

# Second International Caucasian Symposium on Polymers and Advanced Materials



7-10 September 2010  
Tbilisi, Georgia



*Organized by*

Iv. Javakhishvili  
Tbilisi State University

*Auspices*

Ministry of Education and  
Science of Georgia



**ICSP&AM2**



## Welcome

**Dear Colleagues,**

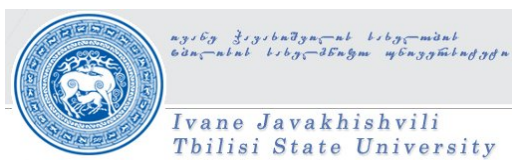
On behalf of the Organizing Committee I wish to extend cordial welcome to all participants of the 2<sup>nd</sup> International Caucasian Symposium on Polymers and Advanced Materials. Three years ago, 2007, this symposium took place in Tbilisi, Georgia. We are delighted to host you this year in the geographical centre of the "Caucasia", 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 2" will help to introduce effectively innovative scientific researches of Georgian, Caucasian and neighboring scientific teams, which are less known for world scientific society.

We hope that this year meeting, gathering almost 100 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

### Sponsors:



### Organizing committee:

Chair – Prof. O. Mukbaniani

Co. Chair – As. Prof. V. Tskhovrebashvili

Co. Chair – Prof. Marc J.M. Abadie

Executive Secretary –T. Tatrishvili, PhD

Conference Secretariat –Doroshenko Mikheil, MSc

**ICSP&AM 2**

# SYMPOSIUM SCHEDULE

*7 September*

**13:00–17:00** Registration

**17:30–19:30** Welcome reception

*8 September*

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

**Co-chairmen:** *Prof. Marc J.M. Abadie and Prof. T. Agladze*

**09:30–09:50** *Marc J.M. Abadie* "Ultra Fast Curing for Aerospace Applications".

**09:50–10:10** *M. Bratychak* "Reactive Oligomers Based on Dianic Epoxy Resins".

**10:10–10:30** *K. Koynov* "Fluorescence correlation spectroscopy studies of dense polymer systems".

**10:30–10:50** *R. Katsarava* "New novel resorbable composite materials for orthopedic surgery: In vivo biodegradation study of polymeric matrix".

*Coffee break 11.00-11.40*

**Co-chairmen:** *Prof. K. Koynov and Prof. N. Lekishvili*

**11:40–12:00** *B. Mamedov* "Synthesis of oligohydroxynaphthylenes and their use in making of heat-stable and electro-conducting rubbers".

**12:00–12:20** *O. Mukbaniani* "Synthesis and Investigation of Polysiloxanes with Reactionable Groups in the Side Chain".

**12:20–12:40** *S. Sedaghat* "Synthesis of Silver-Polyanilinenanocomposite and its Antibacterial Effects".

**12:40–13:00** *N. Durgaryan* "Synthesis, characterization and electrical properties of poly(azobenzophenones)".

*Lunch break 13.00-14.30*

**Co-chairmen:** *Prof. B. Mamedov and Prof. G. Papava*

**14:30–14:50** *M. R. Moghbeli* "Effect of Comonomer and Organoclay Contents on the Microcellular Structure and Elastomeric Properties of the PolyHIPE Solid Foams".

**14:50–15:10** *L. Nadareishvili* "Some Regularities of the Gradient Orientation of Polymers in Heterogeneous Mechanical Field".

**15:10–15:30** *G. Papava* "Diatomite-containing Thermoreactive (Novolak type) Polymer Compositions".

**15:30–15:50** *Kh. Barbakadze* "New Antibiocorrosive Covers and Conservers Based on Bioactive d-Metal Complexes with Sterical Ligands".

*Coffee break*

**16:00–18:00** *Poster session p. 4-41 ("Polymers" and "Advanced Materials")*

## 9 September

**Co-chairmen:** Prof. M. Bratychak and Prof. J. Aneli

**09:30–09:50** Marc J.M. Abadie ” New Ways for Obtaining Biodegradable Thermoplastic Elastomers”

**09:50–10:10** F. Ziaee “The effect of deuterated solvent types in <sup>13</sup>CNMR spectroscopy and splitting of polystyrene para aromatic carbon”

**10:10–10:30** M. R. Moghbeli “Rubber-modification of SAN/Organoclay nanocomposite with Core-shell Rubber Latex Particles”

**10:30–10:50** Yu. Petukhou ” PET films modified by functional carbon nanomaterials”

Coffee break 11.00-11.40

**Co-chairmen:** Prof. S. Hayrapetyan and Prof. R. Katsarava

**11:40–12:00** T. Agladze ”Effect of the Shell on Reactivity of Core/Shell Structured Nanoparticles”

**12:00–12:20** J. Aneli “Modern conceptions on the mechanism of electrical conductivity of polymer composites”

**12:20–12:40** P. Voskanyan “Polymers on vinyl acetate base: present situation and development prospects”

**12:40–13:00** G. Meskhi “Experimental investigation of emitted nanoclusters during laser and ion beam interaction with solids”

Lunch break 13.00-14.30

**Co-chairmen:** Prof. M. R. Moghbeli and L. Nadareishvili

**14:30–14:50** S. Hayrapetyan “Hybrid silica -polymer sorbents for liquid chromatography”.

**14:50–15:10** D. Chkhubianishvili “Study of the Mechanism of Co-Telomerization Reaction”.

**15:10–15:30** D. Gventsadze “Study of Influence Of Georgian Raw Material-Andezite on the Properties of Electric Conducting Polymer Composites Based On Polyethylene”.

**15:30-16:00** L. Akhalbedashvili The ionexchange sorption of ammonium ions on Georgian clinoptilolite.

Coffee break

**16:00–18:00** Poster session p. 42-80 (“Polymers” and “Advanced Materials”)

Closing lecture

## 10 September

**Excursion in old capital of Georgia, Mtskheta and Gori (Stalin museum, etc.).**

**Gala Dinner.**

*Farewell*

## Abstract

### Ultra Fast Curing for Aerospace Applications

*Vanda Yu. Voytekunas<sup>1</sup>, Deborah Jones<sup>2</sup>, Jacques Rozière<sup>2</sup> & Marc J.M. Abadie<sup>2,3</sup>*

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With the development of civil planes with around 50 percent of the primary structure - including the fuselage and wing - will be made of composite materials (Boeing 787 Dreamliner or AirBus A 350 XWB) there is an urgent need to find solutions for repairing structural damages of composite parts as well as other sensitive parts of the plane such as the use of sealants for the sealing of aircraft's windows.

Curing monomers into a 3 dimensional structure i.e. thermosets or duromers can be achieved mainly by thermal or UV/EB process. The second way is more flexible and generally faster, saving energy and therefore cost.

UV has been widely used for thin film technologies but is limited by the thickness – 100 to 250  $\mu\text{m}$ , due to lack of penetration of the light. However the system is quite fast, 0.1 s or 0.001 s in case of the use of Laser. Different techniques have been used successfully such as Differential Scanning Photocalorimetry (M.J.M. Abadie et al.) or real time FTIR (Ch. Deccker et al.) to follow rapid kinetics.

Generally by thermal process, time to fully cure monomers is very long and takes up to a few days. This strongly affects delivery time, as aircrafts are grounded and off of service until structural damages are not repaired.

Thus, the curing time is a very important technical specification for any adhesive/sealant as it can save the waiting time for airplanes that need repairing at the airport and thus reduce the operation cost.

Two directions are followed to speed up the curing time:

- The use of activator or accelerator into the chemical formulation;
- Combine physical treatments such as thermal with UV/EB or microwaves or ultrasounds;
- IR heating and curing;

We present some preliminary results obtained with sealants used for fuel leak repair.



## **Abstract**

### **New Ways for Obtaining Biodegradable Thermoplastic Elastomers**

*Vitali T. Lipik<sup>1</sup>, Sing S. Liow<sup>1</sup>, Leonardus K. Widjaja<sup>1</sup>, Kong Jen Fong<sup>1</sup>, Sujay Chattopadhyay<sup>1</sup>,  
Subramanian S. Venkatraman<sup>1</sup> & Marc J.M. Abadie<sup>1,2</sup>*

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The first thermoplastic elastomers TPE was developed by Shell in the 70s, triblock copolymers named as Kraton® and based on styrene and butadiene or isoprene and later on ethylene/butylene or ethylene/propylene for the soft block. Our challenge was to replace these non-biodegradable elastomers by monomers whose polymers will degrade.

Aliphatic polyesters, such as Polyglycolide (PGA), Polylactide (PLLA), Poly( $\epsilon$ -caprolactone) (PCL) and their copolymers have received great interest in biomedical applications due to their good biocompatibility and bioabsorbability. They degrade mainly by hydrolysis of ester linkages, yield hydroxyl carboxylic acids, which in most cases are ultimately metabolized.

To prepare polymers with variable rate of degradation, most studies have focused on copolymerization. Copolymerization allows blending of two or more polymers, in order to achieve variable degradation patterns. In-depth research of degradation behaviors of the copolymers in different compositions and prolonged synthesis procedure are expected.

If most of the works regarding biodegradable polymers focused on their degradation, no one has been done on the elastomeric properties having at the same time biodegradability behavior.

Coordinated anionic ring opening polymerization has been used to synthesize block copolymers, more precisely diblock, triblock, starblock and multiblock systems based on  $\epsilon$ -caprolactone. Block copolymers include two parts: one is responsible for hardness and rigidity, and another for mobility and softness. It is possible to change their ratio at the synthesis or even one block can be synthesized as a copolymer consisting from two or more monomers. The possibility to vary these parameters allows us to receive polymers with very different properties. The crystallinity of the poly( $\epsilon$ -caprolactone) used as soft segment has been disrupted by incorporating either L-Lactide or trimethylene carbonate (TMC) units.

We have considered different parameters such as the % of crystallinity of each segments, the molar mass, the elongation, the modulus, the maximum tensile stress as well as the recovery. Our studies suggest that soft segment composition does affect the mechanical properties significantly. Elongation can be high as 1500 % with a recovery of 90%.

In this study we report the different strategies which have been applied to develop di-, tri-, star- and multi-block copolymers based on  $\epsilon$ -caprolactone CPL, L-lactide LLA and trimethylene carbonate TMC.

It has been demonstrated that some of our copolymer systems where soft branch is constituted by random copolymer PCL-co-PLLA or PLC-co-PTMC and random copolymer PLLA-co-PCL or PLLA-co-PTMC as hard segment exhibit high elongation with low modulus, showing excellent elastomeric behavior [1].

#### **Reference**

1. Vitali T. Lipik, Leonardo K. Widjaja, Sing S. Liow, Subramanian S. Venkatraman & Marc J.M. Abadie - eXPRESS Polymer Letters, Vol. (2009), N° 32-38 (2010).

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## Abstract

### Thermal Curing of Composites Based Epoxy

Lia Wijayanti Pratomo<sup>1</sup>, Vanda Yu. Voytekunas<sup>2</sup>, Deborah Jones<sup>3</sup> & Marc J.M. Abadie<sup>1,3</sup>

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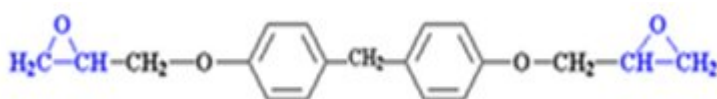
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Thermal curing has been around for many years and yet still dominating in the marketplace because of its applicability to many industrial purposes such as coatings, composites and adhesives. The easy and effective curing of the resin and hardener makes this technique of curing interesting and viable in the area of industry.

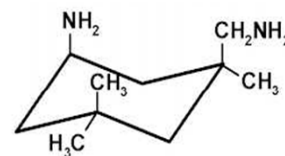
This project investigated the cure kinetics of Epolam 5015 system (see structure below) using differential scanning calorimetry (DSC) under non-isothermal and isothermal methods. Furthermore, the degree of curing (conversion), conversion rate, enthalpy of curing and glass transition temperature ( $T_g$ ) was measured to calculate the kinetic parameters (i.e. activation energy and pre-exponential factor) of the system. Variation of epoxy and hardener ratio of Epolam 5015 system (see structure below) was found to have a significant effect on the cure kinetic parameters. It was found that this optimum system corresponds to 100/30 wt.%/wt.% ratio of resin and hardener, respectively.

The cure kinetic for isothermal curing completely followed  $n$ th-order kinetic model with a reaction order of two. Additionally, non-isothermal curing showed autocatalytic behavior for the system with the optimum amount of hardener (30 wt.%) and above. As the amount of hardener decreases, more complicated cure mechanism including both autocatalytic and first order reactions occur, as it shows the appearance of two exothermic peaks. The nature of these two peaks is suspected due to the amount of hardener is below the optimum system, where the amount of major and minor products of epoxy/amine polymerization (see structure below) is comparable to each other, thus the appearance of two peaks can clearly be seen.

The simulation using the kinetic parameters generated by both methods showed that the kinetic models fitted the experimental data well.



Epolam 5015



Hardener

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## 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 nano-heterogeneous 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 containing soluble carbon nanotubes and fullerenes;
- ❖ Nanocomposites based on liquid polybutadienes.
- ❖ Carbon fiber composites modified soluble astralenes.

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



## Abstract

### Fluorescence Correlation Spectroscopy Studies of Dense Polymer Systems

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Despite of its great potential and high versatility in addressing the diffusion and transport properties of complex systems, so far the utilization of fluorescence correlation spectroscopy (FCS) has been almost exclusively limited to biological studies i.e. aqueous environments [1]. Only very recently FCS was successfully applied to study more “classical” polymer systems, e.g. self-diffusion in polystyrene solutions [2,3], segmental dynamics in polymer melts [4], surface diffusion of adsorbed polymers [5], dynamic of grafted polymer gels [6], etc. In this contribution we will summarize the recent advances of our group towards the development and implementation of FCS as a powerful tool in polymer science. First we used FCS to study the diffusion of single tracers with molecular and macromolecular sizes (dye molecules and labeled polymers) in polystyrene solutions over a broad range of concentrations and molecular weights of the matrix polymer [7]. Then the small tracer diffusion in melts of polyisoprene and polydimethylsiloxane was investigated and related to the segmental dynamic of the polymers [8]. Finally taking advantage of the extremely small detection volume that FCS offers, we studied tracer diffusion in polymer systems with micron sizes, i.e. swollen grafted poly(N-isopropylacrylamide) gels [9] and cross-linked polystyrene micro beads [10].

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## Abstract

### Rubber-Modification of SAN/Organoclay Nanocomposite with Core-shell Rubber Latex Particles

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Poly(styrene-co-acrylonitrile)/organo-modified montmorillonite PSAN/Org-MMT nanocomposites have been prepared via suspension polymerization. The effect of various organoclays on the characteristics of the nanocomposites has been investigated. The microstructure and characteristics of the modified MMT and the resultant nanocomposite materials were determined by X-ray diffraction (XRD), atomic force microscopy (AFM), and transmission electron microscopy (TEM). Differential scanning calorimetry (DSC) and falling dart impact test were also used to determine the glass transition temperature ( $T_g$ ) and impact resistance of the nanocomposites prepared. It was found that depending on the type of used organic modifier, the basal spacing of silicate layers of Org-MMT increased variably. The formation of copolymer chains within the silicate galleries during in situ suspension polymerization caused the basal spacing of org-MMT to increase on some extent. XRD patterns and TEM micrographs showed an intercalated structure for all the nanocomposite materials. Using a typical surface modifier with a double bond in its chemical structure, i.e. 2-(methacryloyloxy) ethyl trimethylammonium chloride (MAETC), resulted in highest impact fracture energy of the prepared nanocomposite. In addition, the nanocomposite powder materials were blended with the core-shell latex to improve their impact resistances. Blending the nanocomposites with the core-shell rubber particles enhanced significantly the impact resistance of the hybrid nanocomposites prepared. TEM micrographs showed the dispersion of the rubber particles as well as the organoclay inside the SAN copolymer matrix.

## Abstract

### Polymer Composites with Gradient of the Electrical Conductivity

*J.Aneli<sup>1</sup>, L. Nadareishvili<sup>2</sup>, G.Basilaia<sup>1</sup>*

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The character of the change of electrical conductivity of films based on poly-vinyl-alcohol filled with carbon black at their stretching along one selected direction has been investigated. The specific volumetric electrical conductance of the initial samples was changed in the interval 10-50 kOhm x sm.

The experiments were carried out on the films obtained on the basis of one and same polymer composite in view of rectangle and trapezium, the thickness of which was no more than 0.2 mm. These films were fixed by special clamps and placed to the furnace. After the films were stretched on 200-300% at temperatures 100-120°C with constant rate (50 sm/min). The stretching was fulfilled for rectangle sample along long side, and for trapezium both in parallel and perpendicular to bases side directions.

In result of the study of local resistances for the rectangle sample it was established that the maximal change of this parameter is fixed in the direction along symmetric axis parallel to the long side of the rectangle. This change has an extremal character (the maximum seems in the central region of the film). The form of this dependence has an view like to Gauss function. The amount of maximum of the local resistances is the higher the lower is concentration of conducting filler and the extent of stretching. Analogical character has the same dependence in the perpendicular to stretching direction, although the last is relatively weak to some extent.

In case of stretching of trapezium in direction parallel to bases the dependence of the value of local resistances on film geometry is more complex, although it is possible to establish the definite laws.

The following investigations were carried out on trapezium with the same form, but in this case to stretching the local resistance only near little base was underwent. In another words here was formed the mechanical field gradient in direction of perpendicular to bases. This gradient was increased from minimum at big base and finished at little one with maximum. It was established that if the form of clamps is linear, than the dependence of mechanical stress or strain on coordinate of the film has the hyperbolic view and, vice versa, if the form of clamps is hyperbolic, this dependence curve has a linear form.

The work results open the perspectives of their application to the creation of the films with desirable anisotropy of local resistances, which may be used in the electronics as the "printed schemes".

## **Abstract**

### **Experimental Investigation of Emitted Nanoclusters During Laser and Ion Beam Interaction with Solids**

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The bombardment of a solid with energetic ions or laser beam leads to emission of atomic species - the flux of sputtered particles, abundant fraction of agglomerates of two or more atoms, multi-atomic formation of so-called cluster –  $A_n^{0,+,-,*}$ , (where A – chemical element, n – the number of atoms in cluster, 0, +, -, \*, - a charge and excited state of cluster). In cluster sputtering “equilibrium” model, a highly energized region of the surface undergoes a “liquid-gas phase” – “plasma” transition upon expanding into vacuum.

Many of physical, chemical and other characteristics of clusters depend on number of atoms and construction types. For different values of n we can obtain metal, semiconductor, or dielectric nanoclusters and when the value of n is large, the environment is condensed. Except for the one-element, an emission of admixture clusters with active chemical elements takes place, investigation of which is quite interesting, especially from chemical, biological and medical viewpoint. Particular interest is attracted by carbon clusters – fullerenes, nanotubes and graphenes – as one of the cluster types with interesting features. As the number of atoms in the system increases, atomic clusters acquire more and more specific properties making them unique physical objects different from both single molecules and from the solid state. Both experimental and theoretical aspects of atomic cluster physics uniquely placed clusters between atomic and molecular physics on the one hand and solid state physics on the other. Metal clusters exhibit electronic level structures which often change completely when the number of atoms in the cluster, n, changes by just one unit. Today one of the topical questions is: what the minimal (nanometric) size of structures of the metallic, semiconducting, or dielectric clusters should be and very important to create materials known beforehand from separated atoms and clusters (Feynman’s prediction).

Investigations of emitted nanoclusters during laser and ion beam bombardment of surfaces are realized using secondary ion mass-spectrometry (SIMS) with energy analyzer, spectrography and optical methods. Under UHV ( $\sim 10^{-9}$  torr) conditions  $N^+$ ,  $O^+$ ,  $N_2^+$ ,  $O_2^+$ ,  $Ar^+$  primary ions with energy (0,5÷50) keV, ( $\mu A/cm^2$  -  $mA/cm^2$ ) intensities and (0-45) $^\circ$  incident angle bombardment of C, NaCl, Mg, Al, Si, S, Ti, GaAs surfaces, negative and positive cluster ions in (1 - 750 amu) mass range are measured using Finnigan - 750 mass-spectrometer. During experiment scanning of sample 5x5 mm<sup>2</sup> by laser and ions and oxygen covering condition is possible. Similarly to ions, under high intensity and power ( $10^8$  -  $10^{15}$  vt/sm<sup>2</sup>) laser interaction of solid surface, high temperature and density “liquid-gas phase” – “plasma” production takes place on near surfaces area and the high temperatures and pressures produced can cause emission of large fragments during the thermal phase.

Energy transferred to the surface is strongly directional and can lead to the simultaneous emission of a group of neighboring surface atoms, which in some cases will remain bounded and form a atomic cluster after emission. The yields of secondary  $Al^+$ ,  $Al_2^+$ ,  $Al_3^+$  and  $Al_4^+$  particles at bombarding of the Al by primary ions with energies  $E_0=5-50$  keV were measured. During de-excitation of excited states of  $Al_2^+$  and  $Al_3^+$  occur the fragmentation of clusters and thus the decrease of their number. Difference between the yields of  $Al_2^+$  and  $Al_3^+$  clusters is sensitive to whether atomic ( $N^+$ ,  $O^+$ ) or molecular ( $N_2^+$ ,  $O_2^+$ ) projectiles are used. The formation of the excited states, which leads to the fragmentation of the clusters  $Al_2^+$  and  $Al_3^+$  in the case of the bombardment with molecular ions is, apparently, more probable.

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## Abstract

### Toughening of Unsaturated Polyester with Core-Shell Rubber Particles

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Preformed core-shell rubber latex particles (CSR) with a soft poly(butyl acrylate), PBA, core and a rather rigid poly(vinyl acetate-co-methyl methacrylate), P(VAc-co-MMA), shell were used to toughen an unsaturated polyester (UP). The effect of shell composition, i.e. VAc/MMA ratio, on the toughening and volume shrinkage of the cured styrene/unsaturated polyester (ST/UP) has been investigated. The results showed that increasing the MMA units in the shell structure up to 50 wt% enhanced significantly the impact strength and fracture toughness of the cured UP/ST/CSR ternary system, whilst beyond this limit the impact and the fracture toughness decreased.

The dispersion of rubber latex particles was studied by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). As expected, increasing the MMA units in the particle shell composition from 0 to 100 wt% changed the dispersion state of the CSR inside the cured ST/UP matrix. In Fact, the increase of MMA units in the particle shell composition resulted in the agglomeration of the rubber particles as bigger rubber clusters in the matrix. This behavior can be attributed to the poor interfacial adhesion between the rubber particle and the matrix. However, the highest fracture toughness was obtained for the blend sample with a partial particles agglomeration. On the other hand, the presence of the rubber particles in the resin decreased the volume shrinkage on some extent.

## **Abstract**

### **Modern Conceptions on the Mechanism of Electrical Conductivity of Polymer Composites**

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During last decades the polymer composites contained the electrical conducting ingredients (metal powders, graphite, carbon black) attract a great attention of the specialists. These nontraditional conducting materials differ from traditional analogous with lightness, high elasticity, corrosion resistance, simplicity of producing technology, etc.

There are considered the existed models of the conductivity of electrically conducted polymer composites (ECPC). The results of the experimental researches of the electrical conducted properties of the polymer composites are compared with the data obtained by theoretical calculations. It is shown that it is no one model capable to explain satisfactorily the processes of charge transfer in various types of ECPC. This situation is due to the high heterogeneity of these materials and to various types and values of interactions between phases of ingredients in them. It is proposed the empiric formula, which describes the peculiarities of polymer composites conductivity with satisfy accuracy. The validity of the proposed model of conductivity of ECPC is tested with some experimental measures of these materials electrical conductivity. On the basis of fulfilled works it is proposed that at investigation of charge processes in ECPC it is necessary to foresee the conception about ratio of values of interactions between composite ingredients of three type: 1) macromolecule-macromolecule, 2) macromolecule – conducting filler particles, 3) between filler particles.

It is considered the dependence of the ECPC charge processes on the environment temperature. This dependence is due to superposition of two separate phenomena – increasing of the material resistance because of thermal widening and increasing of the average distance between conducting particles and decreasing of the resistance because of the increasing of the probability of charge energy. The application of the original experimental method allows to divide the effects of these phenomena. It is established that dependence of the conductivity of ECPC on the temperature may be described by N.Mott well known formulas, which are founded on the conductivity mechanism of the charge transfer by means of jump with variable jump length.

**2<sup>nd</sup> International Caucasian Symposium on Polymers and Advanced Materials  
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## Abstract

### Effect of Comonomer and Organoclay Contents on the Microcellular Structure and Elastomeric Properties of the PolyHIPE Solid Foams

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Highly open porous polyHIPE nanocomposite foams were synthesized by polymerizing water-in-oil high internal phase emulsions (HIPEs) that contain styrene (St), divinylbenzene (DVB), n-butyl acrylate (nBA) comonomer, and organo-modified montmorillonite (org-MMT). The effects of various amounts of nBA and organoclay on the microcellular structure and elastomeric properties of the prepared foams were investigated. The microstructure and characteristics of the nanocomposite foam materials were determined by X-ray diffraction (XRD), Scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Compressive mechanical tests were used to determine the young's modulus and compression set values of the resulting nanocomposite foams. Scanning electron microscopy (SEM) micrographs exhibited that the incorporation of higher levels of the hydrophilic comonomer and organoclay decrease significantly the mean void diameter and intercellular pore size in the resulting nanocomposite foams. The results showed that the use of higher levels of nBA comonomer and organoclay improve considerably the elastomeric behavior of the prepared foam. This behavior can be attributed to the elastomeric nature of the nBA units in the copolymer foam structure. X-ray diffraction (XRD) patterns and TEM micrographs showed an intercalated nanocomposite structure for all the reinforced elastomeric foams prepared.

## Abstract

### PANI/Silver Electropolymerization Nanocomposites: Properties and pH Sensitivity

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An attempt has been made to improve the pH dependence of the electrochemical activity of polyaniline (PANI), desirable for its potential application in sensors, biosensors, bio-fuel cell, and rechargeable batteries, by electrochemical copolymerization of aniline (ANI) with o-aminophenol (OAP), an aniline derivative having two oxidizable groups .i.e. Amino group and hydroxyl group. Copolymerization was carried out with different feed concentrations of OAP with a constant concentration of aniline in aqueous nitric acid solution. Similarly, the doping level can be controlled by varying the current and potential with time, synthesis and deposition of polymer can be realized simultaneously. It has been observed that some properties of PANI can be effectively improved and optimized through the polymerization of substituted monomers or post-treatment. The solution for the electrochemical polymerization of PANI/ OAP/ Ag consists of different concentration of nitric acid supporting electrolyte. This limits its applications to a certain extent. A possible way for solving this problem is to copolymerize aniline (ANI) with o-aminophenol (OAP) and Ag nanocomposite. The present paper reports preliminary results of aniline, o-aminophenol and Ag nano composite copolymers synthesized by electrochemical oxidative method. Few minutes after the reactants were mixed PANI started to precipitate. Voltammetry of poly (aniline-co-o-aminophenol /Ag nano-composite) film in 1M nitric acid solution of pH 9.6 was carried out between -0.20 and 0.62 and the scan rate was set at 6 mV/s. A surprising result was found, in which two anodic peaks and two broadly cathodic peaks appear on the cyclic voltammogram. This is another strong evidence that the copolymer has a good electrochemical activity in the solution of pH 9.6 at the slow scan rate.

## Abstract

### Oligomers Containing Fluorine Atoms Based on Epoxy Resins

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New oligomers with fluorine atoms have been synthesized via chemical modification of dianic epoxy resin with fluorine-containing alcohol-telomers C<sub>7</sub>, C<sub>9</sub> and C<sub>13</sub>, using benzyltriethylammonium chloride + KOH as a catalyst system. Toluene should be used as a reaction medium. Taking into account that quaternary ammonium salts are used for interphase transfer, benzyltriethylammonium chloride and potassium hydroxide were used as aqueous solutions (60 % solution of the salt and 40 % solution of KOH).

The conditions for the exchange of the half of epoxy groups for fluorine fragments in the initial dianic epoxy resin have been established. The synthesis of oligomers containing fluorine atoms and epoxy group was carried out at 343 K and reaction time 10-14 h.

The characteristics of synthesized products are represented in the Table.

Table

**Characteristics of the synthesized oligomers**

Fluorine-containing alcohol-telomer		Reaction time, h	Characteristics of oligomers			
Alcohol-telomer symbol	Amount (in moles) for 1 epoxy group of resin		Oligomer symbol	M <sub>n</sub>	e.n., %	Yield, %
FTS-C <sub>7</sub>	0.5	10	FEO-I	640	11.5	75
FTS-C <sub>7</sub>	0.5	14	FEO-II	820	8.8	84
FTS-C <sub>7</sub>	1.0	14	FEO-III	1270	2.8	85
FTS-C <sub>9</sub>	0.5	14	FEO-IV	880	7.2	82
FTS-C <sub>9</sub>	1.0	14	FEO-V	1750	3.8	83
FTS-C <sub>13</sub>	0.5	14	FEO-VI	1050	8.9	90

The structure of fluorine-containing oligomers was confirmed by IR-spectroscopy. The presence of fluorine atoms in the molecules of synthesized oligomers was determined by the absorption bands at 1212 and 1180 cm<sup>-1</sup>. The presence of epoxy group was confirmed by the adsorption band at 915 cm<sup>-1</sup>. It is proposed to use synthesized oligomers as additives to epoxy-oligoesteric mixtures in amount of 10–25 mas %.

## Abstract

### Reactive Oligomers Based on Dianic Epoxy Resins

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The expansion of polymers application area in the different branches of the industry, as well as the enhancement of demands to the operational characteristics of the goods on their basis, requires the development of new high-molecular compounds and improvement of existing properties.

The structure of the most polymeric systems is formed in the presence of compounds capable to be a source of free radicals under definite temperature conditions. This is, first of all, oligomeric compounds containing free peroxide or hydroperoxide groups.

This work deals with the obtaining of reactive oligomers containing peroxy groups on the basis of dianic epoxy resins. The effect of the nature of initial epoxy resin, hydroperoxide and a catalyst on the synthesis proceeding has been established. Inorganic bases, Lewis acids, ammonium quaternary salts and Crown-ethers were used as the catalysts. In order to improve the operational properties of the goods it is proposed to obtain the reactive oligomers containing fluorine atoms and epoxy group or fluorine atoms and peroxy group on the basis of dianic epoxy resins. The structure of synthesized oligomers was confirmed by the chemical and spectroscopic analyses. The possibility of such oligomers using as active additives to the epoxy-oligoesteric mixtures has been shown.

## Abstract

### New Fine Dispersion Zeolite with Clinoptilolite Structure

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Development of new methods for obtaining fine dispersion zeolites is rather urgent nowadays, since materials obtained by these methods are widely used in many technologies, measures of environment protection and various spheres of medicine, including therapy of malignant tumors [1].

Nano-size zeolite material was obtained by recrystallization of natural zeolite containing rock under hydrothermal conditions. The product obtained by this method represents particles of less than 100 nm. It is distinguished by high phase purity. Groupings of fractions of crystals of this size determine specific external surface activity of zeolites and affect the molecular-sieve, ion exchange, adsorption and catalytic properties.

The present work aimed to find the shortest way of recrystallization of phillipsite-containing rock into fine dispersion zeolite by the use of minimum number of reagents. According to the methodology developed by us the process of hydrothermal crystallization of preliminarily prepared aluminum silicate gel proceeded at lower temperature (98-100°C) and in shorter (20 hr) time in comparison with the existing methods [2]. Rentgeno-diffraction study identified the obtained crystalline material as fine dispersion zeolite, clinoptilolite. Its diffractogram fully complies with the data of literature [3]. Chemical analysis performed by the method of atomic-adsorption spectrophotometry showed that the compensating cation of aluminum silicate lattice of the zeolite is mainly Na. Sorption capacity of the sample (preliminarily burnt at 450 °C for 2 hr) to water and benzene vapor determined by the method of exsiccator, respectively equaled to 8,054 and 0,3 mmol/g (at 0,9 relative pressure).

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2. Tsitsishvili G.V., Krupennikova A.Yu., Maglaperidze A.I. Method of Obtaining of Li-zeolite. Author's Certificate, USSR 45 3907, 1972.
3. Breck D. Zeolite Molecular Sieves. Ed. "Mir", Moscow, 1976, 781p.

## Abstract

### **A study on the Crystallization and Thermal Conductivity of Zinc Oxide (ZnO) Nanoparticle Filled Polypropylene**

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Isotactic Polypropylene (PP) and zinc oxide (ZnO) nanocomposites were prepared by melt extrusion in a twin screw extruder. The influence of ZnO nanoparticles on the crystallization and thermal conductivity (TC) of PP was studied by thermal analysis (DSC) and thermal conductivity analysis (TCA). The introduction of CaCO<sub>3</sub> nanoparticles resulted in crystallinity percent addition. The incorporation of this nanoparticle (up to 15phr) had a significant effect on TC of PP especially in larger filler content. Some of models have been used for prediction of TC of nanocomposites. The experimental results had a good correlation with Ce Wen Nan model.



## Abstract

### New Antibiocorrosive Covers and Conservers Based on Bioactive d-Metal Complexes with Sterical Ligands

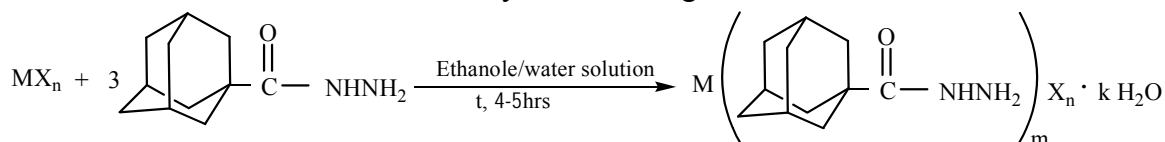
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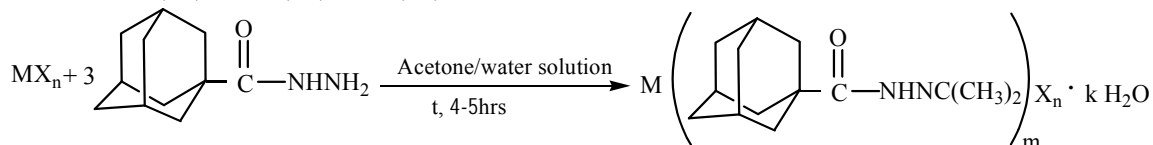
We synthesized adamantane-1-carbonic acid hydrazide and acetone-1-adamantoil hydrazide as organic ligands for obtained of coordinated compounds of d-metals.

By using of a semi-empirical quantum-chemical method of AM1 we calculated geometric parameters (valence angles and bond lengths) and effective charges on the atoms of initial adamantane-containing hidrazisde-hydrazone ligands (scheme). Quantum-chemical calculations were performed by using CS MOPAC (Chem3D Ultra-version 8.03, method AM1 – Austin Model 1).

The synthesis of coordinative compounds on the basis of adamantane-containing ligands and some d-metal salts was carried out by the following schemes:



where, M = Cu, Cd, Co, Ni, Zn; X = Cl<sup>-</sup>, SO<sub>4</sub><sup>2-</sup>, NO<sub>3</sub><sup>3-</sup>, CH<sub>3</sub>COO<sup>-</sup>;  
n = 1, 2; m = 2, 3; k = 0, 1, 2.



Where, M = Co, Ni; X = Cl<sup>-</sup>, SO<sub>4</sub><sup>2-</sup>, NO<sub>3</sub><sup>3-</sup>; n = 1, 2; m = 2, 3; k = 0, 1, 2.

The structure of obtained compounds was analyzed with infrared spectroscopy, thermogravimetric and differential-thermal analysis methods.

The analysis of the infrared absorption spectra of synthesized adamantane-containing ligands and complexes showed that molecule of organic ligand is coordinated with central atoms of metals by means of carbonyl group oxygen and NH<sub>2</sub> group of hydrazide cyclobidentantially, which agrees with the results of quantum-chemical calculations.

Thermogravimetric analysis showed that thermolysis of obtained complex compounds is a difficult process. After loss of water molecules a step-by-step separation of ligand molecules begins. The final result is an oxide or salt of respective d-metal.

The preliminary researches showed that the synthesized compounds have bactericide properties. They may be used against some phyto-pathogenic microorganisms. Synthesized complexes, dropped into the several functional polymer matrixes, may serve as a basis to prepare new bioactive materials and conservers with regular duration of the action.

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## Abstract

### Study of the Possibility of the Obtaining of Nanocomposites Based on Some Bioactive Nano-Phase Fillers

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From arsenic removal the stibium chloride has been synthesized.

The possibility of the obtaining new nano-fillers  $Sb_2O_3$  and stibium-containing complexes based on stibium alkoxides have been studied. The conditions of the obtaining of new fillers were investigated. The bioactivity of the synthesized complexes were studied.

Polymers targeted for creation of substrates for organic-inorganic nano-composites based on acryl and carbofunctional organocyclosiloxanes have been synthesized and studied. Not only classical methods of polymerization but also method of frontal polymerization for the formation of the final polymer nano-composites were investigated.

The preliminary researches showed that the prepared nano-phase fillers can be used for producing materials with biological activity such as antibiocoordination covers and conservators.

## Abstract

### Characteristics of Humic and Fulvic Acids Isolated From Surface Water Sediments

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Humic and fulvic acids (humic acids) are active participants of physicochemical processes in natural waters. Investigation of regularity of their spreading in hydrosphere is the actual matter of environment chemistry. We have detected humic acids in suspension compounds of Georgian fresh surface waters, in bottom sediments and (for the comparison) in the sediments of Indian Ocean.

The extraction of humic acids from sediments was performed with 0,1 M sodium pyrophosphate and sodium hydroxide solution. Concentrates were acidified to pH 2 for coagulation of humic acids. Then the solution was centrifuged to isolate fulvic acid from centrifugate the adsorption-chromatographic method was used. The charcoal was used as a sorbent.

In suspension compounds the concentration of fulvic acids is equal to 0,12-4,0% and is lines bigger than the concentration of humic acids: 0,03-0,07%. The bottom compounds contain less humic acids than suspension compounds, because they are more strict dispersion systems. The concentrations of humic and fulvic acids are correspondingly equal to 0,02-0,5% and 0,2-1,0%. The content of humic acids are 8 times larger than fulvic acids in bottom sediments.

On the bottom sediments of Indian Ocean the quantity of humic acids changes in the narrow range: 0,2-0,5 for humic acids and 0,2-0,8 % for fulvic acids.

The humic acids in turn are dominated by the high molecular weight fraction (>30 000). The elemental composition ranges of humic 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.

We have studied acid-base properties of humic and fulvic acids using potentiometric titration and chemisorption methods. It has been established that pK(COOH) is changed from 4,1 to 4,8 and pK(phen.OH) from 10,0 to 10,6. It is shown that the amount of carboxylic groups changes within 2,0-2,8 mg.ekv/g and that of phenolic hydroxyl groups within 1,9-3,8 mg.ekv/g.

## Abstract

### Investigation of Complexation of Heavy Metals with Fulvic Acids Isolated From Natural Waters

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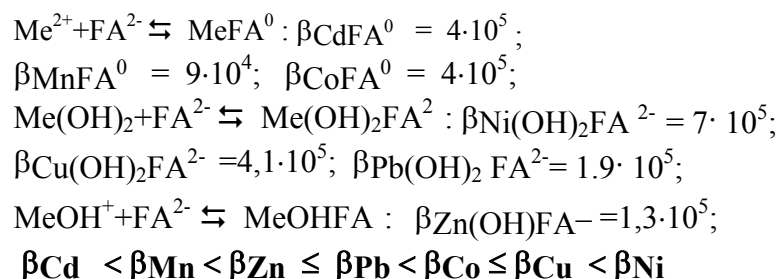
Fulvic acids (FA) take an active part in complexing and sorption processes proceeding in natural waters. The determination of their stability constants is one of the most relevant problems of contemporary analytical chemistry.

The complexation of copper(II), cadmium(II), nickel(II), cobalt(II), zinc(II), lead(II) and manganese(II) with fulvic acids isolated from Georgian surface waters was studied by the solubility method (pH=8,0).

Filtered water samples were acidified to pH 2 and enriched by freezing out. Concentrate was put for 2h on water bath at 60<sup>0</sup> C, for coagulation of humin acids. Then the solution was centrifuged. To isolate FA from centrifugate the adsorption- chromatographic method was used. Desorption of amino acids was performed by means of 0,1M HCl. For desorption of polyphenols the 90% acetone water solution was used. The elution of FA fraction was performed with 0,1M NaOH solution. The obtained alkalic solution of FA for the purification was passed through a cation-exchanger and dried under the vacuum until the constant mass was obtained. There is proposed the formula for calculation of the stability constants of fulvic complexes of heavy metals:

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

It was shown that is expedient to use the average molecular weight (1350) of the “initial associate” fulvic acids, the value of which does not depend on the value of pH. The mean value of the stability constants of the fulvic complexes are:



## Abstract

### Study of Humic Acids Isolated From Bottom Sediments Using $^1\text{H}$ Nuclear Magnetic Resonance Spectroscopic Method

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The  $^1\text{H}$  NMR spectra were obtained on the Varian Mercury Plus 400 spectrometer at 400MHz. In  $^1\text{H}$  NMR spectrum recorded in deuterated water (relaxation time 4 sec, duration of analysis 32 min 48 sec) two regions of chemical shifts are distinguished: 0-5 ppm and 7-9 ppm. In the first region the doublet characteristic for methyl protons joined to amino acetic group is clearly observed with the center at 1.27 ppm. Resonance signal at  $\delta=3.19$  ppm is characteristic for protons of methox group ( $\text{CH}_3\text{-OALK}$ ). Chemical shift at 4.05 ppm corresponds to ( $\text{H}_3\text{C-OCOR}$ ) of carbon acid methyl ether protons. In  $\delta=4.20\text{-}4.25$  ppm regions there appeared quart signal with the center at 4.23 ppm which is characteristic for methin proton of amino acetate group. In the range of chemical shift at 7.50-7.65 ppm there can be observed well expressed signals of aromatic protons corresponding of AA'BB' type 4d group. Wide resonance signals  $\delta=7.73\text{-}7.76$  are characteristic for proton amino groups. As the resonance signals at 7.95-7.99 ppm corresponds to phenolic protons.

In  $^1\text{H}$  NMR spectrum recorded in DMSO- $d_6$  the range of saturated protons is overlapped by signals of DMSO protons residue and adsorptive water. The only thing that can be discerned are signals characteristic for methyl group protons in the range  $\delta=1.12\text{-}1.24$  ppm with centers at 1.14 and 1.22. In the weak part of the field in the range  $\delta=7.56\text{-}7.70$  ppm absolutely symmetric resonance signals of aromatic protons are clearly observed. This group of signals belong to AA'BB' type 4d group of aromatic protons:  $\delta_A=7.64$  and  $\delta_B=7.56$  ppm,  $\nu_A\text{-}\nu_B=30\text{Hz}$ .

Three intensive signals in the range of  $\delta=6.94\text{-}7.20$  ppm with the center at 7.07 ppm can belong to three penta substituted protons of aromatic nuclear.

Thus in  $^1\text{H}$  NMR spectrum of HA recorded by us for the first time there has been fixed the existence of para di-substituting aromatic (AA'BB') and three penta-substituting aromatic fragment. On the basis of  $^1\text{H}$  NMR spectra obtained by us we can assume phenylalanine fragment as one of the probable complex forming site in humic acids molecule.

## Abstract

### Investigation of Humic Acids Isolated From Natural Waters by Thermal Analysis

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The aim of this work was to study the humic 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- $\text{Al}_2\text{O}_3$ , temperature range 20-800 °C. Differential thermal analysis (DTA), thermogravimetric (TG) and differential thermogravimetric (DTG) curves were recorded simultaneously.

The thermograms of both samples were characterized by one endothermic effect, which was mainly caused by dehydration of the humic acids. The effect was registered at 105 °C for HA isolated from the bottom sediments and at 110 °C in the case of HA isolated from the water sample. The loss of mass equals 4 and 8% respectively. Both in low (190-350 °C) and in high temperature range (350-650 °C) the thermograms of two samples are characterized by two exothermic effects (210, 330, 480, 630 and 200, 320, 530, 650 °C). Thus the loss of mass in the low temperature range makes 30 and 38% respectively, but in the high temperature range it equals 62 and 48%.

Exothermic 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 HA molecules accompanied by dehydrogenation and decarboxylation.

Exothermic 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 HA is possible by the value  $z=m/M$ , where  $m$  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 ratio, the more aromatized is the substance. The degree of aromatization of HA, isolated from the bottom is higher ( $z=0,48$ ), than that of HA isolated from the water sample ( $z=0,79$ ).



## Abstract

### Effect of Acidity of the Reaction Medium on Activity of Aromatic Amines in Maillard Reaction

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Melanoidine complex formed as a result of interaction between amines and reducing sugars consists not only from high-molecular products, but its part is a mix of compounds with rather low molecular weights. Aromatic amines actively participate in Maillard reaction with formation of corresponding melanoidines. Our experiments have shown, that from the point of view of dependence from pH of the reaction medium, aromatic amines (aniline, toluidines and aminophenols) participating in Maillard reaction, are similar to aliphatic amino acids - by increase of pH their reactivity increases. In addition, isomeric amines conform to the certain law. For example, at interaction of D-glucose with o-, m- and p-aminophenols in acid, neutral and alkaline mediums, the amount melanoidine formed is increased with increase of pH of reaction medium, and meta-isomer is always less active.

In this respect, in a case of amino benzoic acids opposite regularity is observed - their activity in Maillard reaction with increase of pH decreases, and reactivity of para-isomer is rather low.

The similar picture is observed at the control of reaction by amount of the not reacted amino acid, and by the formed hydroxymethylfurfural. As show the received data, interaction of amino benzoic acids and D-glucose submits to the certain rule. By increase of temperature the amount of the reacted amino acid increases. Thus, in acid, neutral and alkaline mediums m-amino benzoic acid reacts much more actively than p-isomer, and o-isomer in this respect occupies intermediate position. Presumably, such conformity is caused by various values of pKa of isomeric amino benzoic acids.

We investigated distribution of a melanoidine complex formed as a result of reaction of D-glucose with isomeric aromatic amino acids, between low-molecular (< 3500 dalton) and high-molecular (> 3500 dalton) fractions. In contrast to aliphatic amino acids, which react with glucose and form a melanoidine complex rather slowly, the amino benzoic acids and particularly m-amino benzoic acid, in this reaction participates much more actively, and forms a significant amount of melanoidine complex, insoluble in water and in buffer solutions. The reaction activity of p-amino benzoic acid is especially high in acid medium.

That fact, that reactivity of amino benzoic acids in Maillard reaction is reduced by reduction of pH of reaction medium, is the general regularity and proves to be true in case of all aldoses investigated by us. In comparison with aldohexoses, aldopentoses participate in melanoidine formation more actively. For example, aromatic amines including aminophenols, so vigorously react with aldopentoses (xylose, arabinose), that in the mentioned above reaction conditions a great bulk of melanoidine forms an insoluble product.

## Abstract

### The Effect of Deuterated Solvent Types in $^{13}\text{C}$ NMR Spectroscopy and Splitting of Polystyrene Para Aromatic Carbon

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Most of NMR spectroscopy on polystyrene are performed on its solution in  $\text{CDCl}_3$  which is a suitable deuterated solvent. To investigate the effect of solvent, deuterated benzene and tetrahydrofuran (THF) were also used and the spectra of polystyrene para carbon of benzene ring in these solvents were compared. There are three peak regions in  $\text{CDCl}_3$  at 20 °C while, in THF, syndiotactic region is almost separated and isotactic region overlaps with the atactic region. In  $\text{C}_6\text{D}_6$  both syndiotactic and isotactic regions overlap. Based on NMR theories, line width has direct relation with relaxation time of magnetic nuclei in accordance with Heisenberg's uncertainty principle. Short relaxation time cause high uncertainty which is seen as broad peaks in NMR and peak broadening causes overlapping, the fact which is seen during the investigation of polymer stereoregularity. Therefore, by increasing the relaxation time of each sequence which in turn decreases the uncertainty, narrower peaks can be produced and overlapped peaks separate from each other leaving isolated peaks. Type of solvent can have an impact on relaxation time through a complex behavior, the viscosity of solvent, solution and solubility parameters can be effective as well.  $\text{C}_6\text{D}_6$  and hence its polystyrene solution have higher viscosity while all used solvents have almost similar solubility parameter. Therefore, higher  $\text{C}_6\text{D}_6$  viscosity causes lower relaxation time and thus broader peaks, and higher overlapping are produced. Syndiotactic sequences of para carbon in THF and isotactic sequences in  $\text{CDCl}_3$  show better resolution. As a result, motions of racemic rich segments in THF- $d_8$  are higher than those of meso and conversely the mobility of racemic rich segments in  $\text{CDCl}_3$  is lower than that of meso rich segments. In summary, in THF upfield regions and in  $\text{CDCl}_3$  downfield regions show better splitting.

## Abstract

### PET Films Modified by Functional Carbon Nanomaterials

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Composite materials were obtained by *in situ* polycondensation in molten state (i.e. during the synthesis of PET). The process conditions were determined experimentally depending on the matrix type. The presence of CNM (regardless of modification or concentration) in a reactive mixture had no influence on the chemical reactions during synthesis what confirms a usability of the *in situ* method to polymer nanocomposites preparation. CNM were obtained from methane-air mixture upon atmospheric pressure without catalyst on high voltage atmospheric pressure discharge set-up. CNM specimens were studied by scanning (SEM) and transmission (TEM) electronic microscopy. According to SEM and TEM data CNM diameters are within 12-60 nm. PET - based polymer composites containing different kinds of CNM (unmodified and functionalized with -F, -COOH, -NH<sub>2</sub>, -C<sub>2</sub>H<sub>5</sub>, -Fe(C<sub>5</sub>H<sub>6</sub>)<sub>2</sub>, -CH<sub>2</sub>)<sub>15</sub>CH<sub>3</sub> groups) were characterized by following techniques: SEM, DSC, DETA and mechanical tests. The results of dielectric properties measurements of PET films with CNT added in a various ratios are presented. Changes of capacitance and dielectric losses were measured in a frequency range 102-104 Hz at 300 K. Influence of type and amount of CNT in samples on dielectric properties was studied. Capacitance increase from 10 to 20% is observed even for minimal CNT amount (0,05 wt. %). Dielectric losses coefficient is decreased while CNT content increases. Approximation of dielectric spectrum with Havrilak-Negami equation allowed estimating changes of time constants of  $\beta$ -relaxation process.

This work was supported by INTAS - grant N 04-80-6932 "Polymer nanocomposites with the addition of functionalized carbon nanotubes".

## Abstract

### The Coatings on Polyamide Composition Containing Carbon Nanotubes

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Carbon nanotubes (CNT) possess exclusive physical and chemical properties that demonstrate significant potentialities for application in various fields of technology. The results of research of the coatings based on polyamide (PA) containing CNT are presented. Synthesis of multi-walls CNT in high voltage atmospheric pressure discharge plasma are presented. CNT specimens were studied by scanning (SEM) and transmission (TEM) electron microscope.

Utilization of PA 6 powder made by chemical precipitation from solution in  $\epsilon$ -caprolactam is more preferable than utilization of powder made by low temperature mechanical grinding. The coatings containing 0.01, 0.02, 0.05 and 0.1 wt.% of CNT were used in experiments. Polymeric films 200-300  $\mu\text{m}$  thickness was fabricated. The introduction of CNT in PA 6 via suspension in methylenechloride results in solvent evaporation and precipitation during drying process. During the film formation CNT are comparatively evenly distributed in the volume of the melt and alongside with own fetuses of polymer structure. It leads to the formation of the films with higher level of permolecular organization.

Coating were characterized by adhesion and hardness increase on  $\sim 50\%$  and toughness increase on  $\sim 30\%$ .

It is seen that maximum increase of strength characteristics of films are obtained for films with CNT concentration of 0.02-0.05 wt.%.

## Abstract

### Synthesis, Characterization and Electrical Properties of Poly(azoaminophenilenes)

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An efficient synthesis of high molecular weight and processible polymers under mild conditions via diazotation and azocoupling of *m*- and *p*-phenylenediamine with *m*-phenylenediamine with different ratio of amine/sodium nitrite, were demonstrated. The resulting polymers were characterized by <sup>1</sup>H-nuclear magnetic resonance, UV-vis, EPR, Fourier transform infrared spectroscopies and electrical conductivity measurements.

<sup>1</sup>H-NMR spectra support the proposed structure composed a sequence of aminophenylene and phenylene moieties linked together by N=N- bridges in *m*-, *o*- and *p*- positions and the presence of dihydrobenztriazolic units, when diazonium salt of *p*-phenylenediamine was azo-coupled with *m*-phenylenediamine. The solubility tests carried out in solvents such as DMF, DMSO, alcohol, and intrinsic viscosity measurements showed that the lower the sodium nitrite molar content, the higher is the solubility, and lower the molecular weight of poly-azoaminophenylene.

The conductivities of obtained polymers doped with the dopants such as iodine, perchloric acid and hydrochloric acid were investigated as a function of the dopant content.

The iodine- and perchloric acid-doped polymers attained a conductivity of 0.2 Sm/m,  $7.10^{-3}$  Sm/m, correspondingly. Polymers reveal stability towards hydrochloric acid doping. According to electron spin resonance spectroscopy data, the conductivity increase was attributed to the charge carrier (polaron) mobility.

## Abstract

### On the Structure of Poly(*p*-phenylenediamine)

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Some aspects of the chemical oxidative polymerization of *p*-phenylenediamine with potassium peroxydisulfate in a protic acid medium are discussed. It has been established that ammonia is eliminated during the reaction and that the polymer obtained has the polyaniline structure known as pernigraniline as opposed to the polyquinoxaline form. Based on literature reports and our own experimental data, a new scheme for this polymerization is proposed.



## Abstract

### Effect of the Shell on Reactivity of Core/Shell Structured Nanoparticles

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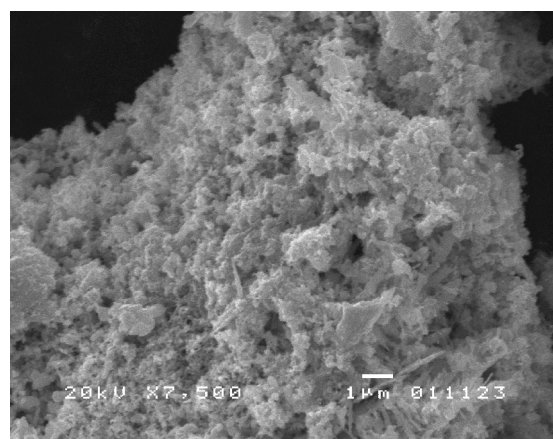
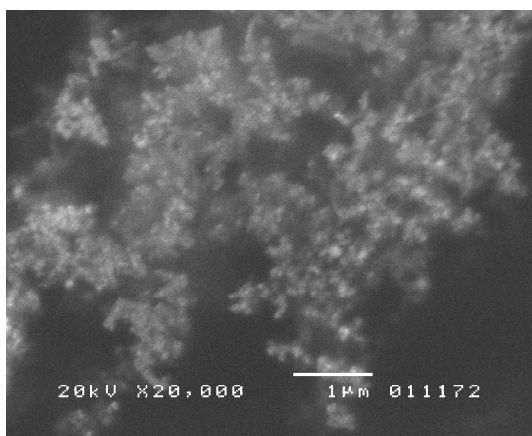
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A dramatic increase in surface to volume ratio of Nanoparticles (NPs) offer a host of unique properties which determine practical and potential use of NPs for biomedical application, in advanced electronic, magnetic and optical devices, energy storage and conversion systems etc. Specific effects displayed by NPs to a great extent originated from the excess of chemical energy of the surface atoms at the interfaces with media. However unbalanced forces are also sources of interactions of NPs with each other and surrounding molecules accompanied by a loss of stability and reactivity of NPs as a result of aggregation and corrosion.

Core/shell structured nanomaterials are characterized by improved chemical and thermal stabilities, are less cytotoxic and possess ability to be embedded in a matrix materials or coatings. Further progress in the development of such “smart” materials to a great extent is determined by knowledge of the nature and structure of shell material and its role in interactions of NPs with chemical and biological media. However only limited information is available on a nature of core/shell interaction on the effect on reactivity of nanoparticles.

According to FTIR spectroscopy data in metal (core) – oleic acid (shell) system molecules of oleic acid are anchored at the core surface by polar carboxylic groups. Kinetics of desorption of shell material and its effect on the apparent and true surface areas testifies significant contribution to adsorption process of micropores formed at aggregated NPs. Effect of structure transformations on antibacterial properties of silver NPs and catalytic activity of nickel NPs were evaluated.

SEM Images of Silver NPs Before and After Desorption of the Oleic Acid



## Abstract

### **Diatomite-containing Thermoreactive (Novolac type) Polymer Compositions**

*N. Gelashvili, G. Papava, Z. Molodinashvili, N. Maisuradze, N. Dokhturishvili,  
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Phenol formaldehyde polymers are widely used in practice in many fields as construction materials: in electrical engineering, machine building, manufacture of everyday designation articles and others.

We were the first who obtained phenol formaldehyde Novolak type oligomers in melts. Composites were obtained by thermal treatment of polymer compositions obtained on their base (hardener - hexamethylene tetramine, filler - natural non-modified diatomite).

The effect of diatomite content on the composite properties was studied. It was proved that high percent content of diatomite (up to 80%) conditions their high heat resistance (350 °C).

Heat resistance of the obtained polymers was studied in dynamic conditions (rate of heating on the air – 4,5 °C/min). It was shown that for the polymers hardened in similar conditions (by 15 mass % hexamethylene tetramine) with the increase of the content of diatomite, the polymer destruction temperature is decreased. This is explained by the fact that increase of diatomite content in the composition impedes close location of polymer molecules, that is, the structure becomes more loose, which makes easier for oxygen to penetrate into polymer and facilitates oxidation processes.

Highly filled polymer compositions were obtained, which contain 30-80 mass % natural diatomite. Various form articles were prepared on their base by compression pressing at 200°C and at 0,7-0,8 MPa pressure.

Physical-mechanical and dielectric properties of the obtained polymer compositions were investigated. It was proved that the composite is of optimal composition when the diatomite content equals to 40-60 mass %. Articles, which were made on the base of such polymer compositions, in some cases are characterized by better indices than the analogous designation phenoplasts known today in industry. It should be stated that the phenoplast that contains diatomite is fire-resistant, refractory; it is neither burnt nor melted.

As is shown by the investigations the costly, deficient organic fillers in polymer compositions can be replaced by cheap and easily accessible local natural mineral material.

## Abstract

### Study of the Effect of Chemical Structure of Bisphenol on Physical Properties of Polymers

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The dependence of properties on the regulation rate of structure of polyarylates obtained on the base of terephthalic acid and the below listed polycyclic Bisphenols was investigated: 4,4'-(2-norbornylidene)diphenol (Bisphenol-1), 4,4'-(hexahydro-4,7-methylenindane) diphenol (Bisphenol-2) and 4,4'(decahydro-1,4-5,8-dimethylenaphth-2-ylidene)diphenol (Bisphenol-3). Structures of polyarylates were evaluated according to the data of roentgeno-structural analysis as well as according to their softening temperature and solubility in organic solvents.

Polyarylate of Bisphenol-1 and terephthalic acid is characterized by partially ordered structure, while polyarylates of Bisphenols 2,3 and terephthalic acid - are characterized by amorphous structure.

Dependence of the rate of regulation of structure of polyarylate made on the base of Bisphenol-1 and terephthalic acid on the method and conditions of synthesis as well as on the treatment of a polymer – was investigated.

The polymer of the most regulated structure was obtained by polycondensation reaction carried out at 220°C in sovol, ditolylmethane and  $\alpha$ -chlornaphthaline. Its amorphous form was obtained at rapid heating of Bisphenol and terephthalic acid chloranhydride in sovol at 320 °C, by further rapid cooling (duration 15-29 min) of reaction mass to room temperature. At low-temperature polycondensation the amorphous polymer was obtained.

Crystalline polyarylate, after re-precipitation from the solution in tetrachloroethane to sulfuric ether acquires amorphous structure. Regulation takes place at thermal treatment of amorphous polyarylate in various high-boiling organic solvents (at 220°C).

Crystalline polyarylate is characterized by softening temperature 360-385°C and is dissolved only in tetrachlorethane and tricresol. Amorphous sample is characterized by softening temperature 310-340°C and is dissolved in wide specter of solvents.

On the base of the above stated we can state that polyarylate of Bisphenol-1 and terephthalic acid tends to crystallization. This is interesting because polycyclic grouping of Bisphenol is neither co-planar nor symmetric, which does not make obstacles to the formation of polymer of the regulated structure on its base.

The above-referred methods of regulation of physical structure, significantly facilitates the problem of treatment of heat resistant, ordered polymers. Preparation of polymers on the base of polycyclic Bisphenols with regulated structure enables us to realize to the higher extent their precious properties, namely, to increase their heat resistance.

## Abstract

### Mathematical Modeling of Optimal Conditions for Treatment of Polymer Compositions

*N. Dokhturishvili, G. Papava, Z. Tabukashvili, N. Gelashvili, N. Maisuradze, Z. Molodinashvili*  
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Thermoreactive, that is, heat-convertible polymer compositions were obtained on the base of resol type phenol formaldehyde oligomers and natural mineral material.

Diatomite content in the compositions was varied from 30 to 80 mass %. Treatment of compositions was performed by compression, by heating. For the treatment of polymer compositions it is necessary to determine the optimal values of the main technological parameters (temperature, pressure, time) in order to realize at maximum the properties of plastic material in the process of treatment, in particular, to realize the advantages inherent to diatomite-containing plastic materials, high heat- and thermal resistance, physical-mechanical and dielectric properties.

Determination of optimal conditions for treatment of polymer compositions is available by the use of factor experiment, by the method of the least quadrants. The specific shock viscosity and the breaking stress at bending were selected as the decisive parameters for treatment of compositions. Optimization is determined according to three factors: temperature, pressure and time duration, which are used at four levels: temperature – 160, 170, 180, 190° C; pressure – 40, 60, 80, 100 MPa; time - 4, 6, 8, 10 minutes. Each factor is varied at four levels. Processing of the results covers summing up of the obtained parameters for each separate factor, for every level. Maximal value of the sum enables us to reveal the most significant factor. Factor analysis covers summing up of the data of separate factors at all levels, which enables us to fix the decisive factor and optimal level for the investigated index.

Table

#	Factors	Specific shock viscosity, kJ/m <sup>2</sup>	Breaking stress at bending, MPa
1	Temperature, °C		
	160	22,5	267,0
	170	20,3	291,3
	180	27,0	325,4
	190	21,7	297,6
2	Time, min		
	4	23,1	293,8
	6	20,3	286,3
	8	22,3	311,1
	10	25,8	290,1
3	Specific pressure MPa		
	40	22,3	307,2
	60	28,8	344,4
	80	23,1	257,5
	100	17,3	272,2

As it is seen from the data given in the Table the specific pressure exerts significant influence on the shock viscosity in the process of treatment. Similarly, temperature affects the properties of plastic material. A sample treated at 180 ° C is characterized by high viscosity.

Optimal parameters were determined as a result of the carried out experiments: temperature – 180 ° C, pressure – 60 MPa, hold-up time – 4 min (per 1 mm thickness of an article).

**2<sup>nd</sup> International Caucasian Symposium on Polymers and Advanced Materials**  
**Tbilisi, Georgia 7-10 September, 2010**

## Abstract

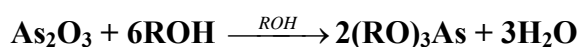
### About a New Method of Extraction of Arsenic-Containing Compounds From Wastes

*G. Chachava, M. Gverdtsiteli, N. Gigauri, M. Rusia, I. Laperashvili*

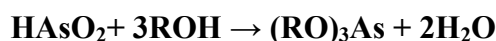
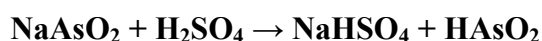
Iv. Javakhishvili Tbilisi State University,

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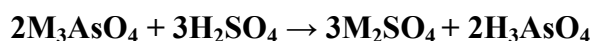
New method of extraction of arsenic-containing compounds from pyrometallurgic wastes was elaborated. The initial material was the waste of gold-production, which was brought in mining-chemical plant of Racha from the Urals („Ural-zoloto”). The average content of arsenic in this waste is 51-65% amyl-, isoamyl- and hexyl-alcohols were used as extragents. As a result of the interaction of these alcohols with arsenous anhydride the ethers of arsenous acids are formed:



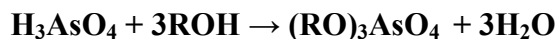
Trialkylarsenites are formed from arsenous acid – as a result of interaction of sulfuric acid and arsenites (III) of metals:



The arsenates (V) of metals are transformed in ethers of arsenic acid:



Where: M is alkali metal.



Water is isolated by azeotropic drying.

After the extraction of arsenic-containing compounds from raffinads, the content of gold in reminder is equal to 6,90 - 7,12 g/ton. So, they can be used for obtaining this noble metal.

The preparation of epoxy-compositions of different type becomes very important in modern electrotechnics. For decreasing the combustibility of polymers antipyrene are inculcated in them. Nowadays the problem of using arsenic-containing alcohol extracts as antipyrene is intensively studied. The covering of this system on epoxy resin makes it fire-proof and firm.

Thus the perspective of reuse of the wastes and obtaining on their basis of arsenic and gold is contemplated.

## Abstract

### Polyamidoarylates on the Base of Polycyclic Bisphenols

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Polyamidoarylates are polyamidoethers obtained on the base of polycondensation of bisphenols, chloranhydrides of dicarbon acids and various diamines. These compounds are characterized by complex properties, which, to a certain extent, are inherent to corresponding polyamides and polyarylates. Variation of these properties is mainly performed by means of alteration of diamine - bisphenol molecular ratio.

Polyamidoarylate properties are substantially conditioned by substituting groups of bisphenol molecule located at the central atom.

The present paper deals with the synthesis and study of such polyamidoarylates, which at the central carbon atom of bisphenol molecule has norbornane type groups in the form of substituting agents.

We were the first to synthesize polyamidoarylates on the base of norbornane type polycyclic bisphenols and to use the low temperature polycondensation method to obtain polyamidoarylates. Some regularities of formation of polyamidoarylates were determined on the example of polycondensation of sebacic acid chloranhydride, 4,4'-(hexahydro-4-7-methyleneindan-5-yliden)-diphenol and hexamethylenediamine. Effect of the factors such as temperature, solvent and tertiary amine nature, reaction duration as well as the effect of ratio of initial components on the process of polycondensation - were studied.

We have obtained also the polyamidoarylates on the base of chloranhydrides of sebacic and terephthalic acids and hexamethylamine with other polycyclic bisphenols with norbornane type card groupings. With this in view, we used 4,4'-(2-norbornyliden)diphenol and 4,4'-(decahydro-1,4,5,8-dimthylenenaphth-2-yliden)diphenol. Synthesis was performed by the method of acceptor-catalytic polycondensation.

A series of new polyamidoarylates on the base of polycyclic bisphenols, which have not been described yet in special literature, have been obtained by us and their properties have been studied.

## Abstract

### Protection of Environment from Pollution due to Nitrogenous Fertilizers

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Intense growth of population demands elevation of production of foodstuff. This is available by means of expansion of lands of agricultural designation, which is limited today because of drastic decrease of such lands thanks to urbanization and industrial progress.

Another way out from this situation is application of intensive technologies. It means sharp increase of fertilizers fixed by agrotechnical norms per unit territory, especially those of nitrogenous fertilizers.

It is known that currently more than 200 mln ton nitrogenous fertilizers are introduced into soil annually in the world. Due to the fact that all of these fertilizers (mainly ammonium nitrate and carbamide) are well soluble in water, at least 50% of these fertilizers are washed out to the soil by ground waters and rain. This results in global pollution of environment (rivers, lakes, seas, water reservoirs, ground waters). As a result of evaporation, nitrogenous fertilizers reach high strata of atmosphere and result in destruction of ozone layer. All these factors, alongside with great economic loss, create extremely dangerous ecological threat to the population and animal world since they contribute to the progress of very dangerous diseases (leukemia and others).

To prevent this problem we have developed a radically differing new type "exchange fertilizers". Principle of action of such fertilizers drastically differs from that of common fertilizers, such as superphosphate, ammonium nitrate, potassium sulfate et al.

Exchange fertilizers consist of not readily soluble components, which are isolated as plant nutrients and are assimilated by plants according to requirement, as a result of buffer effect of chemical reactions going on in soil.

Carbamide is distinguished by high content of nitrogen compared with other nitrogen-containing fertilizers. By its structuring we can obtain not readily soluble nitrogenous fertilizer. Carbamide structuring is performed in melt. As a result of heating aldehyde component suffers intense depolymerization. Created aldehyde instantly interacts with carbamide.

Solubility of the structured carbamide is controlled according to structuring rate, and its regulation is possible by variation of molar ratio of the starting aldehyde component and carbamide. Nitrogen content in the system might be increased up to 20-25%.

The new type nitrogenous fertilizer – structured carbamide, is characterized by advantage over non-structured carbamide, since it is no more washed out into soil and is far more efficient. Since it is not-readily soluble, we can give it dragee form with grain seed (wheat, barley, ray, and triticale) or without it. It does not form concentrated solution around the seed and does not injure the seed.

Dragee is made by special technology. Dragee provides for dosed delivery of nutrients to plants in vegetation period and impedes pollution of environment with nitrogenous fertilizers.



## Abstract

### Development of Neutron Absorbing Composite Polymer Materials and Results of Investigations

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Currently enormous number of radioactive sources of irradiation has been accumulated in the whole world including those of neutron radiation. Therefore great attention is paid to the creation of new constructional barrier materials possessing elevated radiation resistance, mechanical strength and other specific properties.

The possibility of creation of inflexible materials on the base of bisphenol-formaldehyde oligomer of resol type, on the base of 2,2-bis(4-oxypyphenyl) adamantane and formaldehyde - has been considered and the results of their testing - have been offered. Thermally modified diatomite and boron carbide were used as other main composition components.

Simultaneous presence of diatomite and boron-containing components in the polymer composition enables us to resolve some tasks simultaneously: improvement of mechanical indices of the compositions, weakening of neutron current and sorption of helium that is isolated at trapping of neutrons by boron according to reaction  $^{10}\text{B}(n,\alpha)\text{Li}$ .

Thermal modification of diatomite was carried out on the air at 450°C temperature for 4 hrs. At such conditions, alongside with the removal of adsorbed water, we observe burning out of organic compounds and increase of quantity, and correspondingly, total volume of pores ( $V=0,7 - 2,4 \text{ cm}^3/\text{g}$ ).

Experiments were carried out to develop polymer compositions containing diatomite within the limits 5-30 mass % and boron carbide -30-60 mass %. On the base of these compositions, by means of compression pressing, samples of cylindrical and rectangular form were obtained and studied. According to the obtained data introduction of diatomite and boron carbide in polymer composition improves fluidity and strengthening characteristics of the material.

Experiments were carried out at room temperature in the current of thermal neutrons  $2 \cdot 10^6 \text{ n/cm}^2 \cdot \text{sec}$  for 1 hour. Samples of optimal composition show 40-fold weakening of neutron radiation at 4 cm thickness, without changes in their mechanical and electric properties.



## Abstract

### **Metallocomplex Catalysis in Selective Alkylarenes Oxidations to Hydroperoxides. Design of New Effective Ni (Fe) – Catalytic Systems. The Important Role of H-Bonds in the Mechanism of Catalysis**

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A problem of the reduction of activity of homogeneous metal complex catalysts in the course of hydrocarbon oxidation with dioxygen is one of central problems of catalysis, because operation of a catalyst is always accompanied by processes of its deactivation. In connection with this, the increase in the stability of catalysts by their modification becomes the important problem.

One of ways of activating a homogeneous metal complex catalyst is the introduction of modifying ligands. As a rule, the mechanisms of action of the modifying ligands (which are mainly used in biomimetic systems) are not proved, although different explanations of mechanisms were proposed.

Selective oxidation of alkylarenes to the corresponding hydroperoxides, the primary products of alkylarene oxidation, is among the most difficult problems of catalysis, because the majority of the known catalysts are active in ROOH decomposition. The development of efficient catalysts of hydrocarbon oxidation to hydroperoxides attracts keen interest in the context of using hydroperoxides in large-scale production of monomers – propylene oxide and styrene ( $\alpha$ -phenylethylhydroperoxide, PEH), and also phenol and acetone (cumyl hydroperoxide) (the world productions are  $\sim 10^6$  ton / year). We proposed for the first time a method of modifying homogeneous catalysts, complexes of transition metals  $ML_n^1$  [ $M = Ni$ :  $L^1 = acac, enamac$ ;  $M = Fe(II,III)$ :  $L^1 = acac$ ], with electron-donating mono- or polydentate exo ligands-modifiers  $L^2$  ( $L^2 = DMF, HMPA, R_4NX, 18C6$ ) aimed at enhancing the selectivity of liquid-phase oxidation of alkylarenes (ethylbenzene and cumene) to the corresponding hydroperoxides [1]. It has been established that introduction in reaction of ligands-modifiers promotes formation of active forms of the catalyst and hinders or prevents processes, its leading deactivations.

Based on the established mechanisms of formation of catalytically active species and their operation, efficient catalytic systems  $\{ML_n^1 + L^2\}$ , ( $M=Ni$ ,  $L^2$  are crown ethers or quaternary ammonium salts) for ethylbenzene oxidation to  $\alpha$ -phenylethylhydroperoxide were modeled [2]. On parameters selectivity ( $S_{PEH})_{max}$  (95-98%), conversion (20%), and yield of PEH these systems considerably surpass known homogeneous and heterogeneous catalysts of ethylbenzene oxidation to PEH. The high activity of the simulated systems  $\{ML_n^1 + L^2\}$  is associated with the fact that during the ethylbenzene oxidation, the active primary  $(M^II L^1)_x(L^2)_y$  complexes and active heteroligand  $M^II_x L^1_y (L^1_{ox})_z (L^2)_n$  complexes (intermediate products of oxygenation of  $(M^II L^1)_2$ , initiated with coordination of exo ligand  $L^2$ ), are formed to be involved in the oxidation process. The stability of heteroligand  $M^II_x L^1_y (L^1_{ox})_z (L^2)_n$  complexes can be associated with the formation of inter- and intramolecular H-bonds [2]. Studying the effect of addition of small amounts of water to catalytic systems  $\{ML_n^1 + L^2\}$  confirmed the important role of H-bonds in the formation of catalytic species. The introduction of small portions of water ( $\sim 10^{-3}$  mol/l) to catalytic systems based on iron complexes leads to the higher catalytic activity of these systems. (The increase in the initial rate ( $L^2=Me_4NBr$ ), the growth of  $(S_{PEH})_{max}$  (from 65 to 78%) ( $L^2=CTAB$ ). The increase in the initial rate and high selectivity on acetophenone  $S_{R=O} = 70\%$  ( $L^2=18C6$ )) [2]. The activity of Ni, Fe catalysts in micro steps of chain initiation, ( $O_2$  activation), and propagation, at participation of catalyst, ( $Ct + RO_2 \cdot \rightarrow$ ), is assessed for the first time by an original method offered by the authors [1, 2].

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## Abstract

### Thermal Degradation and Combustion Behavior of Polypropylene/ Multi-Walled Carbon Nanotube Composites

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Studies of thermal and fire-resistant properties of the polypropylene/multi-walled carbon nanotube composites (PP/MWCNT) prepared by means of melt intercalation are discussed. The sets of the data acquired with the aid of non-isothermal TG experiments have been treated by the model kinetic analysis. The thermal-oxidative degradation behavior of PP/MWCNT and stabilizing effect caused by addition of MWCNT has been investigated by means of TGA and EPR spectroscopy.

The results of cone calorimetric tests lead to the conclusion that char formation plays a key role in the mechanism of flame retardation for nanocomposites. This could be explained by the specific antioxidant properties and high thermal conductivity of MWCNT which determine high-performance carbonization during thermal degradation process.

Comparative analysis of the flammability characteristics for PP-clay/MWCNT nanocomposites was provided in order to emphasize the specific behavior of the nanocomposites under high-temperature tests.

## Abstract

### The Degradation Heterochain Polymers in the Presence of Phosphorus Stabilizers

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The thermal stability and thermal stabilization of the heterochain polymers were investigated. Analysis of PAI, PSF, PEI degradation and stabilization has allowed an approach to be developed to aid their processing and resolve similar problems with other resins such as polyethersulfone, LCP, etc. Addition of PCA inhibits in heterochain polymers thermal oxidation at high and low temperatures.

## Abstract

### Kinetics for the Chemistry, Biology, Medicine and Agriculture

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Kinetics is powerful and fine instrument in investigations of chemical, biochemical and biological processes, as well as in medicine, agriculture, etc.

This report will present examples how kinetics helps in solving many fundamental and applied tasks due to Research – Development- Production principle (according to data of Institutes of Chemical Physics and Biochemical Physics, Russian Academy of Sciences).

#### Chemistry

1. Making of artificial diamonds from compounds having no carbon;
2. Development of highly sensitive methods of investigation of chemical reactions (chemiluminescence) and analysis of reaction products (for example, determination of a one double bond in a carbochain polymer and its location against 50000 single bonds).
3. Multitonnage chemical production design.

#### Biology – Medicine

1. Cancer and antitumor preparations.
2. Radiation damage (Chernobyl nuclear power plant).
3. Gerontology (how we can live longer).
4. Stress.

#### Agriculture

1. Effect of superfine doses (plant growth regulators – pesticides and their efficiency).
2. Toxicity threshold for chemical compounds.

## Abstract

### Hybrid Silica -Polymer Sorbents for Liquid Chromatography

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Problems of the modification of the surface of micro-spherical silica gel with layers of polymer and the influence of the quantity of the coated polymer on the chromatographic properties of the resulting sorbents have been considered. The polymer modification of the surface of wide-pore micro-spherical silica gel obtained by means of hydrothermal treatment of the meso-porous silica gel under autoclave conditions is described. The polymer layer itself is formed by an octadecylmethacrylate-methylmethacrylate co-polymer. As a result, packings for reversed-phase high-performance liquid chromatography (RP-HPLC) were obtained.

The development of new methods for the synthesis of packing materials for chromatography with the goal of improving its structure and its chromatographic parameters always was and remains significant to the present day. Most often, researchers turn to the different means of modification of the surface of already existing chromatographic systems.

Modern bio-chromatography demands highly sophisticated packings in terms of biocompatibility, selectivity and recovery. Polymers can be designed in a wide variety of properties and therefore deliver solutions to specific chromatographic problems. Thus tailor-made polymer coatings are an alternative to the classical bonded stationary phases. Polymer modification is one of the methods for the elimination of the disadvantages of silica packings (narrow working pH range and "silanol" interactions).

The possibility of varying the pore characteristics of packing materials by means of polymer coatings can be regarded as an important peculiarity of this technique. It is impossible to change the pore characteristics of the initial porous material by classical modification methods ( $C_8$ ,  $C_{18}$ , bonding etc.) since the quantity of the grafted phase is dictated by the properties of the sorbent itself (first of all by its specific surface area).

The influence of the modification on the pore structure and the chromatographic properties of the obtained systems is very important in the modification of porous systems with various modifiers, particularly with polymers. The knowledge of the character of these changes will help to select a suitable initial porous material.

## Abstract

### **Biocompatibility Evaluation of Chitin Based Polyurethane Bio-nanocomposites**

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Chitin based polyurethane bio-nanocomposites (PUBNC) were prepared by emulsion polymerization using poly ( $\epsilon$ -caprolactone) (PCL), 4,4'-diphenylmethane diisocyanate (MDI), chitin, 1,4-butane diol (BDO), dimethyl propanoic acid (DMP) and tri-ethanol amines (TEA) and bentonite nanoclay. A mixture of polymer and bentonite clay enriched in montmorillonite (MMT) was formed, in which MMT dispersed differently depending on interaction of MMT with polymer chains. The bio-nanocomposites (PUBNC) was formulated varying the contents of diisocyanates and mass ratios of chitin and 1,4-butane diol (BDO). Molecular characterization was done using FTIR,  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR techniques. The mechanical properties of these bio-nanocomposites (PUBNC) were improved with increase in the bentonite nanoclay and chitin contents. Cytotoxicity of the synthesized bio-nanocomposites (PUBNC) samples was affected by varying the bentonite nano clay and chitin contents in the chemical composition of the final polyurethane (PU). It is revealed that the final polymers having higher contents of bentonite nanoclay are not preferred candidates for biomedical application although there is pronounced improvement in the mechanical properties with on going investigations into their in vitro biocompatibility and non-toxicity.

## Abstract

### Microstructure and Mechanical Properties of Natural Rubber/Organoclay/Nano-Calcium Carbonate Ternary Nanocomposites: Effect of Mixing Sequence

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In comparison with any of the compounds, polymer clay nanocomposites can show synergistic properties singularly, without any prejudicial impact on any properties of the base material. Rubber nanocomposites containing one type of nanofiller are common, and are widely established in the research field. In this study, natural rubber (RSS-1) based ternary nanocomposites containing both nano-calcium carbonate and organomodified nanoclay have been characterized on the basis of morphology, structure and mechanical behavior. The possible interactions between calcium carbonate particles, organoclay and the rubber matrix have been investigated. The natural rubber nanocomposite samples containing modified layered silicates (Cloisite 15A) and also nano-carbonate calcium (Socal-312  $\text{CaCO}_3$ ) were prepared using a laboratory internal mixer. Effect of the mixing sequence on the morphology and mechanical properties of the samples was investigated. Based on results of morphology and mechanical properties, the addition of nano silicate layers to the system, as the first added filler, leads to lower mechanical properties in comparison with other orders for mixing. Although, simultaneous addition of the two aforementioned types of nanoparticles to the NR compound would lead to better nanocomposite properties compared to other mixing sequences.

## Abstract

### Synthesis of Some Polyesters and Polyamides on the Basis of bis(1H-indol-5-yl)methane, Bis(1H-indol-5-yl)oxide and Bis(1H-indol-5-yl)sulfone and their 2,2'-Diethoxycarbonyl Derivatives

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There are two types of indolcontaining polymers: a) polymers, which contain indole cores in main chain [1, 2] and b) polymers, which contain indole cores as side substituents [3, 4].

In the report are given the synthesis methods of such indole polymers, which contain free highly reactionary  $\beta$ -carbon atoms of pyrrole rings.

According classical E.Fischer reaction were obtain bis(1H-indol-5-yl)methane, bis(1H-indol-5-yl)oxide and bis(1H-indol-5-yl)sulfone 2,2'-diethoxycarbonyl derivatives from 4,4'-diphenylhydrazine pyruvic acid ethylester. By boiling of these compounds with sodium alkali alcoholic solution the corresponding dicarboxylic acid disodium salts were obtained, by interaction of which with phosphorus oxychloride in abs. benzene environment were synthesized dichloride anhydrides. On the basis of these anhydrides, under low-temperature polycondensation conditions were obtained polyesters and polyamides containing indole fragments in the main chain. The countersynthesis of these polymers was carried out on the basis of corresponding activated esters. The powder patterns of the synthesized polymers revealed their amorphous structure.

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## Abstract

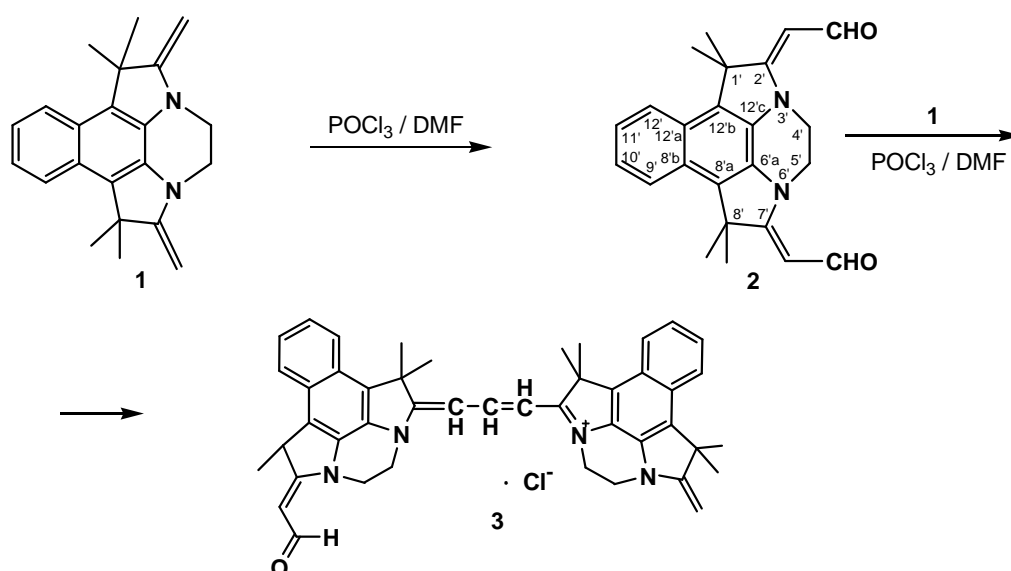
### Biscyanines. Polymethyne Colouring Agents Containing Indole Fragments

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It is known from literature that indoline quaternary salts by interaction with aldehydes result in cyanine colouring agents, which in ultraviolet spectrum give characteristic maximums in long-wavelength part [1]. The cis-trans conformation of naphthodipyrrolenine NH biscyanine derivatives was studied [1]. Carbocyanines containing indolenine fragments were described [2].

In the report are described the possibilities of synthesis of cyanine polymeranalogues by interaction of 1',4',5',8'-tetrahydro-1',1',8',8'-tetramethyl-2',7'-dimethylenedipyrrolo-[1,2,3-d,e:3,2,1-ij]benzo[g]quinoxaline (1) diformyl derivative (2) with excess of Fischer base (1) without isolating the compound 2 from the reaction system:



The model compound 3 was isolated, which structure was established by means of infrared, ultraviolet, nuclear magnetic resonance and mass-spectrum.

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## Abstract

### Polyorganosiloxanes with $\alpha$ -Naphthylcontaining Radicals at the Silicone Atom

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One of the main methods of synthesis siloconeorganic polymers is the reaction of ionic polymerization of organocyclosiloxanes. From literature it is known [1], that the properties of siliconeorganic polymers mainly depends on the nature of organic radicals coupled with silica atom.

In order to synthesize linear polymers with organo- $\alpha$ -naphthylsiloxane rings in the main chain, the reaction of anionic polymerization of synthesized  $\alpha$ -naphthylcontaining organocyclo tri- and tetrasiloxanes was carried out. In particular the reaction of anionic polymerization of  $\alpha$ -naphthylpenta-methyl, 1- $\alpha$ -naphthyl-1,3,5-trimethyl-3,5-divinyl-, 1- $\alpha$ -naphthyl-1,3,5-trimethyl-3,5-diphenylcyclotrisiloxanes and 1,3-di- $\alpha$ -naphthylhexamethyl- and  $\alpha$ -naphthylhexaethylcyclotetrasiloxanes was carried out in the presence of potassium hydroxide (0,1 % of siloxanes weight) at the temperture 80-90<sup>0</sup>C in block. Increasing temperature more than 90<sup>0</sup>C results structurization of polymers, this is obviously caused by detachment of fat-aromatic radicals affected by potassium hydroxide at increased temperature.

In order to investigate the influence of containing  $\alpha$ -naphthyl groups on the properties of synthesized polymers, we studied co-polymerization reaction of  $\alpha$ -naphthylhexamethylcyclotetrasiloxanes with octamethylcyclotetrasiloxanes with molar ratio of initial compounds 1:1 and 1:6 in the same conditions.

Relative reactionability of  $\alpha$ -naphthylorganocyclosiloxanes was established and the properties of synthesized polymers and co-polymers were studied.

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## Abstract

### Syntheses of Sex Pheromone Compositions Using Ring-Opening Metathesis Reaction

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Sex pheromone compositions of more than 600 insect species are known. Among them there are pests dangerous for forests, cereals, orchards, greenhouses, storages, etc. The most understood ones are sex pheromones of *Lepidoptera*, *Diptera*, and *Hymenoptera*. Various schemes have been proposed for preparation of these substances. As a rule they are based on stereo-selective variants of Wittig reaction or on transformation of triple bond into Z-double bond.

We have elaborated a general approach to biologically active natural compounds using stereospecific cometathesis of cycloolefins with  $\alpha$ -olefins as a key reaction especially for preparation of monoenic insect sex pheromone components having a double bond in 6-11 positions. Our way to natural compounds assumes the use of enic hydrocarbon raw materials, which make no troubles in metathesis. Involving cycloolefins of various size C<sub>5</sub>-C<sub>9</sub> with  $\alpha$ -olefins to cometathesis we can prepare 1, $\Delta$ -dienes with desired length, internal bond position and Z-isomer content up to 79 %. Their hydroboration-oxidation sometimes in combination with reactions provided lengthening hydrocarbon chain leads to many real insect sex pheromone components, alcohols, acetates, and aldehydes.

Chemical content of cycloolefin cometathesis products depends on initial mole ratio of cycloolefin to  $\alpha$ -olefin. The proper choice of cycloolefins and cycloolefin excess in starting mixture allow reaching oligoalkenameres of desired length. Their hydroboration-oxidation in combination with hydrogenation leads to the long chain strictly linear primer alcohols - very effective natural plant growth regulators.

The cometathesis of cycloolefins C<sub>5</sub>, and C<sub>7</sub>-C<sub>10</sub> as well as cyclooctadiene with olefins in the presence of heterogeneous catalyst MoCl<sub>5</sub>/SiO<sub>2</sub> in combination with SnMe<sub>4</sub> have been studied. Variation of reaction conditions (mole ratio of starting substrates, catalyst concentration, temperature, conversion, etc) allows performing the process with high selectivity, with respect to target dienes and polyenes of required length and desired stereo-content.

Advantages of cometathesis to many important natural compounds compared to classical fine organic chemistry methods are in the substantial reduction of a number of stages, relative simplicity of techniques and accessibility of raw materials, reagents and catalysts. Our method does not produce any real by-products because practically all of unsaturated hydrocarbons formed in the process can be recycled or converted into functional derivatives of high value.

## Abstract

### Synthesis of Oligohydroxynaphthylenes and their Use in Making of Heat-Stable and Electro-Conducting Rubbers

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The functional aromatic polyconjugated oligomers prepared by oxidative polycondensation reaction of 1-naphthol in the presence of hydrogen peroxide possess high heat- and radiation stability, semiconductivity, catalytic, stabilizing and antistatic activity and paramagnetism. An availability of hydroxyl groups in aromatic nuclei gives to oligomers good solubility, meltability and reactivity in various chemical conversions. Oligohydroxynaphthylenes (OHN) synthesized thus and including reactive phenol hydroxyl groups in each elementary link have been used as an active additive in making of electro-conducting rubbers. The prepared OHNs are powdered products, well soluble in polar organic solvents with melting temperature 383-408 K (depending on conditions of synthesis). Their composition and structure have been established by the methods of elemental and chemical analysis. The molecular weight indices on data of gel-permeating chromatography have the values ( $\overline{M}_w = 820 \div 1540$ ,  $\overline{M}_n = 710 \div 1150$  and  $\overline{M}_w / \overline{M}_n = 1,15 \div 1,34$ ). The experiments showed that oligonaphthols display paramagnetic (concentration of paramagnetic centres (PMC)  $\sim 1,3 \cdot 10^{17} \div 1,9 \cdot 10^{19}$  spin/g) and semiconductor ( $\delta_0 \sim 10^{-8} \div 10^{-4}$  Om.cm<sup>-1</sup> at 298 K,  $E = 1,3 \div 1,67$  eV) properties. The concentration growth of PMC in composition of samples of OHN on 1-2 leads to increase of their electro-conductivity on 3÷5 orders. It has been shown that the samples of OHN show also electron-exchange activity. Consequently, these oligomers can functions as antioxidant in composition and thereby, increasing heat-stability and term of its effective exploitation.

The synthesized OHNs have been used as the active additions for preparation of rubber mixtures on the basis of butyl (BR), butadiene-styrene (BSR) and nitrile (BNR) rubbers. In this case, the rubber mixtures on the basis of these rubbers have been prepared under the standard formulation with only difference, that instead of carbon black (partially or completely) OHNs are used (from 5.0 to 45 m.p. for 100 m.p. rubber). It has been established that an introduction of OHN instead of carbon black in composition of rubber mixtures leads to increase of ultimate strength, specific elongation and decrease of modulus of elasticity of the prepared rubbers. For ex. for rubbers made on the basis of BSR with use of 20-25 OHN instead of carbon black, the ultimate strength is increased to 25.0-26.0 MPa, the specific elongation reaches to 500-560% and the modulus of elasticity at tension on 200%, is decreased from 98÷11 to 45-50 MPa. Along with this it is increased a heat-stability and life time of the prepared rubbers, what has been apparently connected with structural peculiarity of OHN; naphthalene nuclei in chain of aromatic polyconjugation stipulate high heat-stability, and an availability of hydroxyl groups in naphthalene rings – antioxidant activity. Taking into account that OHNs with various content of PMC show high electric conductivity, their joint use with electro-conducting carbon black allows to prepare rubbers with specific surface conductivity  $10^{-8} \div 10^{-6}$  Om<sup>-1</sup>.

The content growth of OHNs from 10 to 30 m.p. (from rubber mass) instead of carbon black and also the increase of concentration of PMC in composition of OHN lead to increase of specific electro-conductivity of the prepared rubbers. The reinforcing properties of OHNs as a part of a rubber composition have been probably stipulated by an optimum combination of such indexes, as small particle size, small density and absence of oxidative-functional groups on a surface of particles.

The dependence of specific volume resistance on displacement time at various contents of OHNs has been established. The main reasons of changes of values  $\rho_v$  of made rubbers are the structurization or destruction of macromolecules. As a result of vulcanization the grid is formed and there arises higher internal stress in rubber. The higher duration of rolling the higher probability of mechanical destruction of the spatially-cross-linked macromolecules, consequence of which is the formation of defective zones in matrix of vulcanizate. The percolation effect is reached at content of 22; 25 and 28 m.p. of OHN for rubbers prepared from BR, BSR and BNR, respectively.

## Abstract

### Printing of Identification Characters on Vanishing Micro-Pattern of Plasticized Polymers as the Means of Polygraphic Protection

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A rapid development of the most diverse consumer goods' counterfeit and adulterations industry is determining the increase of counterfeit package's production volumes. Exactly the package contains the inside's anti-counterfeit features and is most often forged by simple photocopying by applying the small-offset printing methods.

Our development is based on the unique effect of the appearance and disappearance of micro-topography cross-linked rubber and polymer composites accompanying the sorption of "good" solvents. This effect is proposed to be used for marking and protecting against forgery of valuable products or products with limited shelf life. This should make printing images carrying information about the object on the polymer at the time of appearance of micro-relief on its surface. After printing an informative sign, for example, a linear or two-dimensional bar code on the uneven surface of the swollen polymer material and the desorption of solvent from the polymer material, the specific micro relief of the surface disappears (or is smoothed), and an information sign "splits" into pieces, therefore separated by spaces and as a consequence of this, is not perceived by a scanner. Printing of the information sign is done at the moment of maximum distortion of the wavy surface which is plasticized by the liquid polymer. The plasticized surface layer of liquid polymer at the optimal time for printing is created by closed/dense ridges formed by waves, when grooves are at their maximum depth. The solution to this problem will create a so-called temp sensor, which can be used for products with limited shelf life. At the same time, "life" image bar code must match the time and date of the product depending on the properties of the polymer and the volatility of the solvent.

Protection of the products or packaging from forging is provided by the inverse problem solution, hence once the barcode disintegrated into fragments, the polymeric material is exposed to interact with specifically selected solvent, and due to swelling and the formation of relief structures in polymer materials, sizes of cracks are reduced, resulting in the bar code becoming unreadable for the scanner. Search interest to us, the polymer-solvent system, carried out by studying the kinetics and thermodynamics of the interaction of polymers with low-molecular fluids.

#### Conclusions

1. In this paper we propose a unique method of protecting information, which is based on the process of swelling of the polymer material.
2. To find the optimal polymer – solvent system we investigated kinetics of swelling different polymers in low-molecular liquids. Constants of speed, Flory – Huggins parameter, diffusion coefficient  $D$  for each solvent was determined.

**2<sup>nd</sup> International Caucasian Symposium on Polymers and Advanced Materials  
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## Abstract

### Application of the Polymers for Obtaining of Nanostructural Powders of Inorganic Materials

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The polymers and oligomers are widely used for obtaining of nanostructural powders of modern high-technological ceramic materials. Nowadays metal oxides, carbides, nitrides, oxycarbides, oxocarbonitrides, borides, electronic ceramics (isolators, superconductors, and magnetic materials) are synthesized by application of polymeric methods (polymeric precursors, modified sol-gel, polymeric combustion synthesis, polymerized complex methods). Nanostructural powders can be obtained by several methods. Some of them are listed below.

1. Formation of polymers, polymeric gels or polymeric complexes in the course of the reaction and subsequent pyrolysis of the obtained mass.

2. Pyrolysis of organic and organometallic polymers resulting in reception of nanopowders (tubers, cylinders, plats, spherical particles and etc.) with different forms and structures.

With the help of the abovementioned methods we have synthesized a lot of nanostructural powders of many inorganic compounds with particle size of 20-200 nm. For example: I. Carbides and non-oxide cermets WC, W<sub>2</sub>C, WC-Co, Mo<sub>2</sub>C-Ni, (Ti, Mo,W) C-Ni, TiC-Ni are obtained by pyrolysis of mixture of inorganic compounds and carbon-chained polymers (oligomers). Nanophase boron carbide (B<sub>4</sub>C) is obtained by interaction of polymers (oligomers) containing hydroxyl-groups with boric acid and pyrolysis of obtained esters at 400-1400<sup>0</sup>C. II. Luminophors and among them silicates, aluminates, tungstates, molybdates, phosphates, titanates, vanadates, sulphates and others were obtained by sol-gel method. The essence of this method is formation of polymeric gels by interaction of the initial inorganic compounds with polyfunctional organic compounds and their subsequent pyrolysis. Significant scintillated materials like Lu<sub>2</sub>SiO<sub>5</sub>, Y<sub>2</sub>SiO<sub>5</sub>, PbWO<sub>4</sub>, ZnWO<sub>4</sub>, Y<sub>3</sub>Al<sub>2</sub>O<sub>12</sub>, YAlO<sub>3</sub> and others were obtained by gelation of reaction medium by aminoethanols, polyols, citric acid, etc. and subsequent pyrolysis. By this method the monophasic compounds are obtained at the temperature lower by 200-700<sup>0</sup>C as compared to traditional solid-phase reactions.

Silicates of Lu(Y) are obtained as well by pyrolysis of mixture of Lu(NO<sub>3</sub>)<sub>2</sub>, (Y(NO<sub>3</sub>)<sub>3</sub>) and polyethoxy-, polydimethyl- and polydiphenylsiloxanes at 200-1200<sup>0</sup>C. By application of polymeric complex-formers and organic solvents many inorganic compounds are obtained in amorphous state, which can be transformed into nanophasic powders (PbWO<sub>4</sub>, ZnWO<sub>4</sub>) by thermal treatment.

Crystalline phases of the powders were identified by X-Ray diffraction method. The structure and morphology of the synthesized powders are examined with the transmission and scanning electronic microscopes. Thermal analysis (TG, DTG, DT) was carried out by means of Setsys Evolution (Setaram Tag 24).

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## Abstract

### Effect of Modify of the Fillers by Silicon-Organic Substances on the Properties of Polymer Composites

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It is known that the adhesion forces between ingredients in the polymer composites are one of the main factor ensuring both high mechanical and other important exploitation properties of these materials. Therefore at obtaining of lasts a large attention is directed to state of interphase layer between binders (polymers) and filler particles.

In the presented work for increasing of the interaction between macromolecules and filler particles the effect of modify of the surface of mineral filler (basalt) particles by silicon-organic substances (SOS) has been studied. The main idea of the functionalization of this mineral was based on the possibility of chemical reactions between silanol groups localized on the mineral surfaces and silicons functional groups. The composites were made on the basis of two types of polymers – epoxy resin and polyethylene.

The composites was prepared at conducting of the following manipulations: 1) wetting of basalt powders (particle sizes up to 50 micrometers) by tetraetoxisilane during 24 hours; 2) drying of particles at 50-60°C; 3) preparing of the mixture of polymer resin and coated with SOS basalt powder; 4) heating of mixture at 100-120°C; 5) forming of samples for testing with different physical methods in various press forms.

The testing of composites was carried out using apparatus for measuring of the strengthening at compression, thermal resistance by method of Wika, water absorption corresponding to standard. Results of the fulfilled measures show that the composites based on both epoxy resin and polyethylene reveal one general phenomenon – improving all investigated properties thanks to modify of the filler particles of basalt on several time.

Obtained results are described in terms of the structuring peculiarities of composites. Namely, in the composites containing the modified fillers takes place the formation of inter-phase layers created with modify substance molecules, which are chemically bonded with surface active chemical groups of the filler particles. Moreover it is possibility of a formation of chemical bonds between polymer and modifier molecules. The dependence of the studied properties of composites on the concentration of modifier has extreme character – essential improving of the investigated characteristics takes place only at the definite optimal contain of modifier agent.

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## Abstract

### AABB-Poly(depsipeptide)s a New Class of Biodegradable Polymers for Biomedical Applications

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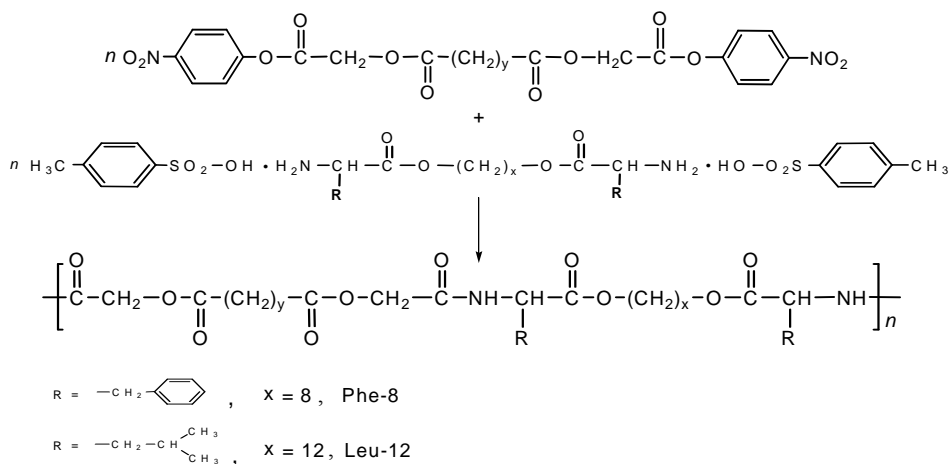
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Poly(depsipeptide)s (PDPs) represent a class of biodegradable polymers composed of  $\alpha$ -amino and  $\alpha$ -hydroxy acids. There are two reported synthetic approaches to the synthesis of AB-type PDPs: a) by solution polycondensation of corresponding di, tri, or higher depsipeptide and b) ring opening polymerization of cyclic monomers like morpholine-2,5-dions - six-membered heterocyclic compounds composed of  $\alpha$ -hydroxy and  $\alpha$ -amino acid. The both ways are too complex and expensive. We have developed a new, third approach to this class of PEAs that leads to AABB-type PDPs free of limitations of AB-PDPs.

Key bis-electrophilic monomers - di-*p*-nitrophenyl esters of O,O'-adipoyl-bis-(glycolic acid) and O,O'-sebacoyl-bis-(glycolic acid) were obtained by direct condensation of corresponding diester-diacids with *p*-nitrophenol in toluene using SOCl<sub>2</sub>/Pyridine as a condensing agent. Intermediate diester-diacids were synthesized by interaction of adipoyl chloride and sebacoyl chloride with glycolic acid in ethyl acetate in the presence of Py.

Di-*p*-toluenesulfonic acid salts of bis-(L-leucine)- and bis-(L-phenylalanine)- $\alpha,\omega$ -alkylene diesters were used as bis-nucleophilic partners of diesters.

The polycondensation reactions of were carried out in N,N-dimethyl acetamide (DMA) in the presence of triethylamine as a *p*-toluenesulfonic acid acceptor at a solution concentration 1.2 mole/L and  $t = 60^\circ\text{C}$ . The polymers were separated from the reaction solution by precipitation in ethanol, washed with ethanol and dried at  $50^\circ\text{C}$  under reduced pressure.



The new polymers have rather high molecular weights ( $M_w$  ranged within 32,000 - 52,500) and narrow polydispersity ( $M_w/M_n$  ranged within 1.36-1.48), and showed good film-forming properties.

The new representatives of amino acid based biodegradable polymers - AABB-PDPs were successfully synthesized for the first time. It is expected that AABB-PDPs will show low immunogenicity due to adirectional orientation of  $\alpha$ -amino acids and a high concentration of ester bonds in macromolecules. This latter can provide with enhanced biodegradation rates of AABB-PDPs that are of interest for numerous biomedical applications.

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## Abstract

### Synthesis of Biodegradable Poly(ester amide)s on the Basis of 2,2'-p-Phenylene-bis-(4-oxazoline-5-on)s, Active Sebacate and Bis-(L-leucine)-1,12-Dodecylene Diester

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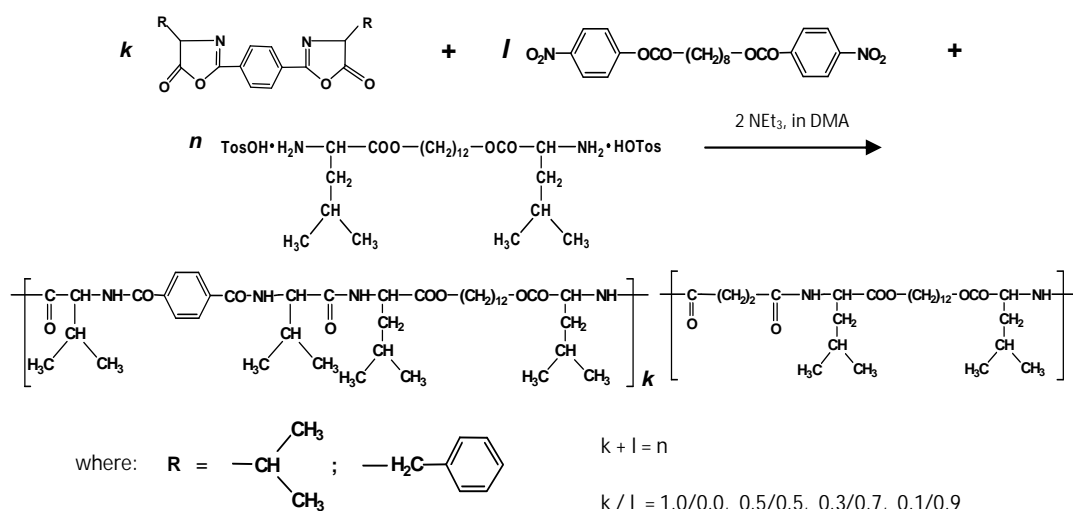
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Bis-azlactones are highly active bis-electrophilic monomers that interact with fatty diamines under mild conditions without liberation any low-molecular-weight by-product. Various high-molecular-weight polyamides having good material properties were synthesized in our previous studies *via* bis-azlactones. These polyamides showed very good biocompatibility, however, their biodegradation rates were too low

To increase the biodegradation rates of azlactone-based polymers we have synthesized poly(ester amide)s by interaction of bis-azlactones (derived from valine, R=CH(CH<sub>3</sub>)<sub>2</sub>, or phenylalanine, R=CH<sub>2</sub>C<sub>6</sub>H<sub>5</sub>) with *p*-toluenesulfonic acid salt of bis-(L-leucine)-1,12-dodecylene diester in DMA at 0-20°C using triethylamine as *p*-toluenesulfonic acid acceptor. Homo-poly(ester amide)s (k=n, l=0) having rather low molecular weights ( $\eta_{red} \leq 0,38$  dL/g in 1,1,2,2-tetrachlorethane/phenol (3/1 w/w) mixture) and poor material properties were obtained that might be ascribed to undesirable side reactions of bis-azlactone with tertiary amines. To decrease the concentration of bis-azlactons and minimize in that way undesirable side reactions we have decided to replace a part of bis-azlactone with other bis-electrophilic monomer – di-*p*-nitrophenyl sebacate that was successfully used in our previous studies for synthesizing high-molecular-weight biodegradable poly(ester amide)s showing excellent material properties. The ratios bis-azlactone/active diester (k/l) used in the present study were 0.5/0.5, 0.3/0.7, 0.1/0.9.



High-molecular-weight ( $\eta_{red} \leq 1.44$  dL/g) co-poly(ester amide)s showing good film-forming properties were synthesized using this approach. The poly(ester amide)s obtained were undergone the enzyme ( $\square$ -chymotrypsin and lipase) catalyzed *in vitro* biodegradation whereas the polyamides prepared by interaction of bis-azlactones and alkylendiamines were quite resistant to these enzymes under the same biodegradation conditions.

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## Abstract

### Comb-type Methylsiloxane Polymers: Synthesis, Properties & Application

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Polysiloxanes are characterized by a number of interesting properties, e.g. excellent heat resistance, low toxicity, biocompatibility, high oxygen permeability, poor wettability, extremely low surface tension, low melting point and glass transition temperature, resistance to radiation, special rheological properties, outstanding electrical isolating properties and others.

Comb type polyorganosiloxanes may be synthesised by two ways:

1. Via hydrosilylation reaction of polymethylhydrosiloxane with allyl or vinyl containing compounds in the presence of platinum catalysts (Pt/C, platinum hydrochloric acid, Karssted's Catalyst, Rhodium and Ruthenium complexes); or using dehydrocoupling reactions of polymethylhydrosiloxane with hydroxylcontaining compounds in the presence of catalysts.
2. The second way for synthesis is the hydride addition of 2.4.6.8-tetramethyl-2.4.6.8-tetrahydrocyclotetrasiloxane (methylcyclotri-, -pentasiloxanes) to allyl or vinyl containing compounds in the presence of platinum catalysts and polymerization of obtained product.

So, synthesis these two ways and possible application of comb-type polymers will be discussed in this work.

## Abstract

### New, Biodegradable Arginine-based Polymers as Potential Carriers for Gene Therapy

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The success of gene therapy fully depends on safe and effective gene delivery systems. Non-viral delivery systems have been introduced in the safety issues and limitations associated with current viral vectors. Synthetic polycations like poly-L-lysine, polyethylenimine, Polyarginine, etc. are widely used as nucleic acid carriers. However, these gene carriers are also far from being perfect. Major limitations of known synthetic polymers are their relatively low transfection efficiency and high cytotoxicity. It is also desirable that synthetic non-viral carriers are biodegradable, and can be easily cleared from the body after their function is fulfilled. Biocompatibility and biodegradability become increasingly important for the long-term gene therapy. Hence, the creation of new cationic polymers/gen carriers free of the mentioned limitations is topical.

We have developed new arginine(R)-based biocompatible and biodegradable polycations of various classes: poly(ether ester amide)s, poly(ether ester urethane)s, and poly(ether ester urea)s. The backbones of these cationic polymers contain the ester bonds that impart biodegradability, and ether bonds that gives the PEG-like structure to these polymers and increase their water-solubility and transfection efficiency (Like Poloxamers).

Newly synthesized R-based polycations were obtained by solution (in DMSO) polycondensation of active diesters of different class with tetra-*p*-toluenesulfonic acid salts of bis-(L-arginine)- $\alpha,\omega$ -alkylene diesters, where “alkylenes” contain ether bonds. The cytotoxicity and DNA binding ability of R-based biodegradable polycations in cervical cancer HeLa cells and mouse breast cancer model 4T1 were studied. These R-based polycations are less cytotoxic than commercially available polycations and form stable and compact nano-complexes with DNA thus demonstrating a high potential for being used as non-viral carriers for gene therapy.

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## Abstract

### Synthesis of Silver- Polyaniline Nanocomposite and its Antibacterial Effects

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Silver nanoparticles (NPs) were synthesized by controlled reduction of  $\text{Ag}^+$  ions and oxidation of aniline monomers in micriemulsion medium at room temperature. Polyaniline loaded with Ag nanoparticles by entrapment of  $\text{Ag}^+$  ions into the polymer network, followed by reduction. The nanocomposite was characterized by scanning microelectronic microscopy (SEM). In vitro antibacterial tests were performed using *Escherichia coli* (*E. coli*) to determine the antibacterial capability of the Ag/Polyaniline nanocomposite.

## Abstract

### Study of the Mechanism of Co-Telomerization Reaction

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It was studied the reaction of co-telomerization of ethylene, carbon oxide, and 4-chlor carbon with initiated tertiary butyl peroxide. It was received as tetrachloralkanes as well as tri-chloralkane chloranhydrides through the reaction. In this reaction carbon oxide plays a dual function: participates not only in the chain increase but also in the chain passing process. The outcome of separate obtained telomeres depends on the proportion of carbon oxide over ethylene and also on telogen proportion over carbon oxide [1].

The content of the reaction depends on the increased selective reaction ability with monomers, carbon oxide and telogen, which is expressed in the proportion of the speed of those reactions. It was concluded that speed constants proportion over  $\text{CCl}_4$  during chain passing  $\sim 30$  times as more than chain passing constant of carbon oxide.

It was researched the dependence of individual telomeres' outputs over the proportion of carbon oxide and monomers. Through experiments it was concluded that the course of polymerization reaction can be tentatively divided into 2 sections. One section spreads on mole proportion  $\sim 2$ . The telomerization reaction mainly takes place in this section with the production of tetrachloralkanes and output of the product is in direct proportion with ratio. In the second section, the product output is counter-proportional of this ratio but the output of carbon acid chloranhydrides is in direct proportion with the ratio. This fact can be explained by the balance of emergence of acil radical:



In the air or liquid phases and in the condition of regular pressure, the emergence of acil radical would have probably no importance. If the concentration of carbon oxide is increased the reaction can run directly, which would increase the output of chloranhydrides. Only copolymer can be emerged on the certain pressure.

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## Abstract

### Thermal Degradation and Flammability of Polyethylene/Graphite Nanosheets Composites Prepared *via* Intercalative Polymerization

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Thermal degradation and flammability of the PE/graphite nanosheets (PE/nG) composites prepared *via* intercalative polymerization technique [1] are discussed. The sets of the data acquired with the aid of non-isothermal TGA experiments have been treated by the model kinetic analysis. An increase of the thermal stability of PE/nG as compared with plain PE has been explained by deceleration of diffusion process on the surface of composites due to the “shielding effect” of graphite nanosheets. The results of flammability tests, especially ignition time delay and gases evolution, lead to the conclusion that “shielding effect” of graphite nanosheets plays a major role in the mechanism of flame retardation of PE/nG nanocomposites.

#### Reference

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## Abstract

### Synthesis and Investigation of Polysiloxanes with Reactionable Groups in the Side Chain

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Functionalized polysiloxanes play an important role in the synthesis of modern materials, among others organic-inorganic copolymers as well as starting materials for many subsequent syntheses [1].

Basic method for the manufacture of functionalized polysiloxanes is based on hydrosilylation processes of the commercial  $\alpha,\omega$ -bis(trimethylsiloxy)methylhydrosiloxane [2], however during reaction not all active  $\equiv\text{Si-H}$  groups participated in the hydrosilylation reaction, which causes branching process through the formation of silsesquioxane bonds and increase in the molecular weights.

In this work we present a new approach of synthesis organosilicon polymers where there are no unreacted  $\equiv\text{Si-H}$  bonds. For this purpose hydrosilylation reaction of 2.4.6.8-tetramethylcyclotetrasiloxane with allylcianoacetate was carried out.

Hydrosilylation reaction of 2.4.6.8-tetramethylcyclotetrasiloxane with allylcianoacetate in the presence of platinum catalysts proceeds with formation of 2.4.6.8-tetra(4-propyloxy-cianoacetate)-2.4.6.8-tetramethylcyclotetrasiloxane. Structure and composition was determined according to the FTIR and  $^1\text{H}$  NMR spectral data.

Ring opening polymerization reactions of synthesized organocyclosiloxanes were carried out using nucleophilic catalyst and termination agent (TA) hexamethyldisiloxane. The synthesized oligomer was a vitreous viscous liquid that was quite soluble in ordinary aromatic type organic solvents and quite stable in time. Structures and compositions of the oligomer were established on the basis of NMR and FTIR spectral data. Molecular weights were determined using GPC. Depending on the ratio of cyclic compound and termination agent (TA) different molecular weight oligomers were obtained.

**Acknowledgment:** The financial support of the Science and Technology Center in Ukraine Grant #5055 is gratefully acknowledged.

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## Abstract

### Methylsiloxane Oligomers with Epoxy Groups in the Side Chain

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Polysiloxanes are characterized by a number of interesting properties, e.g. excellent heat resistance, low toxicity, biocompatibility, high oxygen permeability, poor wettability, extremely low surface tension, low melting point and glass transition temperature, resistance to radiation, special rheological properties, outstanding electrical isolating properties and others.

Polyorganosiloxanes with epoxy side groups have been synthesised by two ways. Via hydrosilylation reaction of polymethylhydrosiloxane with allyl glycidyl ether in the presence of platinum catalysts (Pt/C, platinum hydrochloric acid, Karstedt's Catalyst) it was shown that not all active  $\equiv\text{Si-H}$  groups participated in the hydrosilylation reaction, which causes cross-linking processes. The second way for synthesis is the hydride addition of 2.4.6.8-tetramethyl-2.4.6.8-tetrahydrocyclotetrasiloxane to allyl glycidyl ether in the presence of platinum catalysts and polymerization of obtained product. So, synthesis these two ways will be discussed in this work.

For the purpose of synthesis of organosiloxanes with epoxy groups in the side chain, hydrosilylation reaction of  $\alpha,\omega$ -bis(trimethylsiloxy)methylhydrosiloxane with allyl glycidyl ether at 1:30 or 1:53 ratio of initial compounds was carried out in the presence Karstedt's catalyst.

The reaction of hydrosilylation was investigated without solvent in the presence of catalysts at temperature range 80-90<sup>o</sup>C. In the both cases the hydrosilylation proceeds with an inductive period, after that the reaction autocatalytic with the formation of three-dimensional systems.

Modification 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  $\equiv\text{Si-H}$  groups participated in the hydrosilylation reaction, which causes branching process through the formation of silsesquioxane bonds and explains the increase in the molecular weights.

In this work we present a new approach of synthesis organosilicon polymers where there are no un-reacted  $\equiv\text{Si-H}$  bonds. For this purpose hydrosilylation reaction of 2.4.6.8-tetramethyl-2.4.6.8-tetrahydrocyclotetrasiloxane with allyl glycidyl ether was carried out. The progress of the conversion of active  $\equiv\text{Si-H}$  groups was followed by the disappearance of the  $\equiv\text{Si-H}$  absorption at 2165  $\text{cm}^{-1}$ .

Via ring opening polymerization reaction of obtained product using potassium hydroxide as a catalyst and termination agent (TA) hexamethyldisiloxane the linear methylsiloxane oligomers with regular arrangement of epoxy groups in the chain have been obtained. Some modification reactions of obtained product have been studied.

Structures and compositions of the oligomers were established on the basis of elemental analysis, FTIR and NMR spectral data. Molecular weights were determined using GPC analyzes.



## Abstract

### Synthesis of Organosiloxane Copolymers with Monocyclic Fragments in the Side Chain

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The synthesis of linear organosiloxane copolymers with regular disposition of organocyclosiloxane fragments in the side chain was performed using HFC of dichloroorganosiloxyorganocyclosiloxanes with  $\alpha,\omega$ -dihydroxydimethylsiloxanes and dihydroxydimethylsilane in the presence of pyridine (the acceptor of hydrogen chloride). It is known that application of the acceptor increases of depth of the reaction. The reaction proceeded at room temperature, and at the final stage the reaction mixture was heated up to the boiling point of the solvent used. It was found that at short lengths of linear dimethylsiloxane unit the yields of copolymers are low. Studying the heterofunctional polycondensation of dichloroorganosiloxydiorganocyclosiloxanes with 1,5-dihydroxyhexamethyltrisiloxane after polymer reprecipitation from the mother solution, low-molecular products, corresponded to dicyclic compound were obtained. Depending on the framing groups at silicon atoms, the copolymers represent transparent or slightly opalescent substances, soluble in ordinary organic solvents with  $\eta_{\text{spec}} = 0.04 - 0.4$ . The yield of synthesized copolymers equals to 72 - 95%.

The fractionation of copolymers with methylcyclotetra- (1) and methylcyclopentasiloxane (4) fragments (the length of the linear dimethylsiloxane chain equal to  $n=1$ ) in the chain was carried out and on the basis of fractionation data and determination  $\bar{M}_n$  of fractions and characteristic viscosity  $[\eta]$  the integral curves of distribution according to MW and  $[\eta]$  for copolymer with methylcyclopentasiloxane fragments was constructed. For the same copolymer the value of constant K in the Mark-Kuhn-Howinck-Sakurada equation was calculated  $K \approx (2,38 \pm 0,01) \times 10^{-4}$  as well as the value of the parameter  $\alpha \approx (0,5579 \pm 0,004)$ .

Comparison of the equilibrium rigidity parameter of the copolymer 1 with the volume cyclic substituent in a molecule of copolymer 4 results in an increase in equilibrium rigidity of macro-molecules of copolymer  $A \approx 27 \text{ \AA}$ , compared to that of polydimethylsiloxane  $A \approx 10 \text{ \AA}$  and polydimethyldiphenylsiloxanes  $A \approx 16 \text{ \AA}$ .

For synthesized copolymers FTIR, NMR spectra, GPC, thermomechanical and TGA analysis have been carried out.

## Abstract

### PhagoBioDerm Composition Containing Spray-dried Bacteriophages

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PhagoBioDerm is a novel wound-healing biocomposite preparation consisting of biodegradable poly(ester amide) impregnated with an antibiotic, lytic bacteriophages and other medications. Biodegradable polymer provides slow release of antibacterial compounds and other drugs into the wound. Produced as perforated elastic films or fine powder it was licensed for sale in Georgia. PhagoBioDerm showed a unique wound healing potential and was successfully used for treatment of infected superficial wounds and ulcers (films) [1, 2] as well as deep wounds and osteomyelitis [3]. The powdery bacteriophages used for preparing PhagoBioDerm were obtained by freeze-drying of water solutions (so called "liquid phages") that is costly and long-lasting.

To make PhagoBioDerm and other phage-based preparation cost-effective we have applied spray-drying that is the most widely used industrial process involving particle formation and drying. It is highly suited for the continuous production of dry solids in either powder, granulate or agglomerate form from liquid feedstocks as solutions, emulsions and pumpable suspensions. Therefore, spray drying is an ideal process where the end-product must comply to precise quality standards regarding particle size distribution, residual moisture content, bulk density, and particle shape.

We have selected special carrier materials (fillers) and drying conditions that resulted in products with only 1 log (10) to 3 log (10<sup>3</sup>) reduction in bacteriophage efficacy that is at the same level with freeze-drying.

PhagoBioDerm biocomposite prepared using spray-dried bacteriophages revealed the same bactericidal activity as the first population of the biocomposite consisting of freeze-dried bacteriophages showing spray-drying technology is promising for obtaining cost-effective powdery phage-based remedies.

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## Abstract

### Study of Influence of Georgian Raw Material-Andezite on the Properties of Electric Conducting Polymer Composites Based on Polyethylene

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The elaboration of new electrical conducting polymer composites is very actual now, because these materials are good alternative of the traditional conductors-metals. It is known that sometimes application of some dielectric minerals together with conducting fillers leads to useful results in result of additive powdering of conducting filler, which promotes the enlargement of conducting channels in polymer matrix.

The presented work is devoted to study of influence of the mineral andezite on the conductivity and some physical properties of the conducting composites on the basis of high density polyethylene, filled with carbon black.

It is shown that introduction of dispersive (no more than 50 mcm) andezite to the composite increases its strengthening at compression to 60 MPa, chemical stability in the mixture of 40% sulfur acid and the specific volumetric electric resistance don't exceed 100 Ohm.cm. Therefore thanks to use of dielectric powder of andezite as second additive material to the polymer composite ensures high conductivity of it at relatively low content of conducting filler.

## Abstract

### **Influence of Technological Factors on the Process of Extraction of Lipid Complex of Tea Leaf**

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Analysis of lipid complex of tea leaf (LC TL) showed its high nutritional value and expressed pharmacotherapeutic activity.

To select a LC TL as an extractant chlorinated hydrocarbons have been studied. The maximum effect on output has trichlorethylene (90%) boiling point which guarantees the protection of vitamins and other biologically active substances from the effects of temperature during extraction.

Preliminary laboratory studies allowed choosing the optimization of extraction - output LC TL of 1 ton of raw material and energy consumption for production of 1 ton of raw material. Technological parameters influencing factors - temperature and time of extraction, the ratio of extractant / tea and share a tender fraction in tea raw materials, and their levels and ranges of variation has been established.

Realization of the matrix of central compositional rotatable planning received adequate regression equation in which the method of Lagrange multipliers of unsaturated the optimal levels of factors that give the maximum yield of LC TL at possibly the lowest cost of energy extraction.

## Abstract

### Planning of Experiments and Optimization of the Extraction Processes of Tung Oil

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Tung oil gives a unique in the quality of the film - a strong, flexible, durable and different beautiful shine. Experimentally confirmed that the maximum oil yield have been achieved with extract pre-treated of raw Tung.

The basic factors influencing on the yield of tung oil from the meal, their levels and ranges of variation have been established. The optimization parameters of the extraction of the oil have been proved. The matrixes of rotatable central planning have been implemented and adequate regression equations have been obtained. The problem of optimizing the compromise process of extraction have been solved and optimal values of the factors that ensure the maximum yield of oil per unit of raw material at a fixed energy costs for processing: three-step extraction of crushed oil cake trihloetilenom with a 10 minute duration of each foot, in the phase ratio of extractant/cake 3:1, an extraction at  $70 \pm 5^{\circ}\text{C}$  and the extract mass pulsation frequency of  $2-3 \text{ s}^{-1}$  and the amplitude of the oscillation - 2 mm have been obtained. Yield of the oil with up to 95% from initial, and energy consumption for production of 1 kg of the oil is less than 3,0-3,5 kWh.

## Abstract

### Synthesis of Methylsiloxane Oligomers for Polymer-electrolyte

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Polysiloxanes are characterized by a number of interesting properties, e.g. excellent heat resistance, low toxicity, biocompatibility, high oxygen permeability, poor wettability, extremely low surface tension, low melting point and glass transition temperature, resistance to radiation, special rheological properties, outstanding electrical isolating properties and others.

Polyorganosiloxanes with cyanogen side groups have been synthesised by two ways. Via hydrosilylation reaction of polymethylhydrosiloxane with allyl cyanide groups in the presence of platinum catalysts (Pt/C, platinum hydrochloric acid, Karsted's Catalyst) it was shown that not all active  $\equiv\text{Si-H}$  groups participated in the hydrosilylation reaction, which causes cross-linking processes. The second way for synthesis is the hydride addition of 2.4.6.8-tetramethyl-2.4.6.8-tetrahydrocyclotetrasiloxane to allyl cyanide in the presence of platinum catalysts and polymerization of obtained product. So, synthesis these two ways will be discussed in this work.

For the purpose of synthesis of organosiloxanes with cyanogen groups in the side chain, hydrosilylation reaction of  $\alpha,\omega$ -bis(trimethylsiloxy)methylhydrosiloxane with allyl cyanide at 1:30 ratio of initial compounds was carried out in the presence Karsted's catalyst.

The reaction of hydrosilylation was investigated without solvent in the presence of catalysts at temperature range 80-90°C. In both cases the hydrosilylation proceeds with an inductive period, after that the reaction autocatalytic with the formation of three-dimensional systems.

Modification 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  $\equiv\text{Si-H}$  groups participated in the hydrosilylation reaction, which causes branching process through the formation of silsesquioxane bonds and explains the increase in the molecular weights.

In this work we present a new approach of synthesis organosilicon polymers where there are no un-reacted  $\equiv\text{Si-H}$  bonds. For this purpose hydrosilylation reaction of 2.4.6.8-tetramethyl-2.4.6.8-tetrahydrocyclotetrasiloxane with allyl cyanide was carried out. The progress of the conversion of active  $\equiv\text{Si-H}$  groups was followed by the disappearance of the  $\equiv\text{Si-H}$  absorption at 2165  $\text{cm}^{-1}$ .

Via ring opening polymerization reaction of obtained product using potassium hydroxide as a catalyst and termination agent (TA) the linear methylsiloxane oligomers with regular arrangement of cyanogen groups in the side chain have been obtained. Some modification reactions of obtained product have been studied.

Structures and compositions of the oligomers were established on the basis of elemental analysis, FTIR and NMR spectral data. Molecular weights were determined using GPC analyzes.

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## Abstract

### Modification of the Properties of Composition Materials, Obtained on the Basis of Some Industrial Polymers by Thienyl-Containing Siloxanes

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The siliconorganic compounds, containing the thienyl groups are used for creating the oil-and gasoline-group materials. These compounds can be also used in medicine as silatrans and in agriculture as biologically active substances, or more correctly as repressers of injurious microorganisms of herbs. Liquids containing alkoxy groups are effectively used for making hardly volatile ointment oils. Therefore, it is interesting to study properties of each new compound containing the thienyl groups. In this regard, main objective of our work was to modify properties of composition materials, obtained on the basis of some industrial polymers, by thienyl-containing siloxanes. In particular, we wanted to identify how above-mentioned composition materials are affected by the compounds containing thienyl groups, such as tetrol and oligotetrols.

To all of modified composites have been denoted reductions of wear intensity. This is particularly envisaged in composites which are modified by oligotetrole, namely in the initial stages of the wear rate decreases 6,5 times, and at high speeds of 5 times. When added to markedly decreased the temperature at the surface friction of approximately 85-115<sup>0</sup>C. This phenomenon is very significant for the self-lubricating materials, because they operate in a dry condition and nagevayutsya wear. The less exposed surface, the greater the longevity.

## Abstract

### **New Novel Resorbable Composite Materials for Orthopedic Surgery: *In vivo* Biodegradation Study of Polymeric Matrix**

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Inorganic-organic composite materials are widely used in orthopedic surgery. These materials contain calcium phosphates – tricalcium phosphate and nano-hydroxyapatite as an inorganic phase, and naturally occurring (collagen) or synthetic biodegradable polymers as an organic phase (matrix) that provides the resorption of the material and in that way regeneration/reconstruction of the bone tissue. Current results of multiple investigations of recently utilized polymers revealed that their performance is far from desired strict demands. For instance, natural polymers (mainly collagen) usually elicits allergic reactions while majority of synthetic polymers show lack of desirable mechanical characteristics and/or biocompatibility, and frequently are encapsulated when implanted in the body. It is highly desirable for surgeons to have composite materials of various consistency – from grease-like and elastic cartilage-like materials to strong composites with bone-like mechanical characteristics. Our systematic study is dedicated to the elaboration and practical applications of all three types of Inorganic-organic composite materials.

As an organic phase we have selected original biodegradable polymers composed of naturally occurring  $\alpha$ -amino acids that have a wide range of material properties due to various classes and structural diversity within each class. This allows to select matrices that meet the said strict requirements. Specifically, for constructing bone-like composite material we have selected poly(ester urea) composed of  $\alpha$ -amino acid L-leucine and 1,6-hexanediol (designated as 1L6), for cartilage like composite material - poly(ester urea) composed of  $\alpha$ -amino acid L-leucine and 1,12-dodecanediol (1L12) and poly(ester amide) composed of sebacic acid, L-phenylalanine and 1,6-hexanediol (8F6), and for grease like material low-molecular-weight poly(ester amide) composed of sebacic acid, L-leucine and 1,6-hexanediol (8L6).

At the initial stage of the study we have explored *in vivo* biodegradation mechanisms of the selected matrices without additives. Namely, we have studied poly(ester amide) 8F6 – there to circular discs of thickness 0.12-0.15 mm, diameter  $d=20$  mm, and weigh 33-41 mg were implanted subcutaneously to rats. Four types disc were implanted – (i) monolithic, free of additive, non-sterilized, (ii) monolithic, free of additive, sterilized with a solution of chlorohexidine bi-gluconate, (iii) monolithic, containing impregnated trypsin, sterilized, and (iv) porous, free of additive, sterilized. The sterilized samples (ii-iv) were completely resorbed within < 30 days. Non-sterilized samples (i) were encapsulated though they were also completely resorbed after 2-2.5 months of implantation.

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## Abstract

### Some Regularities of the Gradient Orientation of Polymers in Heterogeneous Mechanical Field

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A major focus of polymer science twenty-first century is to obtain materials and elements with a gradient of different properties. The gradient of the properties in the polymer body may be formed by the gradient of chemical composition, as well using a gradient orientation of polymers.

The idea of the degree of gradient orientation, as a new characterization of polymer material – new structural state (gradient-oriented state) in science was first introduced by us [1]. According to this view, the transition of the polymer in a gradient oriented state makes it possible to obtain polymer materials of new generation, with a gradient of mechanical, thermal, optical, electrical, magnetic, acoustic and other properties. Obtaining materials with desired properties stimulate the emergence of new scientific directions. Gradient-oriented state is created under the influence of inhomogeneous mechanical field on the polymer body.

In the present study investigated to obtain rectangular pieces with a hyperbolic distribution of relative elongations perpendicular to the single axle stretching of the polymer film. Essence of the method described below.

Consider a sector of a circle with two concentric radii  $(O, R)$  and  $(O, r)$ .  $OA = OB = R$ ,  $OC + CA = OA$ ,  $OD + DB = OB$ ,  $OC = OD = r$ . Central  $\angle AOB$  denote  $\alpha$  radian, the length of the  $CD$  chord through  $a$ , the length of  $AB$  arc through  $b$  and  $b/a$  through  $n$ .

Consider the curvilinear trapezoid  $ABCD$ , where the  $CD$  is a segment,  $AC$ ,  $DB$  are arbitrary  $f(x)$  curves, and is arc. For fixed  $a, l$  and  $n$  is calculated  $R, r$  and  $\alpha$ . After simple transformations we obtain the system of equations

$$2r \sin \alpha / 2 = a,$$

$$R = na / \alpha,$$

$$R - r = l,$$

where  $R$  and  $r$  are radii of small and large arcs,  $\alpha$  - radian size of these arcs,  $a$  is small base of trapezoid,  $n$  - multiplicity of stretch of the small base of trapezoid.

To calculate the resulting system of equations based on the secant method we have compiled an algorithm and draw up a program for algorithmic language PASCAL for the personal computer such as IBM.

The calculations are set size of the curvilinear trapezoid. In tension of the sample, placed in the parallel clamps [2], it turns blank rectangular target with a given hyperbolic distribution of relative elongations.

#### References:

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## Abstract

### Some Management Issues Gradient Orientation of Polymer

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Previously we have developed a new understanding of the structural state of linear polymers – to gradient oriented state [1].

In the present study provides decision management laws making the sample base in the segments for any coefficient of single axle deformation.

Consider a sector of a circle with two concentric radii  $(O, R)$  and  $(O, r)$ ,  $OA = OB = R$ ,  $OC + CA = OA$ ,  $OD + DB = OB$ ,  $OC = OD = r$ ,  $AC = BD = d$ . Central  $\angle AOB$  denote  $\alpha$  radian, the length of the CD chord through  $a$ , the length of AB arc through  $b$  and AB chord through  $b'$ . Assume the sample is in the form of a curvilinear trapezoid ABCD, where CD is a segment, AC, DB are arbitrary  $f(x)$  curves and AB - arc. Assume A, B, C, D points are on the same plane. Distance between points A and B denote through  $c$  and  $c < b'$ , i.e. the AB chord of the sample does not coincide with a segment AB. This means that the arc AB does not belong to the plane ABC. Sample stretches so that the ribs were displaced parallel to the original location at a distance  $b - c$  and that after stretching the arc AB aligned with the line AB. For example, after stretching the sample takes the form of a curvilinear trapezoid and  $A_1B_1C_1D_1 \subset (ABC)$ , where  $A_1C_1 = AC$ ,  $D_1B_1 = DB$ ,  $A_1B_1$  and  $C_1D_1$  are segments. After stretching  $A_1B_1 = b$ . Distance between points A and B increased by  $b - c$ , and CD chord stretched on  $b - c$ . If our goal is to spread over upper base  $n$  times, then

$$n = \frac{b-c}{a} = \frac{R\alpha - c}{a} \quad (1)$$

Through simple transformations we obtain:

$$a = 2R \sin \frac{\alpha}{2}, \quad (2)$$

$$b = r\alpha \quad (3)$$

Taking into account (2), (3) and the notation, we obtain:

$$R = r + d = \frac{\alpha}{2 \sin \frac{\alpha}{2}}$$

By inserting this expression into (1), we obtain:

$$n = \frac{\alpha}{2 \sin \frac{\alpha}{2}} + p\alpha = q, \quad (4), \quad \text{where } \frac{d}{a} \equiv p, \quad \frac{c}{a} \equiv q.$$

To calculate the resulting system of equations based on the secant method we have compiled an algorithm and draw up a program for algorithmic language PASCAL for the personal computer such as IBM. These results imply that one can choose the arbitrary  $f(x)$  curves and the length of the CD chord ( $a$ ) for selected distribution of relative elongation.

References:

1. L. Nadareishvili et al., Method of production and investigation of polymer films with a given axial gradient, GEN, 2001, 7, p.73.

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## Abstract

### Reversible and Irreversible Optical Information Recording by Use of Liquid Crystal Polymer Films Doped with Photosensitive Additives

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Photochromic materials have been the focus of intensive investigations for several decades because they have high potential for applications to optically rewritable data storage, optical switching and chemical sensing. Organic photochromic compounds like spiropyrans are particularly interesting targets for the development of new approaches to sensing since they offer new routes to multi functional materials that take advantage of their photo reversible inter conversion between two thermodynamically stable states (a spiropyran (SP) form, and a merocyanine (MC) form), which have dramatically different charge, polarity and molecular conformations. Furthermore, they can be easily incorporated into polymers for improved robustness and ease of handling. In this abstract, we demonstrate the optical properties of liquid crystal polymer film incorporated with photochromic materials. As the photochromic dopants we have used two different species of the photosensitive materials:

1. Spiropyran derivatives prepared and investigated by our scientific group [1,2].
2. Commercially available optically active dopant ZLI-811. By the elaborated method of the micro capsulation were prepared polyvinyl alcohol based liquid crystal polymer films distinguished with advanced properties such as:

High elasticity and homogeneously, good adhesion to any surface, high contrast, perfect resolution and fine gradual changing of the colours. Due to the encapsulation, these films are acquired with good protection upon the external actions and prevent the degradation of the composition providing the long life and multifold exploitation of them. High optical absorption rate and good solubility in liquid crystals provide the spiropyran based films superior photosensitivity [3]. In case of liquid crystal polymer film incorporated spiropyran, a reversible photo-controlled behaviour was observed. This process is fast and shows especially high sensitivity upon visible light irradiation. Another study we have performed is associated with optically active dopant ZLI-811. This photoisomerizable compound has been used as a chiral dopant with a non-photoisomerizable nematic host ZLI-1939 to obtain a wide temperature photosensitive cholesteric mixture and after the encapsulation was prepared liquid crystal polymer film. We found that upon the UV irradiation ZLI-811 undergo a photoisomerisation causing a change of the pitch and thus a shift of the wavelength of the selective reflection band. This photo-tuning effect is irreversible and allows us to write an optical information stable in time. We envisage that in the near future our photochromic liquid crystal polymer films can be considered as an advanced material, which offers an immediate engineering position in the areas, such as: Manufacturing of the optically addressable displays and printers, an environmentally friendly photochromic clothes. Such types of material can be used for reversible and irreversible optical information recording and storage, for photoswitchable sensing devices, photo controllable filters, windows and smart coatings, infrared image converters. Besides, a simple technology promises to fabricate photo chromic material based cost-effective devices.

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## Abstract

### Synthesis and Characterization of Hybrid Nanocomposites of Polyaniline

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The incorporation of metal nanoparticles into polymers has resulted in the origination of a new class of materials that have found fascinating interest in biomedical, catalytic, optical and electronic as well as quantum-size domain applications. Polyaniline metallic nanocomposites with Fe and Pt are prepared in microemulsion medium of sodium dodecyl sulfate (SDS). For this purpose the polymerization of aniline monomers were done by oxidation with  $\text{FeCl}_3$  and  $\text{H}_2\text{PtCl}_6$ . In this method, in-situ oxidation of aniline and reduction of  $\text{Fe}^{+3}$  and  $\text{Pt}^{+4}$  ions are took place, which aniline undergoes oxidation and forms polyaniline (PANi) whereas the reduction of  $\text{Fe}^{+3}$  and  $\text{Pt}^{+4}$  ions resulted in the formation of Fe and Pt nanoparticles in microemulsion medium to result PANI-SDS-Pt/Fe nanocomposite. The nanocomposite is characterized by FT-IR spectroscopy and scanning microelectronic microscopy (SEM).

## Abstract

### Synthesis of Silver-Polyanilinenanocomposite and its Antibacterial Effects

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Silver nanoparticles (NPs) were synthesized by controlled reduction of  $\text{Ag}^+$  ions and oxidation of aniline monomers in micriemulsion medium at room temperature. Polyaniline loaded with Ag nanoparticles by entrapment of  $\text{Ag}^+$  ions into the polymer network, followed by reduction. The nanocomposite was characterized by scanning microelectronic microscopy (SEM). In vitro antibacterial tests were performed using *Escherichia coli* (E .Coli) to determine the antibacterial capability of the Ag/Polyanilinenanocomposite.

## Abstract

### Zeolite Catalyst Cyclosiloxanes Polymerization

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One of the most widespread methods of polyorganosiloxane synthesis is catalytic polymerization of organocyclosiloxanes, where protonic and aprotic acids and strong bases are used as catalysts. It should be noticed that organosiloxane polymerization product requires the following removal of the catalyst by washing or chemical deactivation.

This process, in its turn, is quite labor-consuming power-intensive. Nowadays much attention is paid for creating of high-quality heterogeneous catalysts for polymerization reactions. Possessing all the properties of homogeneous catalysts, they are easily separated from the reaction product. Also possibility is given for their repeated use and for the polymerization reaction continuous process.

The subject of our research work is the elaboration of the new heterogeneous catalyst for polymerization of some organosiloxanes which is made on the basis of natural zeolite using the method of its chemical modification. The possibility of use natural zeolite - clinoptilolite hydrogenic forms as catalysts for octamethylcyclotetrasiloxane polymerization reactions have been shown (Khekordzula, Georgia). Optimal conditions for clinoptilolite chemical modification and organocyclosiloxane polymerization reactions have been defined. In The temperature conditions of 100-150°C and within the time interval 0,5 - 2 hours polydimethylsiloxane with high molecular mass from  $0,5 \times 10^5$  to  $2,3 \times 10^5$  is efficiently produced.

It has been proved that a certain relation between crystalic and amorphous phases is required for catalyst activity. This relation can be regulated by the concentration of hydrochloric acid used for initial natural zeolite patterns processing. It has also been proved that the catalyst can be easily removed from the reaction mass without leaving a trace in the synthesized polymer. In the process of analyzing of thermal oxidation destruction of polydimethylsiloxanes produced in the presence of sulphuric acid modified zeolite catalyst, it has been ascertained that in the second case polydimethylsiloxanes are characterized by higher thermal oxidation stability, the fact that must have positive effect on siloxane polymers service properties. The studied zeolite catalyst presents regeneration capability and for a long period of time (1-5 years) keeps its catalytic activity.

It is possible to conclude, that highly crystalline clinoptilolite of Khekordzula layer, modified into the H- form through the processing of initial clinoptilolite 1N and 2N by hydrochloric acid or the thermal treatment  $\text{NH}_4^+$  - form, represents the active catalyst of the polymerization reaction of octamethylcyclotetrasiloxane.

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## Abstract

### New polymeric composition

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Polymeric materials on the basis of epoxydian pitches ED-20, 22 modified by epoxysiliconorganic oligomers possess complex valuable operational properties: high thermal stability, high dielectric and physico-mechanical properties. A complex specified properties undoubtedly corresponds to those requirements which are presented to them with modern technics and are perspective. Synthesized by us epoxycontaining oligomers 1,3,5,7-tetraepoxy-1,3,5,7-tetraphenylcyclotetrasiloxane has been used for development and research heat-resistant glutinous compositions cold hardening the raised elasticity. For hardening bonding agent with dihydroxydiphenylsilane the ether of a boric acid with following structure:

$(\text{HO})_n\text{B}(\text{OSiPh}_2\text{OH})_{3-n}$  has been recommended.

On the basis of the lead works it is established, that utilization of epoxycontaining siliconorganic compounds as a bonding agent is actual and gives a basic new possibility of creation of glutinous compositions cold hardening working at high temperatures.

# Abstract

## Energetical Description of a Proton Transfer in Polynucleotide Systems

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Energy of activation ( $\Delta E^\ddagger$ ) and energy of reaction ( $\Delta E$ ) of process of a proton transfer in pairs guanine - cytosine (GC) and adenine - thymine (AT) of polynucleotide systems by quantum-chemical nonempirical density function theory (DFT) method are calculated. The calculations were carried out both for electric neutral, and for systems protonated on atom N<sub>9</sub> of purine ring. The results of calculations are given in the table.

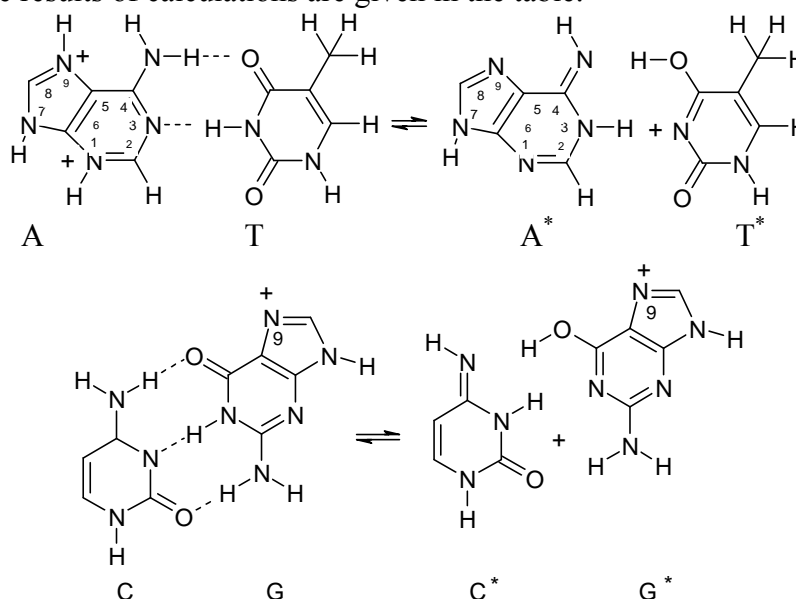


Table. Meanings of energy of activation and energy of reaction of a protons transfer in GC and AT pairs

Bases	$\Delta E^\ddagger$ kJ/mol (kcal/mol)	$\Delta E$ kJ/mol (kcal/mol)
AT - neutral	93.8 (22.4)	51.8 (12.4)
AT - protonated	89.6 (21.4)	44.9 (10.7)
GC - neutral	88.0 (21.0)	41.1 (9.8)
GC - protonated	91.1 (21.8)	50.7 (12.1)

From the table it is visible, that in electric neutral pair GC in comparison with pair AT a proton transfer occurs by smaller energy expenses. Protonated on atom N<sub>9</sub> of pair AT the reduction of energy of a proton transfer causes and for pair GC the opposite effect is observed. This result specifies feature of influence of an electronic structure of the nucleotide bases on them protonoacceptore ability both together with it and on ability of a proton transfer.



## Abstract

### The ionexchange sorption of ammonium ions on Georgian clinoptilolite

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Existing methods and technologies for the removal of ammonia as pollutant/contaminant, i.e. biological and physicochemical, are constantly being either adapted or improved and recent efforts have been made to discover new economically feasible and environmentally friendly alternatives. In this context, the use of natural zeolite for the removal of highly loaded ammonia bearing waste-water appear to have potential due to the advantages and peculiarities over some conventional and expensive ion-exchange resins.

Thus, the main objective of this work is to evaluate zeolite clinoptilolite from deposit of Georgia in thermal treated, Ca- and Na-forms as ion-exchange materials for the removal ammonia from aqueous solutions. Ammonium exchange by natural clinoptilolite was studied at different initial  $\text{NH}_4^+$  concentrations in the range of 25–150mg/L. Exchange capacity increased with increasing of initial  $\text{NH}_4^+$  concentration and this is the result of an increase in the driving force. It was shown that the low-temperature (<300<sup>0</sup>C) treatment doesn't influence practically on ammonium sorption effectiveness, but decreases the rate of ion-exchange reaction. The treatment above 550<sup>0</sup>C makes worse the ion-exchange properties of clinoptilolite. The maximum sorption capacity regarding ammonium increases with the decrease of zeolite fraction size and increase of flow rate. The maximum exchange capacity and distribution coefficients, calculated for dynamic conditions significantly exceed the same parameters for static conditions.

The samples presented fairly high specific surface area, negatively charged zeta potential and 1.02 meq  $\text{NH}_4^+$  g<sup>-1</sup> cation-exchange capacities. The ammonia removal proceeds very rapidly (rate constant of 0.3 min<sup>-1</sup>) through an ion-exchange mechanism at neutral pH values decreasing at pH>9 when gaseous  $\text{NH}_3$  species begin to form. Regeneration tests were done by contacting of 1 N NaCl solution with given weights of ammonium saturated zeolite.

So, ammonium exchange by the natural Georgian clinoptilolite was studied in batch mode and found to be strongly dependent on initial concentration and contact time, and low temperature favors the ammonium uptake on the clinoptilolite.

## Abstract

### Plasma chemical bromination, functionalization and grafting of organic molecules onto graphene-like carbon materials to be purposely used in polymer composites

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The plasma chemical and chemical bromination, proved as highly selective high-yield functionalization method of polyolefin surfaces with C-Br groups, was applied to different carbonaceous materials such as graphene layers (highly ordered pyrolytic graphite-HOPG), natural graphite, C nanotubes and carbon fibres. Polyaromatic sp<sup>2</sup> graphene structures were functionalized by electrophilic addition to covalently bond and sp<sup>3</sup> structured C-Br groups connected with local destruction of the aromatic structure. Atomic Force Microscopy has shown distortions of the surface.

The plasma chemical bromination of HOPG graphene using the bromine plasma yields max. 37 Br/100 C and using the bromoform plasma max. 40 Br/100 C. The bromination yield could be further improved using mixtures of bromine and allylbromide or bromoform and bromine.

Plasma-chemical bromination opens a new and efficient way for grafting of amines, alcohols, glycols, thiols onto C-Br moieties. Linear aminosilanes and diamines were coupled to graphene layer by substitution of Br atoms. About 12-14 molecules of 3-aminopropyltriethoxysilane and 4-5 molecules of diaminohexane molecules per 100 C atoms of the graphene substrate could be grafted. Thus, the compatibility with polymers can be strongly increased and a new class of nanomaterial can be produced with strong chemical interactions between polymer molecules and carbon nanoparticles.

Another topic is the possibility of changing the C-Br functional group into another functional group by hydrolysis or substitution. Thus, in presence of ammonia primary amino groups or using sodium azide C-N<sub>3</sub> groups were formed for click-chemistry etc. Here, the C-Br groups were hydrolyzed under alkaline conditions to hydroxyl (OH) groups. These conversions allow additional modifications for nanotubes and nanofibres.

All the patterns proposed find extensive application in advanced polymer composites for the automotive and aircraft industries.