consist of electron-donating polymers that absorb the sun rays, photogenerate charge carriers, and transport charges and of electron acceptors [1]. The last ones in our work were phthalocyanines [2] and polymethine dyes [3], as electrondonor polymers we studied PPV and carbazole derivatives, mainly their copolymers. Polyvinylbenzocarbazoles as polymeric semiconductors were firstly discovered in our university [4], among them [c] isomer was found to be the most active one [5]. Previously copolymers of n-octyl methacrylate (OMA) with N-vinylcarbazole and N-vinyl-3-iodocarbazole were studied, now new materials have been found – copolymers of OMA with N-vinyl-7H- benzo[c] carbazole with more conjugated electronic structure (Figure 1).

For all copolymers their spectral properties were studied in solutions and in films. The last copolymers have more intensive long-wave absorption than previous ones, the copolymerization causes bathochromic shifts. For films we have found that the nanoparticles are formed as a result of aggregation of dyes molecules in polymer matrixes leading to a bathochromic shift of the absorption of the composite and to an increase in its light sensitivity [2].

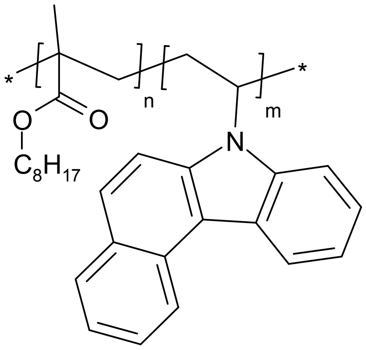

Figure 1. Copolymers.

For these copolymers monomers ratio is 1:1 (m=n).

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Abstract

Comb Type Methylsiloxane Block-copolymers

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In the literature, there are no data about comb-type siloxane-siloxane copolymers with the specified arrangement of linear diorganosiloxane fragments as a lateral group. From another side it's known that in block-copolymers in case of incomepatibility of rigid and flexible blocks two phase systems are obtained.

For the purpose of synthesis of comb-type methylsiloxane copolymers with rigid diorganosiloxane fragments in the side chain in the first stage the monohydroxyl-containing oligomeric diphenylsiloxanes and methylphenylsiloxanes blocked with trimethylsiloxy group were synthesized, by the reaction of heterofunctional condensation of α,ω-dihydroxydiphenyl(methylphenyl)siloxanes with trimethylchlorosilane at 1:1 ratio of initial compounds, in the presence of anhydrous pyridine, at temperature range -5÷0^{0}C in dilute solution of anhydrous toluene.

Comb-type methylsiloxane copolymers with rigid polysiloxane branching side groups were synthesized by catalytic dehydrocondensation of polymethylhydrosiloxane or α,ω-bis(trimethylsiloxy)methylhydridesiloxane-dimethylsiloxanes with α-hydroxyl-ω-trimethylsiloxydiorganosiloxanes at various ratio in the presence of catalytic amount anhydrous powder-like potassium hydroxide (0,1 % total mass of initial reaction products), in anhydrous solution of toluene, at the temperature range 50, 60 and 70^{0}C.

The catalytic dehydrocondensation reaction order, activation energies and rate constants have been determined. The polyorganosiloxanes with rigid polydiorganosiloxane fragments in the side chain, completely soluble in organic solvents have been synthesized. The synthesized copolymers were characterized by ^{1}H and ^{13}C NMR spectra, thermogravimetric, and gel-permeation chromatography, differential scanning calorimetric and wide-angle X-ray diffracttometric methods.

By differential scanning calorimetric and wide-angle X-ray diffractometric methods it was shown that at definite values of the lengths of the flexible and rigid fragments, incomepatibility and microheterogeneous structure in block copolymers was observed. That is means here segregation processes proceed with formation of independent domains both in the main dimethylsiloxane chain, and lateral side groups in parallel plane.

Abstract

Non-Stationary Modes of Frontal Polymerization

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Experimentally it has been shown, that losses of stability in frontal polymerization are caused by heat losses from a reaction zone.

The methods and algorithms of nonlinear dynamics are successfully applied to different scientific fields such as biophysics, biochemistry, electronics, geophysics, neurophysiology, chemistry etc. Processes such as combustion in gases or condensed media, self- propagating high temperature synthesis (SHS) and frontal polymerization, which are realized under the condition of propagation of thermal wave of chemical nature, are of interest as nonlinear phenomena.

In a stationary regime of polymerization the wave structure and front coordinate are stable with respect to various perturbations. As this is not always the case, the velocity and structure of the thermal waves of polymerization are changed and one –dimensional or two- dimensional losses of stability take place during the frontal processes, leading to the formation of various oscillatory and spin modes.

For the processes of frontal polymerization no stationary phenomena in the form of one-, two, and three-headed spin modes were experimentally discovered on the example of frontal radical polymerization.

In this work have been investigated the mechanism of loss of stability of frontal autowaves of Co, Ni, Mn-containing metal-complex monomers have been investigated.

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Abstract

Octamethilcyclotetrasiloxane Zeolite Catalyst Polymerization

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The polymerization reaction of organocyclosiloxanes on natural zeolites has not been studied yet.

There are at present no data about the catalytic activity of natural zeolites in the polymerization reactions of organocyclosiloxanes.

The catalytic activity of modified high-silicone clinoptilolite of Khekordzula layer in the polymerization reactions of octamethilcyclotetrasiloxane is investigated.

During the experiment the effective catalysts of this reaction are revealed.

In particular this is the H-form of clinoptilolite, obtained by action on initial zeolites by the hydrochloric acid solution. The optimal conditions of conducting the reaction and its supposed mechanism are selected.

On the given catalysts, the possibility of obtaining of polydimethylsiloxane with the large output is demonstrated. The study of the possibility of applying natural zeolites as the catalyst in the polymerization reactions of organocyclosiloxanes and the clarification of possible reaction mechanism is the purpose of this work.

Clinoptilolite was used as the catalyst, extended in the territory of Georgia with sufficiently high (8,5-10,5) molar ratio SiO_2/ Al_2O_3 in clinoptilolite. The octamethylcyclotetrasiloxane (D_4) was selected as monomer.

Initial natural clinoptilolite, its modified forms and exhausted catalysts were investigated by the methods of X-ray diffraction analysis and IR spectroscopy. The catalyst surface was also studied by electron-microscopic scanning.

The obtained polymers were investigated by the method of IR spectroscopy. The polymer molecular weight was determined by GPC method

H-form catalyst is optimal for D_4 polymerisation.

D_4 polymerization reaction has cation nature. It goes in the Brünsted's acidic centers. In this process acid centers also manifest catalytic activity, locating on the surface of the crystal phase of clinoptilolite. Results of X-ray structural and infrared spectral analysis and also the electron-microscopic scanning of catalyst surface area confirm our conclusion.

Abstract

Synthesis and Properties of Polyacrylamide Hydrogels Obtained by Frontal Polymerization

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Recently of particular interest are polyacrylamide hydrogels (PAAG) formed by cross-linking of linear macromolecules of functionalized PAAm. PAAG are "smart" polymers capable not only to absorb large amounts of water or aqueous solutions of various substances, but also drastically change its volume with the release of the substances absorbed back into the environment depending on external conditions (temperature, ionic strength of solution, pH value, etc.). Thanks to this ability PAAG are widely used in various fields, especially in pharmacology, medicine as well as in the oil industry for enhanced oil recovery.

In areas related to human health cross-linked PAAG are used frequently synthesized from monomers in the presence of bifunctional organic compounds as crosslinking agents. It is important for the main content of residual monomer (AAm) to be minimal.

Preparation of functionalized PAAm is carried out in industry by well known free radical polymerization or copolymerization of monomers mixture in aqueous solution or in the melt. However, the classical methods of its synthesis are energy intensive and not sufficiently productive increasing the cost of the final product. In addition a residual monomer still remains in the resulting PAAm.

The method of frontal polymerization was used for PAAm Hydrogels synthesis. As advantage of this method one could mentioned a possibility to prepare PAAm Hydrogels containing practically no a residual monomer.

Irregular Biopolymers – the Protein Components of Ion Channels of Plant and Animal Cells

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Among the voltage-controlled ion channels, the external stimulus sensor of which directly is a part of the molecular complex (e.g., glycoprotein) include K^+, Na^+, Ca^{2+}, Cl^- carrying ion channels. In cytoplasmic cell membrane the ion channels connect exo- and cytoplasm, respectively, by the outer and inner apertures. Their function is regulated by changing of the ionic composition under the influence of external or internal factors in the exo- or cytoplasm. The ratio of the Nernst-Goldman relates the change in the ionic composition with the transmembrane potential:

$$\Delta\varphi = f(C_k^i, C_k^e)$$

The change of the transmembrane potential causes a change of the dipole moment of α-helical subunits of the ion channel. The dislocation of charges along subunits – is short-time "gating currents" J_i, which precedes the opening of the ion channel, that have been described by Armstrong C.A., Besanilla F. and predicted by Hodgkin A.L., Huxley A.F.

In the case of appearance of the "gating currents" in α-subunits of neuroreceptor, that are forming the ion channel, mutual almost parallel (collinear) orientation of the subunits provides the unique conditions under which arises mutually antithetical – anti-parallel motion of the charges between them, initiating the development of the mutual repulsive force, which occurs only during the movement of the charges (for example, with the emergence of the "gating currents"):

$$\left|\vec{F}_{ij}\right| = \frac{\mu_0\mu}{2\pi}(\vec{J}_i\vec{J}_j)\frac{\lambda}{R_{ij}}$$

Where $\left|\vec{F}_{ij}\right|$ – the mutual repulsive force between the subunits of neuroreceptor, μ_0, μ – magnetic constant and magnetic permeability, respectively, R_{ij} – the distance between the α-helical subunits of ion channel, $\vec{J}_i, \vec{J}_j$ – the "gating current" in α-helical subunits, λ – length of the interacting fragments.

If accept $\frac{\mu_0\mu}{2\pi} = 2\times10^{-7}$ Hn/m, the mass of the α-helical subunit $m \sim 10^{-27}$kg, the time of the open state of ion channel $\tau \sim 10^{-4}$sec, can get a quality estimate to diameter increase of the ion annel $\Delta R \sim 5\text{x}10^{-10}$m, that indicates a sufficient value for the transmission of hydrated ions Na^+.

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Abstract

Ultra Fast Curing for Advanced Composites

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In the maintenance, repair and overhaul (MRO) of aerospace industry practices sealants are used for joining and sealing purposes.

Some sealants, which are used for the sealing of aircraft`s windows, need a long time (up to few days) to be fully cured. This dramatically prolong the lead delivery time.

We have been interested in developing different techniques to find curing method enabling reduction of cure time of some sealants.

The proposed curing techniques must be able to cure the sealants with less time (less than 2h) compare to thermal curing without chemical modification and without compromising of mechanical properties.

Two curing methods for some aviation sealants have been compared:

- (i) Classical technique using thermal curing kinetic of the sealants where two kinetic models with different curing methods has been proposed for predicting of thermal curing behaviour of aviation sealant;
- (ii) IR curing kinetic of the sealants cured by IR heating.

Shore hardness A measurement of the sealants *vs.* its curing time have been performed at room temperature and at 65 °C in oven as well as using IR.

Keywords: Sealants; Thermal Curing; Infrared Curing; Kinetics; Aerospace

Abstract

Synthesis and Biological Study of New Arginine-containing Cationic Polymers

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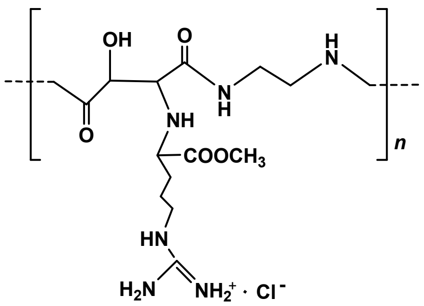
Major limitations of synthetic cationic polymers used as transfection agents for intracellular gene delivery are their cytotoxicity and low biodegradability. Hence, the development of new cytotoxicity free cationic polymers that will degrade under the action of physiological environment is topical. Among synthetic transfection agents those composed of α-amino acid arginine (Arg) are of special interest due to a high transfection activity of the guanidine group [1].

We synthesized a new biodegradable cationic polymer - poly(ethylene malamide) containing L-arginine methyl ester covalently attached to the macrochains in β-position *via* α-amino group:



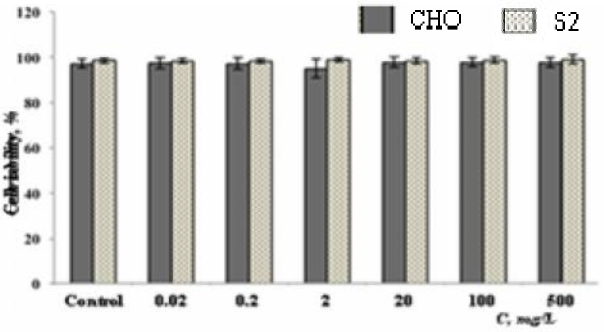


Figure 1. CHO & S2 cells viability

The new Arg-containing cationic polymer was highly water soluble, formed nano-complexes with pDNA at much lower Polymer/DNA weight ratios (WR=5-10) compared to the Arg-based polymers (WR=300-1000) [2,3], and showed no cytotoxicity with Chinese Hamster Ovary (CHO) and insect Schneider 2 (S2) cells within the concentration range 0.02-500 mg/mL for 24 h [4] (Fig. 1).

Acknowledgement. 28071/1 The authors thank Swiss National Science Foundation (SNF) for financial support (Grant # IZ73ZO_1).

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Abstract

Thermooxidative Degradation of the Low-density Polyethylene in the Presence of Fullerenes C_{60}/C_{70}

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The investigation on influence of fullerenes C_{60}/C_{70} on processes of thermooxidative degradation and thermoageing of high pressure low-density polyethylene (LDPE) has been accomplished.

According to heat effects being displayed on the LDPE differential thermal analysis (DTA) curves substantial changes are observed only at high temperatures range. Endo-effects of the polyethylene crystal phase fusing at 378K are almost not changed over maximum temperature and melting heat area as well. This is evidence that fullerenes are distributed in amorphous phase of polyethylene and do not change the polymer crystallinity. Little exo-effect at 508°K connected presumably with re-crystallization processes is not also suffered to marked alteration. Just the heat effects of exothermic thermooxidative processes at area 600K and above are sensitive to the fullerenes presence. The wide and intensive exothermal peak of decomposition of polyethylene degenerates into narrow exothermal one, and as it is displayed from area of respective peaks, the intensity of exothermal processes in some cases lower by order than for the reference polyethylene.

Results obtained are confirmed by the data of thermogravimetry (TG). Temperatures of starting weight loss as well as the area of polymer disruption are shifted to higher temperatures region for the fullerenes contained patterns.

To estimate the efficiency of fullerenes under conditions of thermooxidative degradation there LDPE composites were prepared. The formulations were composed by way of additives introduction to LDPE melt followed by homogenization on laboratory rollers. The LDPE composites were subjected to thermoageing in the air bath oven at temperatures 369-371K for 12 - 96 hours.

The measurements of physical-mechanical features of samples after artificial ageing have shown that tehsile strength, yield piont and relative elongation are in accordance with results of LDPE. thermal analysis. Thus the data indicate high stabilizing activity of fullerene additives which might be compared with activity of impactful commercial antioxidants.

Abstract

A Possible Mechanism of Allosteric Interactions

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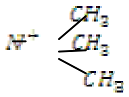
During allosteric interactions the conformation of protein macromolecules changes. which promotes the behaviour of metabolic processes or other biological effects. Allosteric proteins are characterised by two types of key zones: allosteric and active centres; in the simplest case – by one allosteric and one active centre. The impact of the metabolite-receptor (bioenergy-activator) on the allosteric centre causes such deforming effects of protein macromolecule which open the active centre, where its interaction with the adjacent protein macromolecule occurs.

It is accepted to consider the results of the influence of acetylcholine on neuronal nicotinic acetylcholine receptors as allesteric, as it causes the deformative process in the receptor under the influence of a mediator.



Quaternary ammonium groups of acetylcholine, by clinging to the receptor, form the electrostatic field in the area of outer mouth of the receptor. Due to the ability of polarization, the shift if the charges take place in the electrostatic outer field, formed by ammonium charged groups of acetylcholine.

At the same time, owing to the structural peculiarities of allosteric protein (the presence of secondary, system of units α-helical structure), the shift of the charged groups is accompanied by the deformation because of the emergence of the contracting power:

$$F(t) = \alpha \frac{N^2 S}{l^2(t)} \left(\frac{\Delta Q}{\Delta t}\right)^2$$

where α – constant depending on the system of units (in SI system $\alpha = \frac{\mu_0 \mu}{4\pi}$), S, l, N the cross-section, length and number of coils of α-helical subunit $\frac{\Delta Q}{\Delta t}$- shift of charges within Δt. Thus, the conditions which promote the deformation of protein macromolecule, i.e. allosteric effect, are created. In contrast to the proposed models - which describe kinetics quite well - by using the physico-chemical methods we consider the dynamics, i.e. nature of forces, causing the deformation of protein macromolecule under the influence of charged groups of bioenergy-activator, i.e. allosteric effect.

Abstract

Direct Chemical Dynamics and Chemical Reaction Mechanism

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Increasing gasoline prices, depleting fossil fuels, and rising greenhouse-gas emission stimulate global efforts to find alternative transportation fuels. Advanced engine technologies increasingly rely on fuel properties to time ignition and optimize engine performance, so that understanding the fundamental chemistry of alternative fuel candidates is essential. One very important research direction is the search for economically affordable, yet ecologically friendly, renewable biofuels. The efforts include understanding the underlying chemical reaction mechanisms for combustion of novel biofuels, such as alcohols, ethers, esters, furans etc., whose combustion chemistry is known about less and can be significantly different from the more-studied, traditional hydrocarbon based fuels. Complex combustion reactions are characterized by multiple different pathways and some specific details of these reactions cannot be understood and even observed experimentally, thus have to be investigated theoretically, preferably at the molecular level. The processes at the molecular level is governed by quantum theory so that the design of biofuels, tailor-made to combustion engines is neither quick nor easy process. The limitations show up when we attempt to model such processes at the molecular level by means of classical theory and address challenges using the conventional, serial programs and computers. Fortunately, IT industry has already moved to massively parallel pattern, which gives us the choice to apply quantum theory to a real-world problems.

Direct chemical dynamics [1-2] can be used to investigate the short-time dynamics of selected features on the Potential Energy Surface (PES) of biofuel reactions, to check the mechanism of reactions obtained via static – electronic structure theory calculations. In direct dynamics, the trajectories are integrated "on the fly", with the potential energy, gradient, and also Hessian obtained directly from an electronic structure theory without the need for an analytic potential energy function [1].

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The Characterization of Reactivity of Substituted Anilines by σ-constants of Hammett Equation in N-glycosylation Reaction

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The Hammett equation describes a linear free-energy relationship relating reaction rates and equilibrium constants for many reactions involving benzoic acid derivatives with meta- and para-substituents to each other with just two parameters: a substituent constant and a reaction constant [1]. Relative reactivity of isomeric aromatic amines in reaction of N-glycosylation it is possible to characterize on the basis of σ-constants of equation of Hammett.

Aromatic amines used in our experiments are the substituted anilines where as substituent groups act: CH_3, OH, COOH. The methyl group has positive inductive effect, but has no mesomeric effect; Group OH is characterized by weak negative inductive effect and strong positive mesomeric effect; Group COOH is characterized by negative inductive effect and negative mesomeric effect. For reaction of N-glycosylation of substituted anilines, members of Hammett equation $\lg\frac{k}{k_0}=\sigma\rho$ will have the following values: k is a N-glycosylation reaction rate constant (or an equilibrium constant) of substituted compounds (isomeric toluidines, amino phenols or amino benzoic acids); k_0 are the relevant parameters of aniline; σ is a constant of the substituent; ρ is a constant characteristic for given reaction of N-glycosylation, and being a measure of sensitivity of this reaction to the changes of the substituent. In case of isomeric toluidines, amino phenols or amino benzoic acids, this member of equation (ρ) practically changes only insignificantly (or does not vary at all), then for meta and para isomers of substituted anilines the log k will have the following values: meta toluidine 1.16; para toluidine 0.77; meta amino phenol 0.8; para amino phenol 0.18; meta amino benzoic acid -0.43; para amino benzoic acid -0.35. The experimental data received by N-glycosylation of specified substituted anilines, correlate to values of lg k calculated with the help of Hammett equation, and also with other such parameters as values of pKa and values of dipole moment of these compounds [2].

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Abstract

Composites on the Basis of Glycidoxygroup Containing Phenylsilsesquioxanes

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For synthesis of glycidoxy group containing phenylsilsesquioxanes the condensation reaction of cis-2.4.6.8-tetrahydroxy-2.4.6.8-tetraphenylcyclotetrasiloxane and oligotetroles (n=2÷10) in the presence of excess of epychlorohydrin in 25% solution of sodium hydroxide in dry toluene have been carried out and corresponding glycidyl ethers have been obtained. The composition of obtained compounds have been proved via elemental analysis, amount of epoxide groups, determination of molecular masses FTIR and NMR spectra data.

In the FTIR spectra of obtained compounds in the region of asymmetric and symmetric valence oscillation of ≡Si-O-Si≡ bonds bifurcation of absorption bonds with maximum at ν_{as} -1045 cm^{-1}, 1145 cm^{-1} and 1145 cm^{-1} is observed as well a new absorption bands at 820-840, 917 cm^{-1} characteristic of oxirane ring is appeared.

It was established that in the presence of sodium hydroxide the rearrangement phenylsilsesquioxane skeleton takes place and cis-anti-cis structure of silsesquixane structure turn to cis-sindiotactic structure, on which indicate doublet character of absorption bands of ≡Si-O-Si≡ bonds.

Synthesized compounds do not change the characteristic properties within three months, indicating that their continued viability. Glycidyl organosilicon compounds have been used as modifiers epoxy-diane resin ED-22. The compositions were cured at room temperature, as well as amine-type hardeners heating.

The study of oxidative degradation of the resulting composites revealed that the ternary system (ED-22 + glycidoxy phenylsilsesquioxane + hardener) are a high temperature resistant than the cured original epoxy resin. With an increasing chain length of ladder modifier moiety mainly increases the relative thermal stability of composites, which also depends on the structure of the hardener and the highest results is achieve using 4,4'-diaminotriphenyloxide. These composite compounds may be used as a potting material.

Abstract

Tools for modeling of advanced materials

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Atomistic modeling of materials is widely used in industry and academia. Prediction and characterization of geometric and electronic structures are key problems in advanced materials research. It is efficiently addressed with state of the art molecular dynamics and quantum molecular dynamics methods. After reviewing the status of high-performance tools for structure prediction, we highlight the future trends and prospects in the simulation and development of the advanced energy storage materials.

According to these new trends, we developed a multi-scale hybrid method of simultaneous quantum dynamics of electrons and nuclei based on time dependent density functional theory (DFT) for electrons and quasi-classical coherent state (CS) theory for nuclei. The method is founded on mathematically rigorous separation of length scales and physically motivated interface between quantum (finite as well as periodic) and classical regions. Rather than being relayed on the predefined potential energy surface (PES) from electrons, our method calculates the DFT energy of simultaneously moving electrons "on the fly" in atomic, or plane-wave, basis. These two bases enable the realistic treatment of molecular systems attached to a surface.

On the other hand, nuclei can be treated classically using frozen Gaussian wave packet approximation, or quantum-mechanically using Gaussian wave packet approximation with evolving width. The latter is capable of accounting for quantum effects for light atoms, such as hydrogen.

The following accomplishments have been made on the project during the recent period:

- Development of an adaptive radial quadrature grid for efficient and accurate integration of electron density in the outer regions of the molecular systems that has been implemented into the code.

The method will be implemented on a hybrid parallel architecture CPU with Graphical Processing Unit (GPU). We expect to achieve an excellent convergence and overall speedup, which will allow us to scan promising materials for energy storage.

Abstract

Removal of Heavy Metal Ions from Wastewaters by Using of Renewable Bio Sources of Georgia

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The soil, water and air pollution have been dramatically increased by various organic and inorganic substances because of anthropogenic influence. One of the biggest problems is water pollution by industrial, urban and agricultural sewage that reaches 250-300 billion m^3 per year. Because of a large scale pollution, health hazardous heavy metal ions (Cr, Cu, Zn, Pb, Hg, As, etc.) appear in water along with radioactive, bioaccumulative (including carcinogenic) and other toxicants, thats concentration exceed permissible limits. There are plenty of reasons for water pollution by heavy metals; first of all, it should be noted consumer attitude to the nature and low efficiency and high cost of waste water purification systems. The removal of toxic metal ions from waters is difficult and expensive task. Using of many methods for water purification is limited due to high cost of reagents, difficulty of equipment and multiple staging of purification processes. In recent years, great attention is paid to the obtaining of cheap biosorbents from renewable plant raw materials by "green chemistry" methods. Compared with inorganic sorbents, bio-sorbents have the following advantages: low price; high efficiency; simple technological processes for obtaining and etc. Bio-sorbents have high sorption capacity toward heavy metal ions, which exceeds similar ability of inorganic sorbents several times. In Georgia there are many types of renewable bio sources which may be adopted for obtaining of bio-sorbents.

Obtained by us bio-sorbents (from wood processing residues) have been tested for removing of Cr (III) ions from waters. Removal of chromium from waste waters is a highly topical issue, because chromium basic sulfate is used in scheme of leather processing technology of Georgian tanneries. Biosobent allows to liberate chromium ions from wastewater without enrichment with chlorides and sulfates. In water Cr (III) ions undergo hydrolysis and create lots of aqua - and hydroxy complexes with different sorption properties. We have determined that when the water pH = 4, the chromium ions are fixed by carboxylic (not hydroxyl) groups in bio-sorbents, because etherized bio-sorbents reveal 3-4 times less sorption ability. Consequently, partial selective oxidation of biomaterials with formation of the carboxylic groups represents an opportunity for increasing of sorption capacity of bio-sorbents. The influence of adsorbent concentration, pH and a contact time at the effectiveness of chromium ions removal has been studied.

Taking of samples, and preliminary reprocessing was implemented by ISO 11466 standard; determination of chromium in samples was carried out by atomic-absorption spectrometer (NovAA 400 Analytik Jena).

AUTHORS INDEX

Abstract

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