Spring Meeting 2011

Murzasichle, April 13th - 17th, 2011

Students' Section
of Polish Chemical Society

Editorial office

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Welcome to Murzasichle!

The organization committee would like to welcome you to Murzasichle!
We hope you will enjoy your time at the 2011 Spring Meeting.
We wish you an enjoyoable scientific discussion with your fellow participants.

Besides the usual presentations and poster sessions there will be an opportunity to listen to our keynote speakers and to take part in workshops prepared by our sponsors. Moreover, we guarantee lots of fun (as always) amongst the cream of the crop (as always!).

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General Information

Conference Office

Office A **Open on Wednesday, April 7th, 2011. Opening hours: 12:00-20:00.**

Registration of participants

Delivery of conference materials

Office B **Open for duration of conferece.**

Stamping the delegation papers

Organizational issues

Other concernes from the Polish Chemical Society

Meeting Place

Ski Resort „U Zbójnika"
Murzasichle

Accomodation

- 2 to 6-person rooms with bathrooms, TV ,WiFi and a mountain view;
- comfortable conference rooms;
- large dance hall;
- well-stocked, large cafeteria;
- tennis, pool, foosball;
- a spot for firecamp, voleyball,basketball and soccer pitches;
- free parking zone.

Scientific and Social Program

Wednesday April 13th

12:00 -20:00	**Registration**
19:30- 21:00	**Opening Ceremony,** Dinner
21:00 – ...	**Welcome Party**

Thursday April 14th

09:00 – 09:30	Breakfast
09:40 – 09:50	Official opening of the Congress debates
09:50 – 10:40	**Plenary Lecture** **Ph.D. Dorota Gryko** *Conjugation of protoporphyrin IX with vitamin* B_{12} *– novel approach towards NO-free activators of sGC*

Oral Presentations parallel to Y-counsulting Worksops and Zorbing

11:15 – 14:45	**Rajtarski Kamil** *Personal Branding - building a proper image on the labour market*
11:15 – 14:45	**Dudek Kamila** *How to pass through job recruitment process*
16:00 – 19:30	**Rajtarski Kamil and Dudek Kamila** *My role in a team*

Analytical and Environmental Chemistry

Session Chairman: Dariusz Markiewicz

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11:00 - 11:20	**Kłobucki Marek** *Thujone – a magic wand of Green Fairy? Comparison of thujone content in samples of absinthe from market and home distillation*
11:20 – 11:40	**Kocot Karina** *In the world of drops and droplets - dispersive liquid-liquid microextraction in X-ray fluorescence analysis*
11:40 – 12:00	**Rutkowska Małgorzata** *An influence of thermal treatment conditions of hydrotalcite-like materials on their catalytic activity in the process of N2O decomposition*
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Session Chairman: Tomasz Michałowski

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12:55 – 13:15	**Piszcz Michał** *Hybrid polymer electrolytes based on aluminum oxygen core and polyethylene glycol*
13:15 – 13:35	**Wociechowska Karolina** *Synthesis of gold nanorods ligands for biomedical applications*
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13:50 – 14:10	**Staniszewska Emilia** *Raman and IR imaging of a glass painting from the 19th century*
14:10 – 14:30	**Świętosławski Michał** *CCL/Li_2MnSiO_4 - nanocomposite cathode material for safe Li-ion batteries*

Theoretical and Physical Chemistry

Session Chairman: Mateusz Fica

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16:20 – 16:40	**Sienkiewicz Andrzej** *Electrochemical studies of antioxidants activity in micellar systems*
16:40 – 17:20	**Mick Hurrey, Ph.D.** *Integrated Biopharmaceutical, Material Characterization, and Dissolution: Toward Formulation Optimization*
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Biopolymer and Technological Chemistry

Session Chairman: Mateusz Fica

17:35 – 17:55	**Wach Anna** *Thermal degradation of polyacrylonitrile deposited on mesoporous silicas studied by FT-IR and XPS*
17:55 – 18:35	**Csaba Janáky, Ph.D.** *Conjugated polymer based composite materials for renewable energy applications*

18:35 – 18:55	**Łyżwa Dawid** *Organocatalytic Friedel-Crafts reaction under High Pressure*
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Oral Presentations parallel to Reckitt Benckiser Workshops

11:00 – 14:45	**Reckitt Benckiser Workshop**
15:45 – 19:30	**Reckitt Benckiser Workshop**

Biopolymer and Technological Chemistry

Session Chairman: Joanna Narewska

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Session Chairman:Dawid Łyżwa

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13:30 – 13:50	**Furczoń Katarzyna** *Intermediate Temperature Solid Oxide Fuel Cell Membrane formed in Gelcasting Process from Ceria Nanopowder*

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Organic and Supramolecular Chemistry

Session Chairman: Dariusz Markiewicz

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18:25 – 18:55	**Góra Monika** *Self - assembly of gold nanoparticles covered with rod - like liquid crystals*
18:35 – 18:55	**Rybakiewicz Renata** *New air stable and solution processable organic semiconductors for field effect transistors – synthesis and characterization of triarylamine derivatives of arylene bisimides*
19:30 – 20:30	Dinner
20:30 – 21:30	Poster Session 2
21:30-...	Disco

Saturday April 16th

08:00 – 08:30	Breakfast
09:00 – 15:00	Trip to the Tatra Mountains
15:00 – 16:00	Lunch

Organic and Supramolecular Chemistry

Session Chairman: Renata Rybakiewicz

16:00 – 16:20	**Wnęk Katarzyna** *Preparation of conjugated linoleic acid (CLA) isomers*

Biotechnology

Session Chairman: Renata Rybakiewicz

16:20 – 16:40	**Konieczna Anna** *Biotransformations of selected steroid compounds in the culture of Absidia coerulea strain KCh 93*
16:40 – 17:00	**Winiecka Marta** *Application of recombinant lipase from Geomyces sp. P7 in enantioselective transestrification of selected alcohols*

Polymer Chemistry

Session Chairman: Renata Rybakiewicz

17:00 – 17:20	**Gil Małgorzata** *Epoxy resins and their mechanical properties*
17:20 – 17:40	**Strzelczyk Rafał** *Hybrid polymer coatings obtained in simultaneous radical and cationic polymerization*
17:40 – 18:00	**Ślęzak Przemysław** *Novel method of fabrication ceramics shapes: gelcasting*
18:00 – 18:15	Coffee Break
17:55 – 18:35	**FNP Presentation**
18:35 – 19:25	**Markiewicz Dariusz** *Assessment of the personality predisposition in order to enhance the professional activities*
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21:00 -....	Farewall Party

Sunday April 17th

09:00 – 09:30	Breakfast
10:00 – 14:30	**Check out**

Plenary Lectures

Integrated microanalytical systems for cell based assays

K. Ziolkowska, R. Kwapiszewski, E. Jedrych, M. Chudy, A. Dybko, Z. Brzozka*

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Analysis of molecular components and sub-cellular structures in living cell using microfluidic devices has become a major branch of bioanalytical chemistry recently. Investigating the intracellular contents of single cell is essential for understanding physiologic and pathologic processes at the cellular level. Miniaturized versions of bioassays offer many advantages, including small amounts of used solvents, reagents, and cells (critical for valuable samples and for high-throughput screening), short reaction times, portability, low cost, versatility in design, and potential for parallel operation and for integration with other miniaturized devices.

The aim of the studies was to design miniaturized systems dedicated for cell culture, cell lysis, evaluation of enzymatic activity and cytotoxicity of various substances introduced into the microsystems with cells. The geometry of the glass/PDMS device for cell based cytotoxicity assay includes five separate series of chambers for cell culture. The gradient generator integrated integrated on the same chip platform has a "Christmas tree" structure with two inlets and five outlets – simultaneously gives five different concentrations of tested toxic substance in every series of single cell chambers. The device performance was demonstrated using human lung adenocarcinoma epithelial cell line A549. Viability of the cells was monitored with fluorescence microscope. Fluorescein dibutyrate (FDB) and iodide propidine (PI) were used as a markers of viable and dead cells respectively.

Gaucher's disease is a disorder caused by the deficiency of lysosomal β-glucosidase (EC 3.2.1.42) - the enzyme, which participates in the degradation of glycosphingolipids. Another microsystem was designed for enzymatic activity determination followed by on-chip cell (L929) lysis because cell membranes are impermeable for 4-methylumbelliferyl-β-D-glucopyranoside (MUG), which was used as a substrate of enzymatic hydrolysis leading to fluorescent 4-methylum-belliferone and glucose. Obtained results of the kinetic parameters of evaluated enzymatic reaction in the microdevice are in good correlation with those obtained in "macro"-system.

Conjugation of protoporphyrin IX with vitamin B$_{12}$ – novel approach towards NO-free activators of sGC

Dorota Gryko

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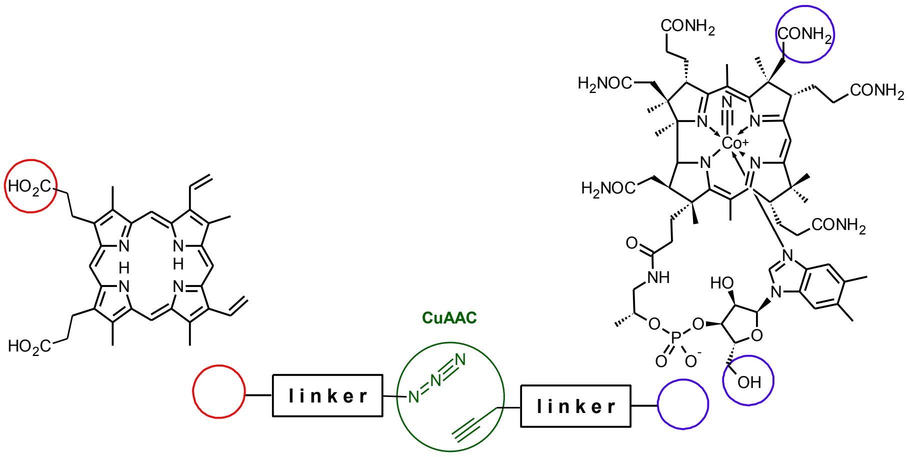
In the continuous battle against heart disease it was found that nitroglycerin and other organic nitrate compounds are among the most effective ones. These compounds operate through a decomposition reaction releasing nitrogen monoxide (NO), which acts as a biological messenger to soluble guanylyl cyclase (*sGC*) causing vascorelaxation.[1] However as with most breakthroughs there was a downfall. Due to overuse the patient would build up a tolerance to the drug. Therefore new and improved NO-free regulators must be examined.

Reports showed that vitamin B$_{12}$ (cobalamine) and protoporphyrin IX promote *sGC* activation *in vitro*.[2,3] Therefore our work concentrates on the synthesis of new tetrapyrrolic derivatives with a focus on hybrid molecules.[4]



References:

[1] Pyriochou, A.; Papapetropoulos, A. *Cellular signaling*, **2005**, *17*, 407.

[2] Martin, E.; Bogatenkova, E.; Bian, K.; Doursout, M. *BMC Pharmacology* **2007**, *7*, 40.

[3] Ignarro, L.J.; *J. Physiol. Pharm.* **2002**, *53*, 503.

[4]Proinsias, K.; Sessler, J.L.; Kurcoń, S.; Gryko, D. *Org. Lett.* **2010**, *12*, 4674.

Application of isotope effects

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Isotope effects are differences in physical and chemical properties that found applications in all branches of chemistry. Of particular interest are isotope effects on rates and equilibria since they allow to learn details about transition states of reactions, species that are not amenable for direct experimental scrutiny.

Basic concepts of isotopic effects will be discussed including the theoretical background and experimental determinations. Then several applications in chemistry, biochemistry, as well as food and environmental chemistry will be discussed.

References:

1.45 Max Wolfsberg, Alexander Van Hook, Piotr Paneth "Isotope Effects in the Chemical, Geological and Bio Sciences" Springer, London,

Conjugated polymer based composite materials for renewable energy applications

Csaba Janáky, **Csaba Visy**

University of Szeged, Faculty of Sciences

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Conducting polymer based nanocomposites are more and more intensively studied since the end of the 1990's. These inorganic–organic hybrids form a promising class of new materials, owing to the advantageous properties of the polymer matrix and the embedded inorganic particles. The combinations often lead to synergistic effects, resulting enhanced properties, making these materials applicable in various fields. Our research group is active in the field of conjugated polymer based hybrid materials since 2004. In this presentation we give an overview on our recent activities, related to novel materials for renewable energy applications.

In the first studies, conjugated polymers such as polypyrrole (PPy), polyethylene-dioxythiophene (PEDOT) and different polythiophenes (PTh) have been successfully combined with different inorganic materials including noble-metal nanoparticles (e. g. Ag) and Bi_2Te_3, leading to nanocomposites with high conductivity and good thermoelectric property[1]. Our concept is to replace the expensive inorganic thermoelectric materials by cheap organic polymers based hybrids.

Nanocomposites of conducting polymers and nanosized metallic oxides are in the focus due to the large variety of their potential applications, such as in electrocatalysis, fuel cell cathodes, or in solar power generation. In the last few years, magnetic iron-oxides, such as Fe_3O_4, □-Fe_2O_3 nanoparticles were incorporated into polypyrrole, polyaniline and PEDOT through different chemical and electrochemical synthetic procedures. The prepared hybrid thin layers have proved to be photo-electro-catalytically active in the O_2 reduction reaction, so they can be exploited as cathode materials in fuel cells[2].

Combination of a p-type semiconductor (organic polymer), and an n-type semiconductor (TiO_2 nanotube array) is a powerful tool to prepare hybrid p/n heterojunction solar cells. By synthesizing these hybrid materials with well ordered structures, their efficiency can be enhanced. By exploiting the advantageous properties of the electrochemical procedures, we carried out the ccompletely electrochemical synthesis.

References:

[1] E. Pintér; Z. Fekete; O. Berkesi; C. Visy et al. Journal of Physical Chemistry C 111(2007) *11872-11878*

[2] C. Janáky, B. Endrődi, O. Berkesi, C. Visy, Journal of Physical Chemistry C*,* 114 (2010) *19338-19344*

[3] C. Janáky, G. Bencsik, Á. Rácz, C. Visy, K. Rajeshwar et. al. Langmuir, *26* (2010) *13697–13702*

Acknowledgment: The support, through the project TÁMOP-4.2.1/B-09/1/KONV-2010-0005 is gratefully acknowledged.

IR-study of interaction between penetrant and polymeric matrix

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The membrane gas separation (MGS) is one of the physicochemical separation and purification methods. MGS is widely used in different areas of chemical technologies [1], i.e. separation different binary system, such as N_2/O_2, CH_4/CO_2 and many others. "The heart" of the membrane module is the membrane, which should be choosing very carefully. During the separation of some mixtures there might be some interaction between separation gases, which is penetrating through the membrane and its polymeric matrix.

For example, ammonia in aromatic polyamides, polyheteroarylenes which is characterized by electron acceptors character of active groups of these polymers. Also donor-acceptor interaction in which the penetrants acting as electron acceptor is might be realized in sulphur dioxide – polyeher(ester)ureas system. Hydrogen bonds might be cause of such interaction in hydrogen containing fluorocarbons in polyurethanes. Despite the fact of wide and common use of membrane gas separation for above mentioned problems it is needed to explore the process for the case of interaction between the separated gases and membrane matrix. In this case the separation effect might increase or decrease.

In the present work we represent the results of investigation interaction between ammonia and cellulose acetate glassy polymer membrane. Ammonia and some permanent gases permeability were measured [2]. It is shown that ammonia and water interaction with cellulose acetate membrane is of reversible nature. Features of this process determine the thermo dynamical and kinetic properties of the system penetrant (ammonia and water) – polymer caused by the types and energies of interaction realized in the system [3].

IR-spectroscopy was used for proving specific interaction in investigated system. The tested system was obtained by ammonia and water purge through cellulose acetate up to sorption equilibrium at certain temperature. As we were known the donor-acceptor character of interaction of these polymer membrane matrix/penetrant can be proved by change in IR spectrums of polymer in sorption equilibrium with interacting penetrant, also by high values of partial molar enthalpy of dissolved penetrant.

The obtained IR-spectrums of ammonia – cellulose acetate and water-cellulose acetate systems are characterizing by significant increase in absorption peak which are not present in cellulose acetate without ammonia and water.

As a result the investigation of penetration of gases interacting with membrane was proposed for practical realization in the new separation method - absorbing pervaporatoin [4].

References:

1. Vorotyntsev V.M., Drozdov P.N., Vorotyntsev I.V. *Desalination.* **240**. 301-305. (2009)
2. Vorotyntsev I.V., etc., *Russian Journal of Physical Chemistry*, **80 (12)**, 2020-2023, (2006).
3. Vorotyntsev I.V., etc., *Russian Journal of Physical Chemistry*, **83 (5)**, 818-821, (2009)
4. Vorotyntsev I.V., etc., *Desalination*, **200 (1-3)**, 379-381, (2006)

This work has been financially supported by the State contract № P2537

Integrated Biopharmaceutical, Material Characterization, and Dissolution: Toward Formulation Optimization

Mick Hurrey

Senior Scientist, Pharmaceutical Physics

Materials Discovery and Characterization,

Pharmaceutical Development

Vertex Pharmaceuticals

Since the human genome has been sequenced, active pharmaceutical ingredients are being developed in a different way. Biologists have identified gene targets that are responsible for a particular disease, and then searching for small molecules that bind specifically to a protein or enzyme that inhibit a particular indication. While this has lead to advances in drug discovery, the number of new medicines has been slowly declining because these new materials are harder to formulate into commercial products. In part, this is due to low solubility of these new class of compounds, which requires complicated manufacturing and control strategies to develop a final dosage form. This talk will discuss some of the strategies necessary to obtain a soluble, stable, and bioavailable solid-oral dosage form, when the disease target requires an active ingredient with poor physical chemical properties.

Workshops

Y-Consulting

Kamil Rajtarski

Business Development Manager, Human Resources Advisor, Career Consultant and Business Trainer. Specialist in creating a professional image of employees and employers. Practitioner of analyzing the level and development of employees competencies.

Since 2006 he has been associated with the business consulting in the area of training and recruitment services. He has extensive experience in the specialist, managers and senior managers recruitment in many sectors across the Poland and East – Central Europe. He has also worked with several reputable firms offering projects in the field of human resource management within the organization.

He manages sales and marketing areas in training and coaching company, responsible for business development, project management, marketing strategy and employer branding. He pursues independent projects of staff selection and recruitment.

Trained in psychology, pedagogy, teaching methodology and interpersonal communication skills at studies and in many additional courses. Participant of numerous conferences and dozens of training courses focused on the team management, leadership, coaching and processes of talents, projects and change management.

Actually he creates and develops strategy of Y-Consulting company. Manages projects in the field of organizational and personnel consulting. Conducts trainings in management processes, employee development, motivation, recruitment, sales and interpersonal skills based on his own scenarios, tools and exercises.

Y-Consulting

Kamila Dudek

Development Projects Manager, Recruitment Consultant, Diagnostician, Assessor, Trainer, Psychologist, specialist in human personality and admirer of development methods. Graduated from Administration at the UPH, studied at the Faculty of Economics and Business at the University of Maribor in Slovenia and Psychology at the UKSW. She speaks English fluently.

She has consulting experience in conducting executive selection & recruitment processes in sectors of IT, finance, FMCG and logistics. Working in a global corporation in the FMCG sector she was responsible for staff administration, recruiting and working with people managing the personnel policy. She implemented her own program of Outplacement directed to the supply chain employees.

She has experience in team management and organizing several conferences and symposias. She has clinical practice in the field of personality and psychological diagnosis in mental health institutions.

In Y-Consulting company she is involved in consulting projects in the field of human resource management. Creates and conducts trainings supported by its own tools and exercises related to interpersonal skills, HR processes and recruitment.

Reckitt Benckiser

We are the global leader in production of household detergents and a leading company in the sector of personal care and non prescription drugs.

We have business units in 60 countries and sell our products in 180 countries. Our success is a result of efforts of 25 000 people working around the globe, including 2 500 in Poland.

Each day millions of people around the world buy our best quality products: Finish, Vanish, Airwick, Cillit Bang, Harpic, Woolite, Calgon, Bryza, Dosia, Lovela, Dettol, Scholl, Durex, Veet, Strepsils, Nurofen, Gaviscon.

We invite you to get acquainted with Reckitt Benckiser!

Participate in a presentation and cases prepared by employees of the largest Reckitt Benckiser factory in the world, which is located in Nowy Dwór Mazowiecki near Warsaw. You will learn what it is like to work at the factory, how to start an internship at RB and what we offer in relation to developing and shaping your career. You will also have a chance of checking your skills solving a case entitled:

"Product development process"

You will face real problems taken from everyday work of the employees of Research and Development Department. You will have a chance of demonstrating your creativity and motivation which allow to achieve appointed goals as well as your exceptional analytical skills.

FNP

Foundation for Polish Science

The Foundation for Polish Science (FNP), formed in 1991 is celebrating its 20th anniversary this year. The Foundation is an independent, self-financing, non-profit, non-governmental organization, with a mission of supporting science in Poland. It is the largest source of science funding in Poland outside the state budget. Its budget for 2011 is 120 m PLN.

The main objectives of FNP are:

- to support excellent scientists and research teams,
- to facilitate technology transfer,
- to support various investment initiatives serving science in Poland.

The Foundation realizes these objectives by:

- awarding individual prizes and scholarships to scientists,
- awarding grants for the modernization of scientific facilities and the protection of scientific collections,
- grants for the transfer of scientific achievements to industry,
- otherwise supporting important undertakings in the service of science (e.g. through conferences and publishing programmes).

The Foundation also plays an increasingly active role in supporting international scientific cooperation, taking actions to facilitate the exchange of scientific ideas, and increasing the scientific independence of the younger generation of scientists.

The Foundation's principles for awarding support are as follows:

- fundamental motto: "*Supporting the best, so that they can become even better*".
- competitive procedure – all grants, prizes and scholarships are awarded on a competitive basis.
- *peer-review* method – the achievements of those taking part in competitions are assessed by academics.
- scientific excellence – the most important criterion for the awarding of support.
- the "*hard money*" principle – high selectivity in awarding support under all programmes, strict procedures for settling accounts for the amounts awarded.

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Assessment of the personality predisposition in order to enhance the professional activities

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Many studies (McKenney and Keen, May/Jun 1974; Rosenberg, Mead and Kelleher, May/Jun 1996; Pentland, Jan/Feb 2010) were conducted to assess and account which treats are responsible for outperforming people's successes. According to Marcus Buckingham and Donald O. Clifton (2001) the most efficient way for professional development is to explore and maximize the value of personal strengths. However, it is common that the young people, especially students, are not fully aware of their fundamental advantages.

During the presentation general, quick and accurate test on all participants will be executed, aiming to evaluate the personality and natural predisposition for development in work environment.

The expected outcome of this presentation will be the information for students which personality attributes they exhibit and which approach they apply for problems' solving. Based on this information, specific strategies to all students for boosting their talents will be provided. Consequently, some general advice how to achieve professional fulfilment and satisfaction will be proposed.

References:

1. Clifton, Donald O., and Marcus Buckingham. "*Now, Discover Your Strengths"* New York: The Free Press, 2001
2. McKenney, James L., and Peter G. W. Keen. "*How managers' minds work*" Harvard Business Review, May/Jun 1974: **Vol. 52** Issue 3, p79-90,
3. Pentland, Alex. "*We Can Measure the Power of Charisma*" Harvard Business Review, Jan/Feb 2010: **Vol. 88** Issue 1/2, p34-35
4. Rosenberg, Richard, Dana Mead, and Herb Kelleher. "*What's Personality Got to Do with It?*" Harvard Business Review, May/Jun 1996: **Vol. 74** Issue 3, p114-114

Oral Presentations

Oral Presentations

Analytical and Environmental Chemistry

The use of stripping voltammetry for testing heavy metals in rivers at Lodz Hills Landscape Park

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Created in 31 December 1996, Lodz Hills Landscape Park covers an area of 10,747 ha. It is located to the northeast of Lodz in two cities - Lodz and Brzeziny and five municipalities - in the area Nowosolna, Stryków, Brzeziny, Dmosin and Zgierz. Such location, apart from the benefits of tourism, entails risks associated with a strong anthropo lakes in the above area.

Since 2000 Students Scientific Society of the Department of Chemistry, University of Lodz, monitoring the surface water for their chemical composition. From time to time, on an annual basis, studies are performed, among others. heavy metals like lead, cadmium, zinc and copper. The last such cycle began in May 2010.

Research are carried out using the method of anodic voltammetry inversion, with mercury film electrode. This method is characterized by a high sensitivity and selectivity.

The first determination stage of need a special preparation of samples, designed to remove disturbing compounds in the process of analysis.

Proper determination is carried out in two stages. In the first stage - concentration, is followed by separation of marked substances on the mercury film. During the second stage - digestion, as a result of electrode process, metals are digestied. Voltammetric curve is recorded in the form of peaks corresponding to the presence of the metal. Quantitative determination of metals is carried out with standard addition method or the double standard addition method.

According to test results, can it be stated that, due to the studied ions, waters surface of Lodz Hills Landscape Park can be classified in the first class quality.

References:

1. A. *Cygański, Metody elektrolityczne*, WNT, Warszawa, **1995**.
2. W. Szczepaniak, *Metody instrumentalne w analizie chemicznej*, PWN, Warszawa, **2008**.

Thujone – a magic wand of Green Fairy? Comparison of thujone content in samples of absinthe from market and home distillation

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Absinthe is a high-proof alcohol distilled from macerate, which recipe mainly consist of flowers and leaves of wormwood and green anise. The first report of its production comes from Switzerland from 1792, and the development of the first recipe is attributed to Dr. Pierre Ordinaire, who produced it as a cure for all ailments.

Due to the psychoactive activity and its green color, absinthe is popularly called the "green fairy". Thujone, a chemical compound responsible for the all hallucinogenic effects of absinthe consumption, occurs naturally in wormwood, the main component of the macerate.

Increasing popularity of absinthes is observed particularly among young people. Because of its specific effects on the human brain, manufacturing and sale of absinthe has been prohibited for many years in many countries. Now, due to regulatory changes, it can also be bought legally even in Poland. However, because of high price, there are different ways of domestic production of this beverage, comprising: a prepared blend of suitable herbs (mostly wormwood - *Artemisia absinthium*) for maceration and distillation, or an extract of absinthe which needs only to be dissolved in alcohol. Low costs of these methods makes them increasingly popular.

The aim of this study was to determine the concentration of thujone using solid phase extraction (SPE), GC analysis and GC-MS evaluation [1] in different absinthes from domestic production: macerated and distilled from a mixture of herbs and made from extracts, and to compare results with two samples of commercially available beverages. The results have also been confronted with the EU standards [2] and the concentration of thujone claimed by the manufacturer of raw materials for the production of absinthe at home.

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In the world of drops and droplets – dispersive liquid-liquid microextraction in X-ray fluorescence analysis

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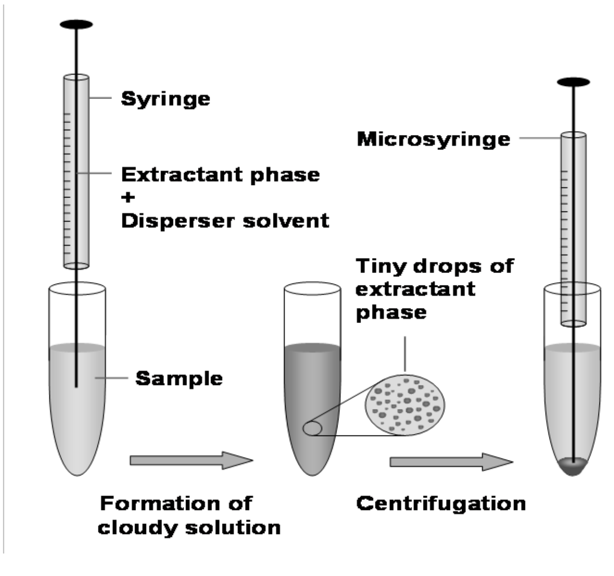
Liquid–liquid extraction (LLE) is widely used as a pre-treatment technique for separation and preconcentration of organic and inorganic analytes from aqueous samples. Despite its widespread use, LLE has several drawbacks, such as emulsion formation, multistage operation procedure or the use of large volumes of toxic organic solvents, which makes LLE an expensive and environmentally unfriendly technique. To overcome these problems new sample-preparation techniques, such as liquid-liquid microextraction (DLLME), were developed. These techniques can be considered as simple, low cost, rapid procedures, requiring low sample and extractant volumes. Moreover, they offer high recoveries and enrichment factors and easy linkage to most analytical methods [1,2].

In this work, the combination of DLLME with X-ray fluorescence spectrometry (XRF) is proposed for preconcentration and determination of the trace elements such as V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Se and Pb. Compared to electrothermal atomic absorption spectroscopy, XRF enables the simultaneous determination of many elements, which additionally reduces the time of analysis. In the developed procedure, an appropriate mixture of methanol (disperser solvent) and carbon tetrachloride (extraction solvent) was rapidly injected into the water sample containing analytes in the form of their complexes with ammonium pyrrolidinedithiocarbamate [3]. After centrifugation, 10 μL of the sedimented phase containing enriched analytes was pipetted onto the Millipore filters and measured using XRF spectrometer. The obtained results show good precision and accuracy of the method, low detection limits and high enrichment factors. DLLME was successfully applied for the XRF determination of metals in water samples.



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Tea as a source of dietary metals

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Tea is one of the most widely consumed beverages in the world, next only to water. Depending on the treatment of tea leaves, we can distinguish several types of tea like black, green, and less popular in Europe oolung tea. All types are produced from the same plant - *Camellia sinensis*. Green tea processing includes a step to inactive oxidizing enzymes, such as polyphenol oxidase, which partially converts monomeric polyphenols (mainly catechins) into dimeric/oligomeric compounds, such as theaflavins and thearubigins, responsible for the characteristic aroma and colour of black tea. Black tea is fully oxidized whereas oolong tea is a result of oxidation being stopped somewhere in between that of green and black tea and therefore contains flavonoids that are found in both teas. Tea is known for its healthy properties, because of the presence of tea polyphenols, mainly flavonoids. Drinking tea prevents platelet aggregation, reduces the risk of atherosclerosis and cancer, slows the effects of aging by removing free radicals, has antibacterial, antiviral properties. In addition, tea is rich in minerals such as Al, Ca, K, Mg, Mn. The content of metal ions in the infusion depends on both type of tea and water which is used for brewing.

The work is about determination of some metal ions such as Cu, Fe, Zn, Cr, Co, Mn in the in three kind of commonly consumed bagged teas: black, green and fruit. Microwave-assisted acid digestion procedure was used for dissolution of the samples and metal contents were determined by ICP-MS and FAAS. The levels of metals varied between tea types. The highest content of Cu, Cr, Fe and Co was found in black tea leaves, while fruit tea was a good source of Zn. To study the effectiveness of metal transfer from dry tea matter to infusion, different kind of water (deionised, tap and spring) were used for brewing. The efficiency of extraction using tap water was the lowest for Cu and Zn, but the highest for Fe and Cr (only from black tea). Natural water extracted the highest percentage of Cu and Zn from all studied teas.

An influence of thermal treatment conditions of hydrotalcite-like materials on their catalytic activity in the process of N_2O decomposition

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Nitrous oxide is known as strong greenhouse gas, and its global warming potential is about 300 times as high as that of carbon dioxide. N_2O is also responsible for destruction of ozone in the stratosphere. Each molecule of this gas emitted into the atmosphere has an average life time of about 150 years. One of the major anthropogenic sources of N_2O emissions are nitric acid plants, where N_2O is formed as a by-product in the ammonia combustion process. The catalytic decomposition of nitrous oxide is shown in the equation No. 1.

$$N_2O \rightarrow 1/2O_2 + N_2 \qquad (\Delta H^o = -163\ \mathrm{kJ/mol}) \qquad (1)$$

Hydrotalcite-like materials containing apart from magnesium and aluminum also copper and cobalt were prepared by co-precipitation method. These layered double hydroxides were calcined at 600, 700, and 800 °C, and additionally doped with various amount of potassium (0,9; 0,09 wt%). Obtained mixed metal oxides were characterized by powder X-ray diffraction, thermogravimetric measurements, BET surface area measurements, Uv-vis-DR spectroscopy, X-ray photoelectron spectroscopy and scanning electron microscopy (fig. 1). The prepared materials were tested as catalyst for low temperature (250-500 ˚C) N_2O decomposition.

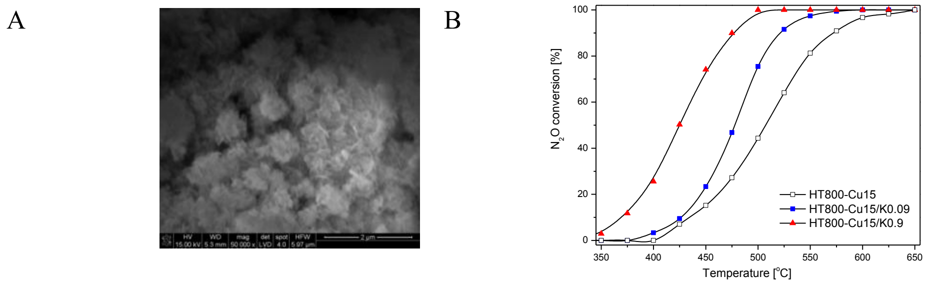

Fig.1. A – SEM images of the sample HT800-Cu15/0,9K, B- results of the catalytic tests for the sample HT800-Cu15 modify with different amount of potassium

The best results obtained for the copper-containing catalysts. An increase in the calcination temperature significantly activated the cobalt-containing catalysts. The opposite effect was found for the samples containing copper. The activation of the cobalt-containing samples was related to the formation of the catalytically active spinel phase (Co_3O_4). Additional introduction of potassium improved catalytic activity of the samples (fig. 2).

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Oral Presentations

Biotechnology

Biotransformations of selected steroid compounds in the culture of *Absidia coerulea* strain KCh 93

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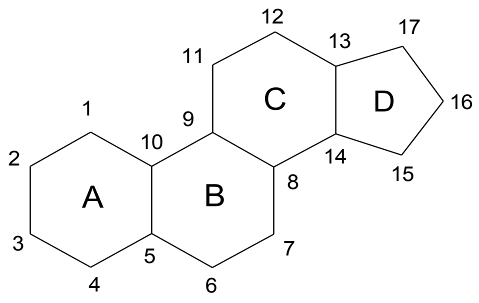
Steroids are a group of natural organic compounds present both in plants and animals. The basis of their structure is the steran skeleton (**1**). In addition, they contain specific functional groups, mostly carbonyl and / or hydroxyl and methyl at positions C_{10} and C_{13}, which determine their biological properties [1, 2].



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Depending on the location of these groups in the molecule, they may show, among others, such features as: being anti-inflammatory, sedative, anti-oxidant and anti-cancerous. They can be natural components to produce compounds useful in pharmaceutical and cosmetic industries. Preferred transformation of fungi may lead to demonstrating the ability to introduce a hydroxyl group to a molecule of substrate by cytochrome P450 [3].

As a result of biotransformation of 11α-and 17α-hydroxyprogesterone and androstendiol carried out with the Absidia coerulea KCh 93 strain, substrates hydroxyderivatives were achieved. Hydroxylations occurred respectively in positions 6β, 11α and 11β and 7α and 7β.

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Application of recombinant lipase from *Geomyces sp. P7* in enantioselective transestrification of selected alcohols.

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Lipases are one of the most versatile enzymes. They are used in the pharmaceutical, cosmetic, dairy industries and their industrial importance and usage continues to grow. Therefore, unprecedented was the discovery by the Institute of Biochemistry Research Group at the Technical University of Lodz unique properties of lipase from the Antarctic strain of filamentous fungi *Geomyces sp. P7*. It was found out that this strain is the best catalyst of enantioselective transestrification of 1-phenylethanol with vinyl acetate in cyclohexane. Despite these interesting properties industrial using of native enzyme will be almost impossible because of difficulties in cultivation of the strain producing this enzyme. It is characterized by the very slow growth, low biomass yield, and relatively low optimum growth temperature of around 10^0C. For this reason it was decided to expression of this enzyme gene in the host such as *Saccharomyces cerevisiae* and *Escherichia coli*. The aim of my work was to determine the feasibility of recombinant lipase catalytic transesterification of chiral, secondary and tertiary alcohols.

Oral Presentations

Coordination and Inorganic Chemistry

Optical versus photoinduced electron transfer (OET vs. PET) in TiO_2 photosensitization

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Titanium dioxide based materials are often used as a photocatalysts in various reactions. This semiconductor is highly photoactive upon UV irradiation conditions but application of visible light requires its modification affording the photosensitization effect. It can be achieved in different ways – by ion doping, synthesis of composites with other semiconductors or by surface modification with various compounds – transition metal complexes or organic compounds with donor groups.

In the presence of surface modified materials two types of photosensitization mechanisms can be distinguished. In the first one the surface modifier excitation is followed by interfacial electron transfer from the excited state to conduction band. This type of photosensitization is called Sakata-Hashimoto-Hiramoto process (*1*) or a photoinduced electron transfer (PET). It is fundamental for dye sensitized solar cells, but can also be observed for TiO_2 modified with metal complexes (e.g. $PtCl_4$ (*2*), ruthenium dyes). The second type of mechanism involves excitation of a surface titanium(IV) complex – The electron is transferred directly from the surface modifier to the conduction band of titanium dioxide. This process requires good electron donors immobilized on TiO_2 sufrace (e.g. catechol derivatives or cyanoferrates (*3*)). The mechanism of such photosensitization may be called as an optical electron transfer (OET) or Creutz, Brunschwig and Sutin model (*4*).

Experimental data show that OET mechanism can be observed for nanocrystalline TiO_2 modified with catechol or salicylic acid derivatives. Transparent colloidal solutions of these materials appeared to be capable of photocatalytic degradation of azur B (thiazine dye) and methyl orange. Properties and photocatalytic activity of such systems together with details of mechanistic studies will be presented and discussed.

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Nanocomposite catalysts for removal of the volatile organic compounds (VOC)

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Nowadays a vast majority of population is subject to harmful substances introduced into the environment due to the emission of contaminated fuels used in various branches of industry. Volatile Organic Compounds (VOCs) are the group of compounds which are always present in outlet gases. Present technology attempts to counteract this problem through seeking innovative solutions. The most common way for the reduction of themes emission is thermal oxidation of VOCs. However this method is not very efficient and may lead to the formation of many undesirable by-products like NO_x. That is the reason why more eligible path for removal of VOCs is catalytic oxidation. Catalysts used in air pollution control are currently in grate interest of researchers who are developing new catalytic systems based on nanometric materials characterized by new properties. One of the most promising catalysts is nanosized material based on cerium (IV) oxide. Mixed valences of Ce ions in ceria and formation of oxygen vacancies are the reasons why CeO_2 shows high catalytic activity in redox reactions [1]. It was also reported that catalysts containing selected transition metal oxides may present the activity similar to that found for the precious metal based systems.

In this work precursors of the nanostructured materials based on cerium (IV) oxide were prepared using a modified reverse microemulsion method [2]. Three series of materials were synthesized: pristine CeO_2, CeO_2 doped with cobalt, and Co_3O_4 doped with cerium. The obtained precursors were subjected to thermal analysis (EGA – TGA/DTG/SDTA) in order to determine optimal calcination conditions. The structure of the obtained nanostructured powders was estimated from powder XRD measurements. Analysis of elemental composition of obtained catalyst was performed by Optical Emission Spectroscopy with Inductively Coupled Plasma (ICP-OES). Surface morphology, specific surface area and pores distribution were evaluated on the basis of the N_2-BET method. The morphology of the obtained nanoparticles derived from different precursors differs from each other. The ceria doped materials formed mono phase solid solutions of fluorite–like structure.

All of the obtained materials were catalytically active in the incineration of selected VOCs molecules (methanol).

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Intermediate Temperature Solid Oxide Fuel Cell Membrane formed in Gelcasting Process from Ceria Nanopowder

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Solid Oxide Fuel Cell (SOFC), are the most efficient (up to 70%) energy sources [1]. The most important part in SOFC devices is solid electrolyte membrane. Actually, commonly used material for such the membranes is yttrium stabilized zirconia (YSZ). Operating temperature for this material is about 1000˚C, which make impossible to use SOFC in transport or another application, where is a problem related to heat conversion. That is why the scientists are looking for materials which can operate at intermediate temperature (around 500-800˚C). According to present knowledge, most promising ones are cerium (IV) oxide doped with trivalent cations [1-5]. The SOFC membrane must be strong, durable, gas-proof and thin as possible, without deterioration of its mechanical properties.

Gelcasting is a process for formation of complicate shapes from ceramic powders [6]. This process was applied to produce the thin ceramic films from ceria nanopowder. The nanopowders reveal high surface energy what leads to lowering of sintering temperature [7]. The optimal sintering temperature was determined from dilatometry technique (TMA). The morphology of the starting powders were characterized by N_2-BET (low temperature nitrogen adsorption) and DLS (dynamic light scattering) methods. Crystallite size was calculated from X-ray diffraction data using Scherer formula.

Shapes prepared in gelcasting process from ceria nanopowders were later fired at different temperature, then characterized by scanning electron microscopy (SEM) and atomic force microscopy (AFM). To show an influence of formation method, a standard uniaxially pressed pellets were formed from the nanopowder, fired in the same conditions and finally characterized. The transport properties of the ceria membranes were characterized by high temperature electrical conductivity (EC) as well as by impedance spectroscopy (IS).

Acknowledgement:

This work has been financially supported by the Polish Ministry of Science and Higher Education under grant no. N N209 099337. The part of the measurements was carried out with the equipmentpurchased thanks to the financial support of the European Regional Development Fund in the framework of the Polish Innovation Economy Operational Program (contract no. POIG.02.01.00-12-023/08).

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Synthesis and investigation of new molybdenum compounds containing the molybdenum clusters

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Transition metal oxides, such as molybdenum oxides, are used in many industrial applications and have gained interest both from technological and scientific points of view [2]. The main fields of industry where they are applied are catalysis, sorption, energy storage, molecular electronics, optical materials, and ceramics [3, 4]. An interesting example of this compound group are molybdenum oxides, which have a great industrial interest due to their optical and electronic properties. In fact these transition metal oxides can be switched between two different optical states prompted by photochromic, thermochromic or electrochromic effect. Compounds that contain molybdenum oxides substructures modified by organonitrogen ligands were classified as fifth class of oxides, in which organic materials play a significant structural role [5].

Polymorphism is commonly known, but relatively rare existing phenomenon [6]. Polymorphic transition influence many properties of a compound, for example: physical stability, chemical stability, manufacturability, or in case of drugs, change the kinetics of oral absorption. Relatively small changes in crystal packing may lead to significant differences in the crystal packing density and other properties of polymorphs[7,8].

Compounds containing many independent molecules in the unit cell of inorganic-organic compounds seem to be currently a subject of great interest both for pure science and for its industrial consequences, especially for pharmaceutical production and technical applications [9]. In the recent literature is observed an increasing amount of reports dedicated to the development of new compounds possessing Z'>1 and to study of their properties [10,11].

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Beyond the limits: A Brief Introduction to Superacids

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The concept of acidity is one of the first things that are being taught about reactivity of compounds. There are three definitions of acids – one given by Svarte Arrhenius in 1884, which is very limited in it's applications. Johannes Nicolaus Brønsted and Thomas Martin Lowry independently came in 1923 with the idea of tying acidity to a transfer of a proton. A third, conceptually different approach was conceived at the same year by Gilbert Newton Lewis, who recognized acid as a lone electron pair acceptor.

The main measure of acidity of a solution is the pH. In most cases in biological and chemical systems we may use the Henderson–Hasselbalch equation:

$pH = pKa + \log([A^-]/[HA])$

It is not without limitations – there is a number of approximations used. One cannot use it when there is a very strong acid or base, a very diluted or concentrated solution or a ratio of acid to base very far from 1.

For very concentrated solutions of strong acids we use the Hammett acidity function:

$H_0 = pK_{BH+} + \log([B]/[BH^+]$

where BH^+ is the conjugate acid of a very weak base B, with a very negative $pK_{BH}{}^+$.

The H_0 value is a solvent-independent quantitative measure of acidity and it allows to ignore the leveling effect and directly compare the acidity of different compounds.

Brønsted superacids are compounds which have the H_0 value lower than that of 100% H_2SO_4 (H_0 = -12). There is for example the fluorosulfuric acid which is about 1000 more times acidic that H_2SO_4. There are also Lewis superacids defined as compounds with Lewis acidic properties stronger than $AlCl_3$ like SbF_5. Very low H_0 values are obtained by mixing both kinds of superacids.

Superacids are used in both inorganic and organic synthesis due to their specific properties.

Alkaline earth metals coordination compounds with model amines possessing stiff conformation. Structural, thermal and spectroscopic properties.

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The coordination chemistry of alkaline earth metal ions is an active area of research due to their potential application possibilities in various fields such as biochemistry and environmental chemistry [1]. The magnesium and calcium are the metals of most interest [2] but other alkaline earth metals, like strontium, are also important. After the development of the drug - strontium ranelate - which reduces the incidence of fractures in osteoporotic patients, an increasing awareness of the biological role of this metal has grown [3]. Taking it into consideration, the investigations of coordination chemistry of these metals group is crucial not only due to the need of biologically active compounds of clinical applications but they are also important in terms of obtaining new, environmentally and human friendly (most magnesium and calcium compounds are low toxic [4]), materials of other usage.

To understand the properties and structures of the compounds of alkaline earth metals with 1,10-phenantroline (phen) and hexamethylenetetramine (hmta) and to find out about the differences in coordination ability of these metals according to slightly different electronic properties, the study was performed. Magnesium, calcium and strontium complex compounds with phen and hmta were obtained. To investigate the properties and structural differences imposed by the anion properties, the different salts of these metals were used and these are: sulphates, nitrates and halogenates. The structures of these complexes were determined and their characteristics were investigated. The TG analysis was used to study their stability and thermal decomposition. FT-IR, and, in case of phen, UV-VIS and fluorescence spectroscopy studies were also conducted.

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Influence of dopant concentration on electrical proprieties of Sm or Y doped ceria

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Solid oxide fuel cells (SOFC) are used to produce electricity from fuel oxidation process. Briefly, the fuel cell is an electrochemical device which combines hydrogen and oxygen to produce electricity, with water and heat by-product [1]. These cells are composed of anode, cathode materials separated by ceramic solid oxide as an electrolyte. They have the advantage of high efficiency, stability, flexibility in the type of fuel used and low cost. Their disadvantages are high operating temperature due to which start-up of the operation takes a long time and strong mechanical stresses during heating up and cooling down of the cell. For this reason, it is important to find new electrolyte to reduce the operating temperature of SOFCs and make these fuel cells more viable.In the literature it appears that in recent decades ceria doped with gadolinium has been used as material for SOFC electrolyte due to its high ionic conductivity at low temperatures and can be applied as oxygen sensors or oxygen membranes. The ionic conductivity of pure CeO_2 is comparatively low and dependent on purity of the precursor material, therefore, doping of ceria may be used for increase the ionic conductivity of ceramics.[2]

In this work a series of Sm or Y (3-24%) doped ceria was obtained using a reverse microemulsion method assuring formation of fine grains ceramic nanopowder. The doped ceria nanopowder was pelletized under uniaxial press and then sintered at 1100°C. The transport properties of the obtained materials were characterized by electrical conductivity measurements (EC) as well as impedance spectroscopy (IS).

Acknowledgement:

This work has been financially supported by the Polish Ministry of Science and Higher Education under grant no. N N209 099337. The part of the measurements was carried out with the equipment purchased thanks to the financial support of the European Regional Development Fund in the framework of the Polish Innovation Economy Operational Program (contract no. POIG.02.01.00-12-023/08).

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Catalytic activity of nano-$Ce_{1-x}Cu_xO_2$ as a function of electronic and defect structure

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The problem of Volatile Organic Compounds VOCs is becoming one of the most important environmental problems discussed by scientists around the World. Every year the Environmental Protection Agencies reduced the allowable emission limits for VOCs. In many cases it is impossible to eliminate completely emissions of volatile organic compounds. The most common practice for removal of VOCs is adsorption, mainly on an activated carbon. This is just a half of solution, because there is always problem of regeneration of the adsorbents. The easiest way would be the high-temperature oxidation of the adsorbed molecules. This method, is expensive and environmentally unfriendly, since at high temperatures, harmful byproducts like thermal nitrogen oxides (NO_x) can be formed. An alternative method is to use catalysts which lower temperatures of the reaction. One of the materials for catalytic low temperature incineration of VOCs can be cerium (IV) oxide. Ceria shows high catalytic activity in redox reactions thanks to many structural defects caused by doping or activation procedure.

In this study a series of materials based on cerium (IV) oxide dopped with copper (II) ions were obtained. Precursors of the oxide were synthesized using technique of reverse microemulsion (w/o) [1]. The optimal conditions of the calcination process were determined by the thermal analysis methods coupled with evolved gas analysis (EGA-TGA/DTG/SDTA). The morphology and the structure of samples were characterized by XRD and BET analysis. The morphology of the nanoparticles obtained from different precursors differs from each other. The ceria doped materials formed mono-phase solid solutions with fluorite–like structure. The electronic structure of the prepared catalysts was determined from high –temperature (T, pO_2) measurements of electrical conductivity.

The obtained materials were catalytically active in the incineration of selected VOCs molecules (ethylene, methanol or acetone). It was shown that better catalytic performance was gained for compounds with higher amount of copper (II) ions. The correlation between high-temperature electrical conductivity and the catalytic activity in VOCs incineration was found. The optimal defect structure of the catalyst has been proposed.

Acknowledgement:

This work has been financially supported by the Polish Ministry of Science and Higher Education under grant no. N N209 099337. The part of the measurements was carried out with the equipment purchased thanks to the financial support of the European Regional Development Fund in the framework of the Polish Innovation Economy Operational Program (contract no. POIG.02.01.00-12-023/08).

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Oral Presentations

Interdisciplinary

Electrochemical Impedance Spectroscopy results analysis – Genetic Algorithm application

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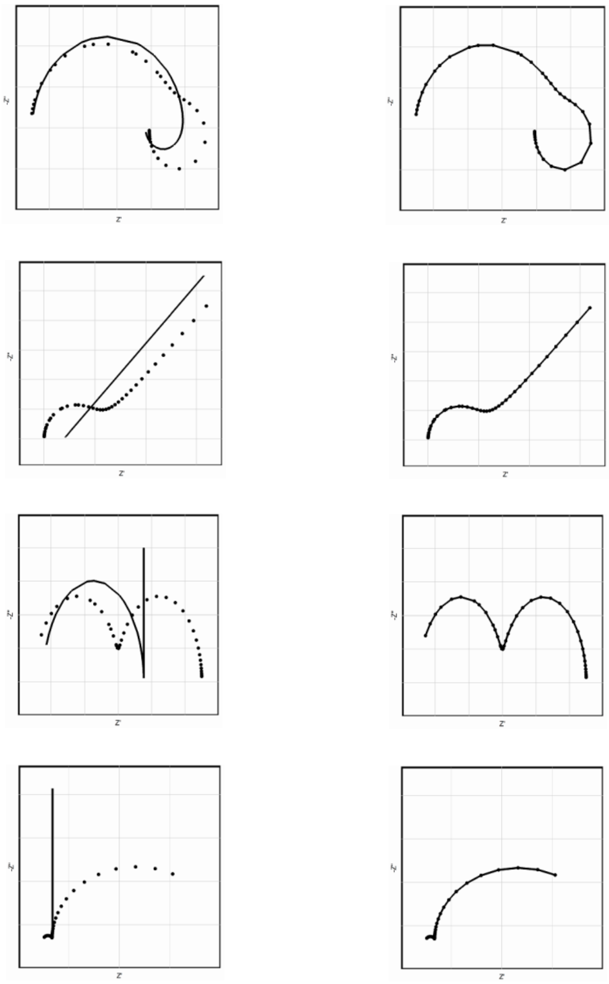
Standard procedure of Electrochemical Impedance Spectroscopy experiment results analysis, is to fit Equivalent Circuit parameters to experimental data. This is done most often by classic, deterministic algorithms of optimization (the most common is Complex Nonlinear Least Squares algorithm), the efficiency of which strongly depends on starting point.

In presented work, the hybrid algorithm was proposed, based on evolutionary algorithm (Genetic Algorithm) cooperating with classic, deterministic algorithm (Leveberg-Marquardt algorithm). The efficiency of proposed solution in delivering proper values of fitted parameters, in most cases exceeds 95%.



A B

Exemplary fitting results found by classic algorithm (A) and by hybrid one (B).

Hybrid polymer electrolytes based on aluminum oxygen core and polyethylene glycol

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Novel polymer electrolytes based on methylalumoxanes (MAO) and various chain length polyethyleneglycols (PEG) were successfully synthesized and pre-characterized[1]. In the current work $LiCF_3SO_3$ was added to the system with salt concentration fixed at 1 mol/kg level. Simple substitution reaction were carried between methylalumoxane and pelyethyleneglycols. The methyl groups bonded to the aluminum atoms belonging to the aluminum-oxygen core react here with the hydroxyl groups forming Al-O-C moieties. Multi branched (highly viscous) or crosslinked (plastic solid) hybrid polymer matrix were synthesized. Addition of lithium salt to the substrates leads in one step of reaction to the organic-inorganic polymer electrolytes which are here analyzed as potential systems for battery applications. Fully amorphous electrolytes were obtained for short analogs of PEG's as confirmed by DSC. Thermal properties with no sudden conductivity drop in temperature range from 70 to $-20^{o}C$ were obtained for samples of highly viscous, rubbery and bridle solid constitution. Above mentioned mechanical forms were characteristic for branched and crosslinked electrolytes respectively. Contrastively, for electrolytes without MAO content thermal changes were observed in DSC thermo grams originating from matrix freezing and resulting in the conductivity drop. This observation suggests existence of interaction of PEG with the MAO core. According to Hard-Soft Acid-Base principle suggested by Pearson where hard base interact with soft acid the explanation of the thermal properties of matrix can be attributed to the fact that ether (C-O-C) moiety is a hard base and Al-O-Al structure present in the core is a soft acid. Some discreet changes were observed in FT-IR spectra in area characteristic for C-O-C bond vibrations. After addition of salt where additional fractions of acidic and basic centres appear in the electrolyte being competitive verus the already present ones. Higher salt dissociation rates were observed with increasing MAO content in the matrix according to FT-IR data. To apply the electrolyte in the metallic lithium containing secondary battery passivation layer has to be characterized. When passivation layer was formed during annealing of system Li|LiX|Li without current flow a stable state was achieved with no further changes during electrochemical measurements. No changes of SEI layer were observed for current flow or voltage applied (chronopotentiommetry and chronoamperommetry regimes). Experiment was carried on up to 400 cycles during 15 minutes each. Preliminary stabilization of the SEI layer allows the determination of the diffusion coefficient dependency versus temperature for all studied electrolytes omitting disturbances originating from SEI formation during the measurements. Additionally viscosity of electrolytes was determined in temperature dependence to correlate with transport process in bulk of electrolyte. Results will be discussed and presented

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Raman and IR imaging of a glass painting from the 19th century

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The identification of components used in formation of a paintwork helps to better understand the techniques used in the past, and is also used in the art restoration or authentication of a work of art. IR and Raman spectroscopies are commonly associated with analysis of pigments, minerals, and organic materials and provide important advantages for the characterization of the art objects. Moreover, the information obtained from the vibrational spectra serve as diagnostic tool for the identification of original and degradation products that occur during aging and deterioration of the art object. Additionally, both methods work in imaging mode that reveals spatial distribution of components, if a sample constitutes cross section of the investigated object. In this work, we present IR and Raman studies of the glass painting "Ecce Homo" from the Ethnographic Museum in Cracow. This painting was painted in the middle of 19th century by unknown artist from the Orava region.

The aim of this investigation is to recognize the inorganic (fillers and pigments) and organic (pigments and medium) compounds in complex multi-layered build-up. The imaging profiles were recorded by using FT-Raman mapping and supported by Raman spectra collected with excitation lines at 514 and 633 nm. The ATR FT-IR and reflection FT-IR imaging were also performed. In this way the stratification of the art work and the distribution of the pigment and medium within layers is preserved. Results obtained by these methods have given an insight in distribution of these compounds in the paint layers. For instance, the Raman spectra reveal only the presence of inorganic pigments, whereas the IR profile indicates the presence of some pigments and organic compounds used as a paint binder or formed due to degradation processes.

CCL/Li_2MnSiO_4 - nanocomposite cathode material for safe Li-ion batteries

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Rechargeable Li-ion batteries, due to their high energy density per weight and volume unitare key components ofthe portable electronic devices required by today's mobile society.[1] Increasing public awareness of environmental problems and searching for pure energy entail fast development of electric and hybrid vehicles (EV/HEV) market. Technology of EV/HEV require safe, efficient, environmental friendly and cheep batteries.

The family of dilithiumorthosilicates Li_2MSiO_4 (M = Mn, Fe, Co, Ni) is a group of potential polyanionic cathode materials for Li-ion batteries. Their theoretical capacity which is almost two times higher than commonly used lithium cobalt oxide and high chemical stability makes Li_2MSiO_4promising material for Li-ion cell cathodes.[2] The most serious limitation of dilithiumorthosilicates is their poor electrical conductivity. Conductivity of electrode material can be improved by coating with conductive carbon layer (CCL) and minimizing grain size.[3]

Dilithium manganese orthosilicate was successfully synthesized by sol-gel Pechini method. CCL/Li_2MnSiO_4 composite was produced in a one-step process using organic precursor matrix as a source of carbon.Choosing appropriate conditions of calcination allowed to control the thickness of formedcarbon layers. Obtained composites were investigated using EGA-TGA/DTG/SDTA, XRD, IS, BET and electrical conductivity measurements.

Acknowledgement

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The part of the measurements was carried out with the equipment purchased thanks to the financial support of the European Regional Development Fund in the framework of the Polish Innovation Economy Operational Program (contract no. POIG.02.01.00-12-023/08).

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Synthesis of gold nanorods ligands for biomedical applications

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Nanotechnology is a rapidly expanding field of science, the biomedical applications of which are steadily increasing. Recently, thanks to their unique properties, nanostructures have begun to play an important role in the Photothermal Therapy [1]. This approach, used in cancer treatment, is an alternative to Photodynamic Therapy. The basis for this therapy are structures having the ability to convert absorbed light energy into heat with high efficiency [2].

Attributes which provide nanostrucures (mainly nanoparticles, nanorods and nanospheres) with interest of researchers in the context of Photothermal Therapy are: high conversion efficiency of absorbed visible or infrared light into heat, the ability to tune the spectral range of absorption and high photostability [**Błąd! Nie zdefiniowano zakładki.**]. Moreover, large capacity of nanoparticles functionalization with biologically active compounds [**Błąd! Nie zdefiniowano zakładki.**, 3] extends the field of their therapeutic applications to antibacterial and antifungal therapy.

Ligands useful in this project are signal peptides [4,5], which facilitate the internalization of nanoparticles attached to them into the cells of microorganisms, as well as sugars [6] and their analogs – iminosugars involved in intercellular interactions.

The aim of this study was synthesis of signal peptides (**Błąd! Nie można odnaleźć źródła odwołania.**) and iminosugar derivatives (**Błąd! Nie można odnaleźć źródła odwołania.**), as well as synthesis of gold nanorods and attempt to modify them using the obtained ligands. Resulting material would have potential antimicrobial activity [7].

Cys – LINKER – PEPTIDE

Figure 2 Structure of synthesized signal peptides.

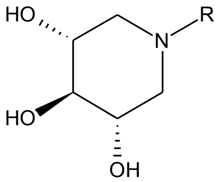

Figure 1 Structure of synthesized iminosugar derivatives: N-alkylated-1,5-dideoxy-1,5-iminoxylitol.

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Oral Presentations

Organic and Supramolecular Chemistry

Asymmetric Organocatalytic Synthesis of γ-Nitroketones with a Quaternary Stereogenic Centers

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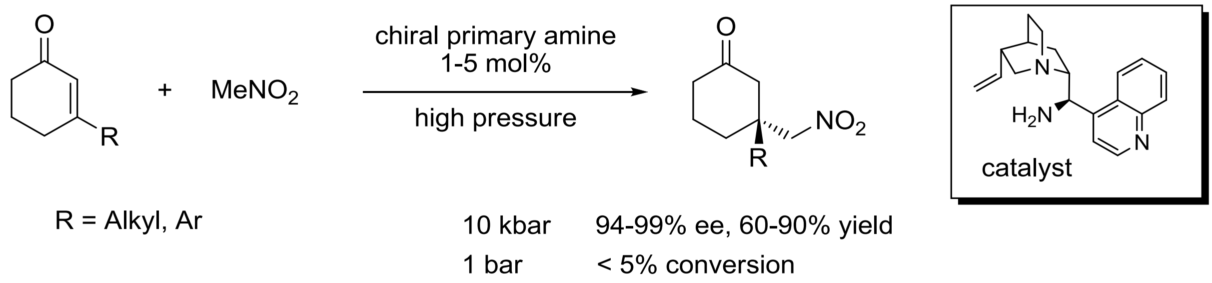
Development of new asymmetric organocatalytic methods and processes[1] has become an important direction in modern stereoselective organic synthesis. Conjugate additions to α,β-unsaturated carbonyl compounds belong to the most important and versatile reactions, successfully carried out in organocatalytic manner.[1] However, this type of asymmetric transformations is practically restricted to β-mono-substituted Michael acceptors. We focused our attention on reactions of prochiral β,β-disubstituted enones with various carbon nucleophiles, leading to products containing quaternary stereogenic centers. Until now β,β-disubstituted cyclic enones were successfully employed in organocatalytic hydrogenation[2] and epoxidation.[3] 1,4-Conjugate addition of nitroalkanes is also possible, however is limited to 3-*n*-alkylcyclohexenones and require long reaction time and 20 mol% of catalyst.[4]



In this communication we present examples of enantioselective conjugate addition of nitroalkanes to cyclic and selected acyclic enones, catalyzed by chiral primary-amines. We found that high pressure (*ca.*10 kbar) remarkably accelerate investigated reactions with low loading of catalyst and very high enantioselectivity.

Acknowledgements: Many thanks to Professor Janusz Jurczak for his help and encouragement. Financial support from the Ministry of Science and Higher Education (grant no. N N204 145740) and Foundation for Polish Science are gratefully acknowledged.

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Asymmetric Organocatalytic Friedel-Crafts Reactions under High Pressure

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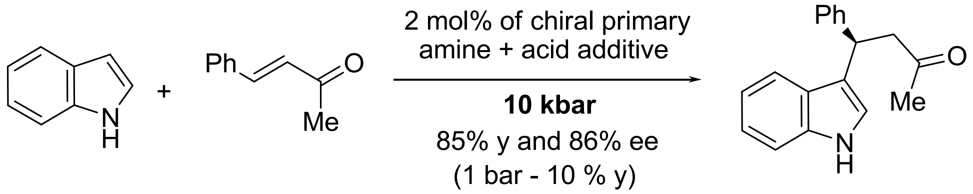
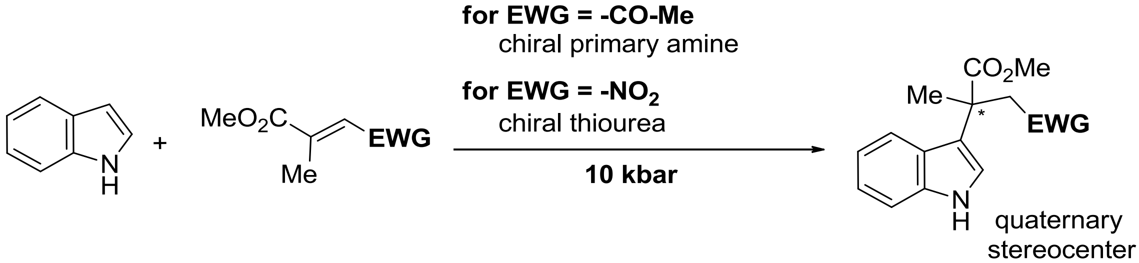
Asymmetric organocatalysis is a very attractive way to produce chiral molecules, however, in many reactions the limitations concern high loading of catalyst, long reaction time, and narrow substrate scope. In our opinion, combination of organocatalysts with **high-pressure methodology can increase efficiency** of some reactions.[1]

The goal of our research is to investigate the influence of high pressure (up to 10 kbar) on asymmetric organocatalytic **Friedel-Crafts alkylation of indoles with α,β-unsaturated ketones and nitroolefines** in the presence of catalytic amount of chiral primary amines and thiourea derivatives.[2] The high-pressure Friedel-Crafts reaction is efficient even with 1-2 mol% of catalyst.



We also found that very difficult reactions of indole with β,β-disubstituted enones and nitroolefines, leading to products containing **quaternary stereogenic centers**, can be successfully performed under high pressure conditions.



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Self – assembly of gold nanoparticles covered with rod – like liquid crystals

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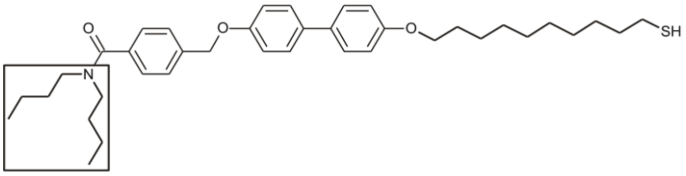
Moving from macro to nano scale can reveal previously unknown properties of a substance already well known, so that it can find a completely new applications. Nanotechnology is engaged in the manufacture of objects with sizes in the range of several nanometers (e.g. carbon nanotubes, metallic nanoparticles), as well as their examination. Much attention is dedicated to metal nanoparticles, including gold. Gold nanoparticles (AuNPs) are the most stable of all of the metallic nanoparticles. Thanks to nanoparticles' ability to modify their surface, they can be used in catalysis, medicine or photonics(**1**).

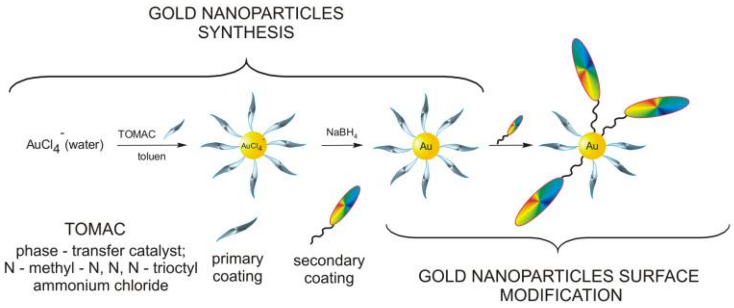
Liquid crystals (LC) compose a state of matter that has properties between those of a conventional liquid and those of a solid crystal. For instance, an LC may flow like a liquid, but its molecules may be oriented in a crystal-like way.

In many cases size of nanomaterials influenced their properties and potential applications, so it is obvious that we need to precisely control AuNPs dimensions. The bottom – up approach (used in my work) and self assembly (which is possible due to the presence of liquid crystals) promise solution to this challenge.



Scheme 1.

During my work (**2**) I synthesized mesogenic / promesogenic, rod – like ligands with identical tricyclics cores and thiol groups (one of them is presented above – ***Scheme 1)***. Part of the molecule, which was different for every ligand, was the type of the terminal substituent – amide groups, obtained from various secondary alkyl amines. Those compounds were subsequently used to modify the surface of AuNPs, exploiting modified Brust – Schiffrin method (***Scheme 2***). In my speech I will discuss *if* and *how* new mesogenic (or promesogenic) ligands can influence self – assembly of gold nanoparticles



Scheme 2. Synthesis of AuNPs.

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H- and Π-shaped liquid crystals: synthesis, molecular structure and phase properties

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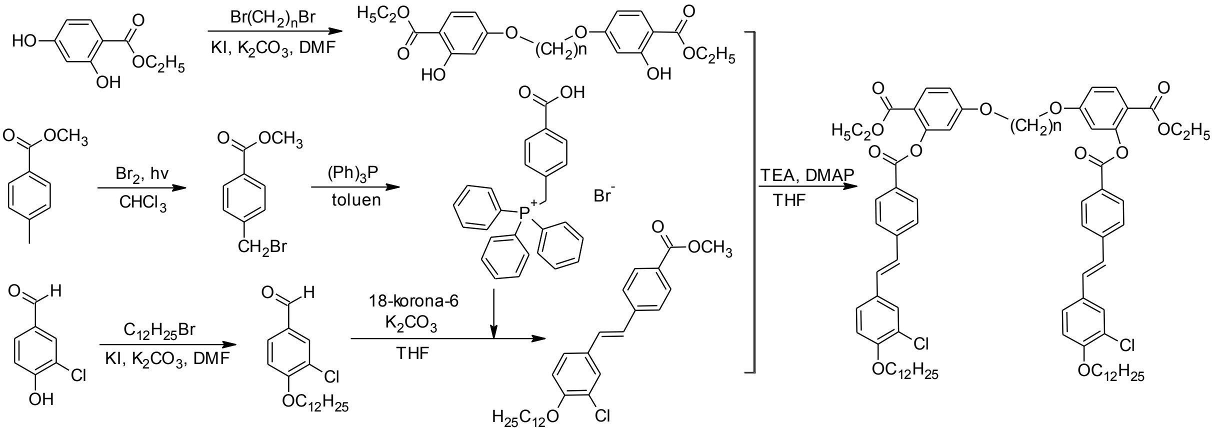
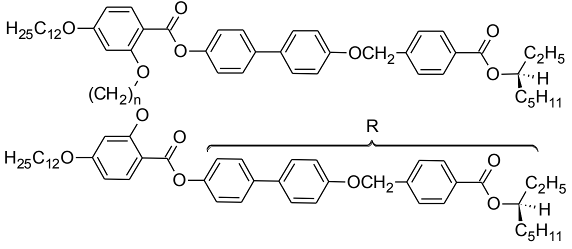
One series of new Π-shaped and six series of new H-shaped liquid crystalline dimeric molecules were synthesized and their thermotropic properties were studied by DSC and polarizing microscopy. These compounds consist of two identical mesogenic units linked through a flexible spacer containing 1 ÷ 6 methylene groups.

Representative procedure of the synthesis of Π –shaped dimer, comprising of two parts, is outlined in **Scheme 1**.

Scheme 1



Scheme 2



Representative molecular structure of H-shaped dimers is outlined in **Scheme 2.**

The analytical data, as well as experimental details, can be found in ref. 1 and in the supplementary information.

- ✓ Most of the obtained compounds exhibit nematic and / or smectic (A, B, C) phases (probably it is the first smectic A and B behaviour of H- and Π- shaped mesogens)
- ✓ An odd - even effect of the central polymethylene spacer on the transition temperatures as well as on the thermodynamic parameters for phase transitions has been observed (in comparison, ΔH_{iso} and T_{iso} increases for odd-membered, but decreases for even dimers).

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New air stable and solution processable organic semiconductors for field effect transistors – synthesis and characterization of triarylamine derivatives of arylene bisimides

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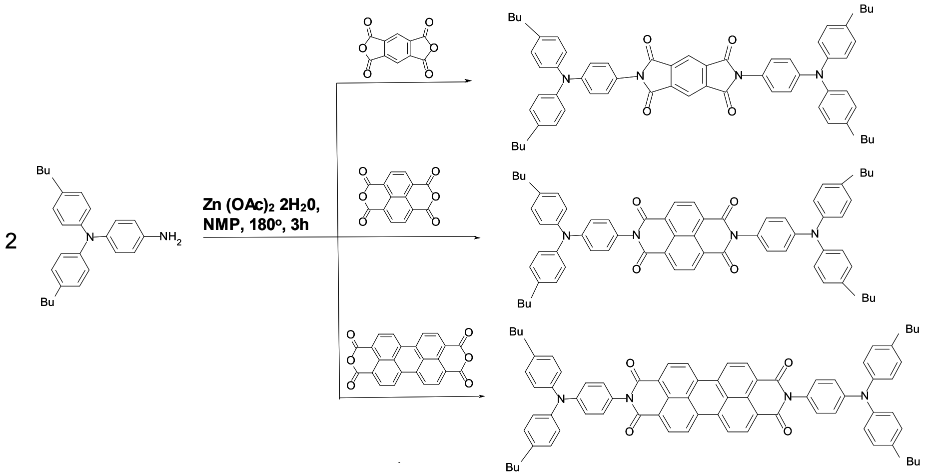
New solution processable organic semiconductors, consisting of pyrromelitic, naphthalene or perylene bisimide core and triarylamine N-substituents, have been synthesized. All three compounds are electrochemically active and undergo reversible oxidation and reduction as evidenced by cyclic voltammetry investigations. The oxidation process involves the transformation of the triarylamine substituent into a radical cation as proven spectroscopically and spectroelectrochemically. The reduction process occurs at the arylene bisimide core leading to the formation of a radical anion and eventually a dianion in the second step. This is in perfect agreement with DFT calculations which show that in all three molecules the HOMO orbital is located on the triarylamine moiety whereas the LUMO one on the bisimide core. In all molecules the electrochemically determined positions of the HOMO levels are below -5.0 eV *vs* the vacuum level, whereas the LUMO levels are close to -4.0 eV. Taking into account these values, the new compounds seem appropriate for fabrication of single component, air operating ambipolar transistors. However, contrary to the expectations, they show the field effect only in p-channel FETs with no effect in the n-channel configuration. The hole mobility measured in the saturation regime of all organic (CYTOP dielectric) FETs approaches 10^{-4} $cm^2V^{-1}s^{-1}$ – the value slightly exceeding that measured for low molecular weight, amorphous triarylamine semiconductors.



Acknowledgement

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Preparation of conjugated linoleic acid (CLA) isomers

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Conjugated linoleic acids (CLA) are a family of positional and geometric isomers of octadecadienoic acid (C18:2), with two conjugated unsaturated double bonds at various carbon positions in the fatty acid chain. The natural source of CLA are milk and dairy products.

An increasing interest of CLA is attributed to its potential health benefits. It has been reported in studies on animals that CLA have anti-cancer properties. Researchers have also found that isomer 9-*cis*, 11-*trans* of CLA can decrease the risk for cardiovascular disease and risk of inflammation. Nevertheless CLA is best known for its body weight management properties, which include reducing body fat and increasing lean muscle mass.

The aim of the presentation are biological properties of CLA, its commercial applications and methods of chemical synthesis of CLA isomers. We will also show selected spectroscopic data analysis of CLA.

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Oral Presentations

Polymer, Biopolymer and Technological Chemistry

Synthesis of chitosan nanoparticles using ultrasound

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Polymeric materials have been used for many decades in biomedical applications such as drug delivery, implants, contact lenses, vascular grafts, dental materials, and select artificial organs. Their useful and tunable mechanical properties have offered broad utility in the structural support or replacement of tissues or in controlled retention and release of drugs. The development of nanoparticulate systems for drug delivery allows drug release to be carefully tailored to the specific treatment site through the choice and formation of various drug-polymer combinations. In recent years, chitosan-based microspheres have been widely studied for the controlled release of drug systems such as antibiotics, proteins, peptide drugs or vaccines [1-2].

Chitosan is a natural origin polysaccharide which meets the criteria of biocompatibility and bioavailability. Its nanoaggregates may be used as a drug carrier or as well as bioactive substance alone - the results of some studies indicate its possible immune system stimulating properties [3] and ability to suppress tumor growth [4].

Many methods of synthesis chitosan nanoparticles are known e.g. complexation in the protonated state with polyanionic electrolytes [5] or water-in-oil emulsion based strategies [6].

In this study, physical nano-sized aggregates of chitosan were obtained in reverse emulsion using ultrasound in the absence of cross-linkers which are often regarded as toxic in parenteral administration. The impact of molecular weight of chitosan on particle size and size distribution was measured. The influence of freeze-drying on the structure and size of particles was investigated.

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Epoxy resins and their mechanical properties

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On the basis of the mechanism of photoinitiation, photopolymerization reactions can be broadly divided into free radical and cationic systems. In most popular free radical systems, light-sensitive photoinitiator molecules present within a monomeric liquid react with photons of light to generate highly reactive free radicals [1]. These radicals initiate the polymerization process, attacking reactive double bond groups in monomer molecules and converting them into a polymer. Multifunctional monomers or oligomers that contain multiple reactive groups are commonly used to create solid networks of polymers in rapid cross-linking reactions. A wide variety of commercially available monomers and oligomers can be used in this process. The most popular are epoxy-acrylates, acrylourethanes, polyesters containing acrylic polymerisable groups at the chain ends, and unsaturated polyester resins obtained by diluting unsaturated polyester in acrylated monomers (reactive diluents) [2,3]. Monomeric acrylates and methacrylates are less frequently used because they are relatively volatile, toxic, and have an unpleasant odour [4]. Solid monomers, obviously have lower toxicity.

In this work photopolymerization of commercially available bisphenol A epoxy diacrylates with bis[4(2-hydroxy-3-methacryloyloxypropoxy)phenyl]sulfide - the monomer synthesized by us is presented. As this compound is solid at room temperature, in its polymerization reactive diluent N-vinyl-2-pyrrolidone (NVP), which is also comonomer, has been applied. As photoinitiator 2-hydroxy-2-methyl-1-phenylpropan-1-one (Darocur 1173) was used. Thermal and mechanical properties of the obtained compositions were studied.

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Adsorption of methyl-ethyl ketone on polymer-derived carbon supported on MCM-41-type silicas with various pore size distributions

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Volatile Organic Compounds (VOCs) are one of the most hazardous group of gaseous pollutants discharged into the atmosphere. Their negative influence on the human health (related to mutagenic and carcinogenic properties of some VOCs) as well as the role in smog formation and stratospheric ozone devastation has been recognized. VOCs are responsible for inducing of many incurable dangerous illnesses, e.g. various types of cancer, heart disease, asthma, liver and the central nervous system damages. Thus, there are rigid acts regulating the permissible concentration of VOCs in indoor air and industry exhaust gases and opening the necessity of intensive study on the development of efficient ways of VOCs' elimination.

A large number of different methods of VOCs removal, based on catalytic and thermal oxidation, cryogenic condensation, biofiltration and gas permeation, can be used in an industrial scale. Nevertheless, adsorption seems to be the most effective, cheapest and environmentally friendly technique which additionally provides the recovery of adsorbed VOCs. The commercial adsorbents of VOCs are activated carbons obtained by carbonization and activation of biomass or coal. Unfortunately, microporosity of activated carbons results in diffusion limitations and excluding adsorption sites located on the inner surface of these materials to be active in the process. In our approach we extend an accessible surface of carbon by deposition of polymer layers on MCM-41-type mesoporous silica supports followed by thermal activation. The influence of pore size distribution of MCM-41 support on the adsorption capacity in the removal of methyl-ethyl ketone (MEK) vapour was studied.

Three MCM-41 (C_{12}, C_{16} and C_{18}) silica sieves with various pore size distributions were obtained by soft-templated synthesis using dodecyl-, hexadecyl- and octadecyltrimethylammonium chloride, respectively, as pore forming agents. The hybrid PAN/MCM-41 materials were prepared by an introduction of various amounts of polyacrylonitrile onto a SiO_2 surface by precipitation polymerization in an aqueous slurry of required support [1]. The range of intended PAN/MCM-41 mass ratios was 0.1 – 2.0. The resulting precursors were carbonized under the previously optimized conditions (350°C, 4 h) in an argon atmosphere [2].

The samples were characterized with respect to textural properties and coating effectiveness. Adsorption tests for the MEK elimination were performed under dynamic conditions. MEK was chosen as a probe molecule representative for a wide family of ketones being frequently components of emitted VOCs.

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Adsorption of Fe(III) cations on poly(sodium acrylate)/poly(acrylamide)/montmorillonite nanocomposites

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In recent years polymeric gels have attracted great attention in many fields of science. Hydrogels have an intermediate state between liquid and solid providing an ability to absorb and store water and aqueous solutions. Due to these properties, they are widely used in hygienic products, horticulture, drug-delivery systems, removal of heavy metal ions from waste water and stabilization of mineral sediments [1]. It was shown that an introduction of some inorganic species, e.g. layered clays, improves widely the swelling ability and sorption capacity of hydrogels. The most usable clays are smectite-type layered silicates including montmorillonite. Some examples of the synthesis and characterization of acrylate/montmorillonite nanocomposites can be also found in literature. These hydrid materials are obtained by in situ polymerization in aqueous slurries containing 5-10% of clay. Many studies on the swelling properties, the cationic dyes sorption as well as the abatement of cations of heavy metals from water solutions were performed [2-4]. The so called superabsorbents, synthesized on the basis of acrylate monomers exhibited high absorbency of distilled water in range of 120-150 $g_{water}/g_{nanocomposite}$. Moreover, high adsorption efficiency in the elimination of cations, for example Pb(II), Ni(II), Cd(II) and Cu(II), was observed for these materials [4].

A series of hydrogel/clay nanocomposites based on acrylamide (AAm) and sodium acrylate (SA) as well as acrylamide/sodium acrylate copolymers was synthesized in the presented work. Acrylic acid was neutralized using the equimolar amount of NaOH (30% solution in distilled water) in ice/water bath. The same amount of crosslinker MBA (N,N'-methylbisacryamide) and initiator APS was used during all the syntheses. The raw clay (montmorillonite Wyoming or Zębiec) and monomers were mixed at mass ratio of 1:1. The polymerization reaction was carried out at 65°C for 3 h to ensure the full conversion of the monomers. The composition and structure of the synthesized nanocomposites were examined using DRIFT, elemental analysis and powder X-ray diffraction. The obtained materials were tested in a role of adsorbents of Fe(III) cations from an aqueous solution. The sorption capacity was determined using the spectrophotometric thiocyanate method. The Langmuir adsorption model was found to be the best appropriate for a description of Fe(III) adsorption on the tested nanocomposites.

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Oxidative dehydrogenation of ethylbenzene to styrene over carbon based catalysts

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Styrene, beside ethylene, propylene and vinyl chloride, belongs to the most important monomers in the plastic industry, and is used for the production of polystyrene (PS), polystyrene-containing copolymers, polyester resins, synthetic rubbers, latexes, lacquers and paints. The annual world production of styrene exceeding $13 \cdot 10^6$ tons [1] is based on two main processes: dehydrogenation of ethylbenzene (about 90% of the worldwide production) and epoxidation of propene.

The equilibrium-controlled ethylbenzene dehydrogenation is performed in the presence of excess of steam at relatively high temperatures (above 550°C). The thermodynamic limitations caused that alternative ways of transformation of ethylbenzene into styrene are developed. The oxidative dehydrogenation of ethylbenzene seems to be the most promising among the proposed methods. In opposite to the endothermal commercial technology, the oxidative dehydrogenation is a strongly exothermal process, which omits the thermodynamic barriers in the ethylbenzene conversion. This process can be carried out over two types of catalysts. Firstly, the catalysts with medium strength acidity (e.g. alumina, zeolites or carbon molecular sieves) can be applied. It has been proved that in this case the high activity is caused by the presence of so called 'active coke' onto the catalyst surface. The redox-type catalysts based essentially on $MgO\text{-}V_2O_5$ are another type of catalysts active in the oxidative dehydrogenation of ethylbenzene The reaction over the redox oxide systems proceeds via the Mars-van Krevelen mechanism: the lattice oxygen oxidizes ethylbenzene molecules, and air is responsible for reoxidizing the reduced catalyst [1, 2].

In the presented work, highly ordered mesoporous carbon (CMK-3) was tested as a catalyst for the oxidative dehydrogenation of ethylbenzene to styrene in the presence of oxygen. The CMK-3 carbon was obtained by the hard-template synthesis using mesoporous silica sieve SBA-15 and sucrose as a carbon source. Highly ordered mesostructure replicated from SBA-15 was formed after a removal of silica template by dissolving with hydrofluoric acid. The porosity of the resulting carbon material was constituted by well-ordered hexagonal, cylindrical mesopores interconnected by micropores. The value of BET surface area for the CMK-3 carbon achieved 1270 $m^2 g^{-1}$ and total pore volume equaled to 1,28 cm^3g^{-1}. Our study demonstrated that the ordered mesopores of CMK-3 can be efficiently used for the oxidative dehydrogenation of ethylbenzene to styrene. The experiments showed that the 'active coke' formed during the activation of the CMK-3 surface in the oxidizing atmosphere plays a significant role in the catalytic activity.

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Thermal degradation of polyacrylonitrile deposited on mesoporous silicas studied by FT-IR and XPS

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The organic–inorganic composites as precursors of carbon layers deposited on supports have attracted wide attention over the last decade. Because of high effectiveness and low manufacturing costs these materials have gained a wide range of applications, especially in adsorption and catalysis. They can be also applied to eliminate different pollutants from air and wastewater, mainly volatile organic compounds (VOCs).

In the presented work, carbon/silica composites obtained by carbonization of polyacrylonitrile deposited directly on the surface of mesoporous supports (silica gel and MCM-41) are studied. Such materials exhibit highly developed surface area and porosity. Additionally, they show no diffusion limitations in the case of large molecules adsorption. The studied C/support composites were prepared by the radical, precipitation polymerization of acrylonitrile (AN) in an aqueous suspension of an inorganic support and then carbonized under controlled conditions.

Thermal decomposition of synthesized materials was studied by thermogravimetry (TG), X-ray photoelectron spectroscopy (XPS) and diffuse reflectance infrared Fourier transform (DRIFT). TG analysis showed some stages of carbonization of the PAN/support precursors in an inert atmosphere, which could be assigned to the chemical transformations by DRIFT and XPS:

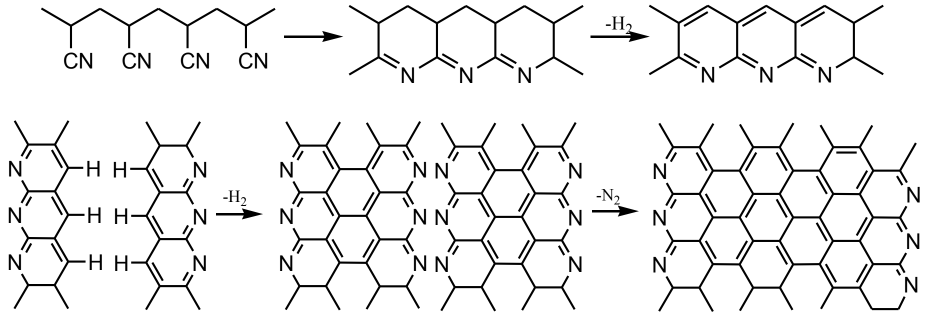

Fig. 1. Mechanism of thermal decomposition of PAN [1]

DRIFT measurements gave insight into the changes of the functional organic groups, whereas XPS experiments provided quantitative information regarding the element concentration in the uppermost surface layer.

This work was supported by the Polish Ministry of Science and Higher Education under the grant no. N N507 553238. Rafał Janus wishes to thank the Foundation for Polish Science MPD Programme co-financed by the EU European Regional Development Fund for the financial support.

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Hybrid polymer coatings obtained in simultaneous radical and cationic polymerization

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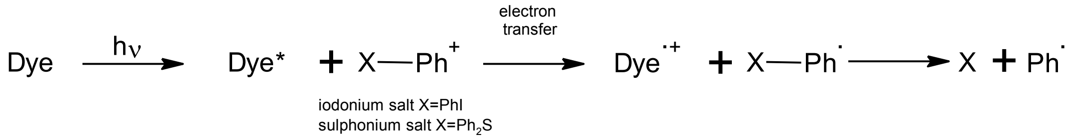
Radical and cationic light-induced polymerization is of high interest due to its convenient process conditions. It is controlled by manipulating the intensity and wavelength of radiation [1]. Photopolymeriztion has gained a use in stereolithography, photocurable varnishes, inks, adhesives, optoelectronics and medicine [2].

Dye initiating systems that undergo oxidizing sensibilization, are able to initiate radical and cationic polymerization [Scheme 1]. In a such mechanism, an excited molecule of a dye is an electron donor that undergoes an oxidation process forming a cation-radical. A co-initiator present in a formulation is reduced with simultaneous decomposition [3]. In order to achieve polymerization process under visible light onium salts as photosensitizers and dyes as photosensibilizers are used. Onium salts like sulphonium and iodonium with non-nucleophilic anions generate stable, strong Broensted acid that induces cationic polymerization. The photolysis of the sensitizer gives radical products inducing radical polymerization [4]. Presented research is associated with application of dyes, derivatives of 12H-quinoxalino[2,3b][1,4]benzothiazine as photoinitiators of radical and cationic polymerization in hybrid systems. Radical systems are based primarily upon acrylates and cationic mainly on epoxides. The introduction of hybrid systems gives higher reactivity and lower sensitivity to moisture than such formulations alone [5].

Photoredox pairs consisting of a dye and an onium salt are effective initiators in photoplymerization process.



Scheme 1

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Novel method of fabrication ceramics shapes: gelcasting

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In previous years ceramic nanopowder has achieved special interest. Using nanoparticle ceramics in comparison to micrometric ones has many advantages like reduced times and temperatures of sintering. Moreover, the ceramic may be produced by a gelcasting process and formed in many complex shapes.

Preparation of material with high mechanical properties, complex shaped demands applying the gelcasting method. It is a process of ceramics forming without using clay minerals. Instead, there is a powder (e.g., Al_2O_3, ZrO_2, SiC, CeO_2) suspension in aqueous monomer solution with cross-linker. Colloidal solution is homogenized for few hours, activated and casted into an appropriately designed mould. Then the mixture is "in situ" polymerized to form a polymer-water-ceramic gel which immobilizes the dispersed ceramic particles in the defined shape. Prepared gelly material is dried to give the so-called "green body" and removed from the mould. Finally it is fired giving durable and strong material in defined shape.

In this study the gelcasting process was applied to formation of SOFC cerium oxide(IV) membranes, as well as to formation of catalyst support aluminium oxide rods.

The surface of materials was characterized by scanning electron microscopy (SEM) and atomic force microscopy (AFM) techniques. Low temperature nitrogen adsorption (N_2-BET) were used to characterize porosity of prepared samples.

Acknowledgement:

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Oral Presentations

Theoretical and Physical Chemistry

Hyaluronan binding by CD44: A preliminary molecular dynamics study

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CD44 is a major cell surface receptor for hyaluronan (HA), i.e. a high–molecular weight copolymer of N-acetylglucosamine (GlcNAc) and glucuronic acid (GlcUA), (□-1,3-GlcNAc-□-1,4-GlcUA)$_n$. The molecular dynamics (MD) simulation of the murine CD44 in complex with a HA heptasaccharide was performed basing on the crystal structures obtained by Banerji et al. [1]. The results confirm that the contact of CD44 with HA is dominated by hydrogen bonds and van der Waals forces. In addition, the two conformational forms of the HA$_7$-CD44 complex reported experimentally can also be observed during MD simulations. These structures differ mainly in the degree of contact between HA$_7$ and the Arg45 residue. The ligand-induced order-to-disorder transition of the C terminus of CD44, reported by Takeda et al. [2] was not observed. Additionally, some thermodynamic parameters accompanying to HA binding by CD44 were estimated.

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Experimental and theoretical studies of complex formation by antioxidants in the micellar solutions

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It is well known that the activity of antioxidants depends not only on their molecular structure but also on the character of the medium in which the oxidation process occurs. In this communication the results of systematic studies of vitamin C activity in different media by UV-vis spectroscopy are presented [1,2]. As follows from the studies, in diluted surfactant solutions (SDS, CTAB) vitamin C undergoes atmospheric oxidation more readily than in pure water. However, in the concentrated surfactant solutions (much above the CMC) the process becomes more difficult. In the SDS/pentanol/water microemulsions the oxidation rate is larger than in the aqueous solution and increases with the increasing pentanol content. For the CTAB/octane/butanol/water microemulsion the opposite effect is observed. The stability of vitamin C is much higher than in pure water and reaches its maximum with the composition corresponding to the becontinuous phase. We studied also the influence of vitamin C on the antioxidative activity of vitamin E in the SDS/pentanol/water microemulsion. Our studies confirmed an enhanced antioxidant capability of the mixture compared to single antioxidants. The reason for it may be the formation of 1:1 complex between the vitamin C and vitamin E molecules. Some evidence for the complex existence comes from the isosbestic points observed on the UV spectra.

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Electrochemical studies of antioxidants activity in micellar systems

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The activity of antioxidants depends on their redox properties. The electron-donating ability of antioxidants can be quantitatively assessed from their electrochemical features. This knowledge may lead to better understanding of the antioxidant activity in the systems of practical use. Among different electrochemical methods, cyclic voltammetry with the glassy carbon electrode has been widely used to study the behaviour of antioxidants in different micellar systems.

This presentation shows the results of our studies concerning the electrochemical oxidation of hydrophilic ascorbic acid – AA, in surfactant solutions, in the mixed aqueous-organic systems: water+ACN (3:2 v/v) and water+EtOH (1:1 v/v) containing surfactants and in the microemulsion region of SDS/ pentanol/ water and CTAB/ octane/ butanol/ water mixtures (both microemulsion regions include the W/O, BC and O/W phases).

A general conclusion drawn from our investigations is that surfactants shift the AA oxidation potential and the peak current value. The magnitude and direction of the shift depends on the surfactant type. The oxidation potential of AA decreases and the peak current increases in the CTAB solutions. The non-ionic TX-100 and anionic SDS give opposite effects. In general, the oxidation of AA proceeds more readily in less acidic solutions.

Discussing the results of AA electrooxidation in the mixed aqueous-organic systems, the influence of organic solvents on the surfactants micellization process should be taken into account.

The electrooxidation of AA in the microemulsions is less efficient when the concentration of the organic phase increases. AA exhibits the highest electrochemical activity in the electrolyte solution and the lowest in the BC system.

Our investigations can be helpful in designing of new cosmetic and pharmaceutical formulations.

Poster Presentations

List of Poster Presentations

Thursday April 14th	
P1	**Andrzejczak Olga** The variety of structure and healthy properties of polyphenolic compounds.
P2	**Bagan Roża** Toksykologia środków uzależniających
P3	**Borzęcka Wioleta** Synthesis and coordination properties of derivatives and analogues of 8-hydroxyquinoline
P4	**Brodaka Małgorzata** Pyroelectric and piezoelectric effect in crystals
P5	**Chomicki Adam** Vertical leaders
P6	**Czochara Robert** Synthesis and thermal stability of fullerene C_{60} derivatives
P7	**Denisiuk Wioleta** Studies on the methods of chemical and enzymatic synthesis of the S-adenosyl-L-methionine
P8	**Dziełak Anna** Medical application of organophosphorus compounds
P9	**Fica Mateusz** Characterization and corrosion properties of electrodeposited Ni-W, Fe-W and Co-W alloys
P10	**Filipczak Paulina** Raman spectroscopy of Si nanowires
P11	**Grucela Marzena** New aliphatic-aromatic liquid crystalline polyimide
P12	**Guillaume Poisson** New Tris-ACE-α-cyclodextrin tripods: first results
P13	**Gwóźdź Kamil** Galvanic cells – evolution in time
P14	**Janicki Robert** Capsaicin – spice up your life!
P15	**Kamel Karol** Determination of detonation velocity of CHNO explosive compounds by means of multiple linear regression – an old method, but new results

P16	**Kamel Katarzyna Anna** Molecular farming - plants as bioreactors for production of recombinant proteins.
P17	**Kamiński Ireneusz** Peptide bond synthesis in the aqueous milieu.
P18	**Kelm Anna** Surface-Enhanced Raman Spectroscopy in detection of Neurotransmitters and Neuromodulators
P19	**Kędzia Magdalea** The investigation of the microwaves on fatty acids' isomerisation
P20	**Kiryluk Kamila** Low energy electrons and bromoderivatives of nucleobases. A DFT study.
P21	**Kołodziej Agata** Structure, occurrence, isolation and the importance of phospholipids in nature and a variety of industries
P22	**Koper Anna** The Use of Resin in Elimination of Interferences from Surface Active Substances in Voltammetric Determination of Trace Amounts of Selected Elements
P23	**Korzun Urszula** Comparison of fatty acid composition of phospholipids from poultry yolks
P24	**Kotomska Natalia** Microbiological transformation of 11α- and 17α-hydroxyprogesterone
P25	**Krężel Jakub** The Waters of Kozienicki Landscape Park
P26	**Krogul Agnieszka** Catalytic activity of $PdCl_2$ complexes with pyridines in nitrobenzene carbonylation
P27	**Kundys Anna** Synthesis of biodegradable linear copolymers of L-lactide
P28	**Kustra Klaudia** Biotransformation of 16-dehydropregnenolone in cultures selected strains
P29	**Laszuk Anna** Photoconductivity of 2,4,7-trinitrofluorenone and poly(N-vinylcarbazole)
P30	**Letmanowski Rafał** Synthesis and characterization of modified glassy proton electrolytes which can be used in fuel cells
P31	**Lewiński Bartłomiej** 1,10-phenanthroline coordination compound containing zinc bromide
P32	**Łozińska Iwona** MTDLs (multi-target-directed ligands) as a drugs in Alzheimer disease

P33	**Madaj Witold** Beginnings of nutrigenomics on the market.The case of proanthocyanidins.
P34	**Madej Daria** Diastereoselective photocyclization of 2,3-dibenzylidenesuccinic acid derivatives
P35	**Mazur Marcelina** Biotransformations and anitbacterial activity of iodolactone with metoxyphenyl ring
P36	**Mazurek Magdalena** Optimization of the oligocarbonate diols synthesis
P37	**Misiak Natalia** Preparation of pyrolytic carbons from polymer precursors

Friday April 15th	
P38	**Nagórniewicz Beata** Radiation synthesis of nanogels derived from microemulsion
P39	**Nowak Anna** Archaeological glass analysis by means of LA ICP MS
P40	**Nowak Ewelina** Selected properties of spelt starch illuminated with ultraviolet and linearly polarized visible light
P41	**Olech Kamila** New anthracene derivatives for optoelectronic materials
P42	**Olesińska Magdalena** New anti-cancer drugs analogues for the modification of multifunctional nanocarriers
P43	**Orzeł Joanna** Chemometric in analysis of fluorescence fingerprints
P44	**Osypiuk Alicja** „Blondzik, tipsik i solara- o środkach i zabiegach upiększających z chemicznego punktu widzenia"
P45	**Pawłowska Dorota** Microcontact Printing (μCP) of fluorescent proteins using porous PDMS stamps
P46	**Piecyk Karolina** Chemically Capped Spliced Leader RNAs - a usefull tool for studies on Function of the Nematode Spliced Leader

P47	**Pietras-Ożga Dorota** X-ray Photoelectron Spectroscopic Studies of Carbon Fiber Surfaces
P48	**Popławski Daniel** The phenomenon of electroporation of lipid membranes
P49	**Sawicki Piotr** Influence of organic dyes on sonochemical degradation of DNA. The way to sonodynamic cancer therapy
P50	**Siatecki Grzegorz** Application of europium and terbium complexes to build fiber-optic sensors of UV radiation
P51	**Sierański Tomasz** Ab-initio systematic analysis of stacking interactions in benzene-benzene, benzene-pyridine and pyridine-pyridine supramolecular compounds
P52	**Skonieczny Kamil** Excited-State Intramolecular Proton Transfer in aryl-imidazole molecules with chromophore modifications
P53	**Słupska Marta** Synthesis of cyclic analogues of tryptophan by the Pictet-Spengler condensation of chiral aminoaldehydes with β^2- or β^3-homo-Trp derivatives
P54	**Smusz Sabina** Hybridization of ligands as a way of generating combinatorial libraries of drug candidates
P55	**Smykowski Daniel** DFT calculations of CO_2 - zeolite interactions: adsorption and molecular dynamics simulations
P56	**Sobota Tomasz** Transformation of quinine and quinidine to β-amino acid derivatives – potential catalysts of asymmetric synthesis
P57	**Sowiński Sebastian** Synthesis and Characterization of CdSe Quantum Dots
P58	**Stachniuk Justyna** The investigation of $Fe(CN)_6^{3-/4-}$ system on 4-mercaptopyridine self assembled monolayers on gold
P59	**Starzyńska Zuzanna** Anthocyanins, carotenoids, chlorophyll - health hidden in colors
P60	**Stasiak Aleksandra** Properties of elastomeric nanocomposites containing montmorillonite (MMT)
P61	**Steinborn-Rogulska Izabela** Direct melt/solid polycondensation of L-lactic acid to poly(L-lactic acid) with high molecular weight
P62	**Surma Łukasz** Carbon dioxide in the MTG technology – Fuel of the Future

P63	**Szymańska Jolanta** Solvent effects on enzymatic deamination of L-alanine
P64	**Tomczyk Karolina** Multicomponent aliphatic-aromatic copolyesters
P65	**Tomczyszyn Aleksandra** Synthesis of platinum(II)-tachykinin peptides complexes for potential antitumour applications
P66	**Truchlewski Adam** Search for new tuberculostatics. an x-ray study
P67	**Uber Dorota** Foldability of peptides derived from N-terminal beta-hairpinsof 1E0L protein (WW domain)
P68	**Węcławski Marek** Novel fused porphyrin with aromarics moiety obtained by intermolecular oxidation - synthesis and optical properties
P69	**Węglarz Ewelina** Neutral aminopeptidases - the role, function and transition state inhibitors
P70	**Wojciechowska Magdalena** Selective oxidation of ammonia to nitrogen and water vapour over mixed metal oxides obtained from hydrotalcites
P71	**Wojtkiewicz Justyna** Bioactive hydrogel dressings containing angiogenesis – stimulating factor
P72	**Zabost Dariusz** Synthetic preparation of proton conducting glasses for hydrogen fuel cell applications
P73	**Zdrowowicz Magdalena** PCR Synthesis of Double Stranded DNA Labeled with 5BrdU. A Step Towards Finding a Bromonucleoside for Clinical trials
P74	**Zielińska Anna** Modelling of solvent effect on nitrogen NMR chemical shifts in thiazoles and thiadiazoles

The variety of structure and healthy properties of polyphenolic compounds.

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Polyphenols are a large and very diverse group of secondary plant metabolites that arise during the transition of the shikimate pathway with L-tyrosine and L-phenylalanine. They belong to the group of phenols and they have two or more hydroxyl groups attached to aromatic ring. Scientists know a few thousand natural plant polyphenols which differ in structure, molecular weight, the physical, chemical and biological agents. Taking into account the carbon skeleton including simple, soluble forms of polyphenols is distinguished by hydroxybenzoic acids, hydroxycinnamic acids, coumarin, naphthoquinones, xanthones, stilbenes and flavonoids among which we can distinguish particular anthocyanins. Polymerized derivatives of these compounds are tannins and lignin. Polyphenols are antioxidants, substances low concentrations of which counteract or significantly retard the oxidation of the substrate. They fulfill an important role in preventing and counteracting the effects of oxidative stress. The oxidative stress is a state of imbalance between production of reactive oxygen species generated by various processes taking place in living organisms and processes for their liquidation. It is the base of numerous diseases among which include cardiovascular diseases, neurodegenerative diseases, cancer and eye disease, which could include glaucoma, cataracts and age-related macular degeneration (AMD). Numerous studies indicate that polyphenols can be extremely useful not only in prevention but also in the treatment of these diseases.

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Toksykologia środków uzależniających

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Using intoxicants accompanied the man since the dawn of history of mankind. At first they were using extracts of such plants as the opium poppy or the thorn apple. However, with the development of civilization and chemistry, next agents were being discovered. Some of these drugs cause hallucinations, facilitate falling asleep or stimulate. Concept of „ Intoxicants " includes the group of compounds with very diverse structure and different interactions on receptors in the human body. Therefore, we are meeting with a few means of their division. It is possible to classify these substances according to others depending on their origin or also consequences of action.

As the significant division is recognized the division according to the World Health Organization (WHO), and - regarded as the most popular- division according to physiological action. In it we distinguish 8 types of toxic mania: type of morphine, type of amphetamine, type of khat, type of cocaine, type of alcohol and barbiturates, type of volatile solvents, type of cannabis and type of hallucinogens.

This poster includes basic information about the most popular intoxicants known for our civilization.

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Synthesis and coordination properties of derivatives and analogues of 8-hydroxyquinoline

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8- hydroxyquinoline is one of the best green luminescent materials in organic light-emitting diodes (OLEDs) up to now, which can also chelate many metal ions, the corresponding complexes possess high luminescent efficiency. Colour and charge-transporting properties of complexes can be changed by varying the central metal ion, the ligand structure and the number of ligands [1]. So we design and synthesize two-photon absorbing chromophores of dipolar and quadrupolar structure based on 8- hydroxyquinoline framework which has high molecular absorption cross-section and fluorescence quantum yields. These molecules have promising optical properties for versatile applications such as the fluorescent sensing of metal ions, biological molecules or organelles based on two-photon excitation fluorescence microscopy *in vivo*.

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INSTYTUT CHEMII ORGANICZNEJ
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Pyroelectric and piezoelectric effect in crystals

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Phenomenon of pyroelectricity, based on inducing electric charges on the surface of crystal caused by change of the temperature, has been discovered in eighteenth century. An inverse phenomenon called electrocaloric effect, when crystal is cooled or warmed by placing it inside electric field, also exists. Piezoelectricity occurs when external mechanical stress applied to some of the crystals induces electric charge proportional to the strength of the mechanical stress. An inverse effect, i.e. mechanical oscillation of the crystal placed in the external electric field, is also observed.

Pyroelectric and piezoelectric effects have found wide practical application. The biggest development of applications of these phenomena occurred during the Second World War. Applying the pyro- and piezoelectric materials in submarines as the transmitters and receivers of ultrasound waves in water initiated the development of physics and technology of ultrasound. Intensive research on these materials led to the discovery of reliable ceramic materials known as intelligent materials. Highly valued piezo- and pyroelectric crystals are used in the sensors of force, temperature, pressure, stress, and also in everyday objects such as microphones and sonars.

In the following study mechanism of these phenomena at a molecular level have been associated with properties of the crystals revealing the piezo- and pyroelectric effects. Examples of the crystals and polycrystalline materials with above mentioned effects have been presented. Applications of these materials in science as well as everyday life are also presented. The possible applications, such as substitutes of human tissue and intelligent materials, of crystals and synthetic polymers are described.

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Vertical leaders

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Viagra was a turning point in the treatment of erection dysfunction. Nowadays, many other preparations have a similar effect (among others Maxigra, Levitra, Cialis) but they are medicines available only on prescription. As a result, men with this problem have to visit the doctor.

For this reason, preparations available without a prescription in pharmacies become more popular. The producers of these medicaments promise that they have efficacy similar to the drugs mentioned above. In this group of pharmaceuticals there are for example: Liderin, Permen, Vitasteron, Penigra. They are dietary supplements mainly contain: amino acids, plant extracts, vitamins and minerals.

It should be noted that these preparations are recommended for men who cannot get full satisfaction from sexual life caused by overwork, poor diet, sedentary or stressful lifestyle. However, drugs like Viagra should be taken by people with serious physical dysfunction.

The most common ingredients in these tablets and their effect on the body will be shown in presentation.

Synthesis and thermal stability of fullerene C_{60} derivatives

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Since their discovery in 1985[1], fullerenes and carbon nanotubes have been the subject of pure and applied research leading to development of nanotechnology - a new field linking science and technology in which material properties are dependent not only on their molecular structure but also on the particle size. Chemical modifications of fullerenes and nanotubes are interesting due to potential applications in many fields of science, industry and medicine, i.e., new superconductors or insulators, strong nanofibers, drug delivery agents, inhibitors of the HIV-1 protease[2,3].

The aim of our studies is to synthesize organic derivatives of fullerene C_{60} containing polar groups: hydroxyl, nitro and polycyclosulfate groups (Fig.1).

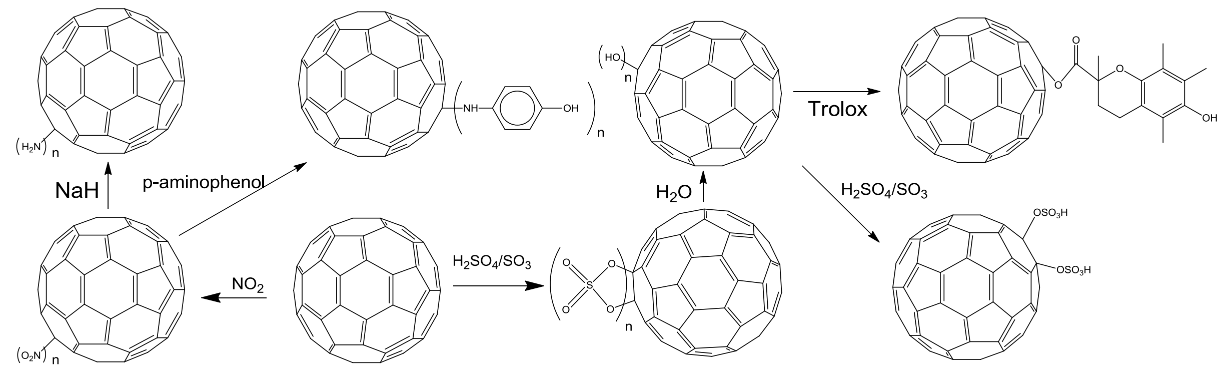

Figure 1. Examples of obtained Fullerene C_{60} derivatives.

In this work we present the results of $C_{60}(X)_n$ (where X=substituent group) characterization by the means of infrared, UV-Vis, thermal analysis, NMR, MS methods.

This work was supported by Ministry of Science and Higher Education, grant N N507452937.

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STUDIES ON THE METHODS OF CHEMICAL AND ENZYMATIC SYNTHESES OF THE *S*-ADENOSYL-L-METHIONINE

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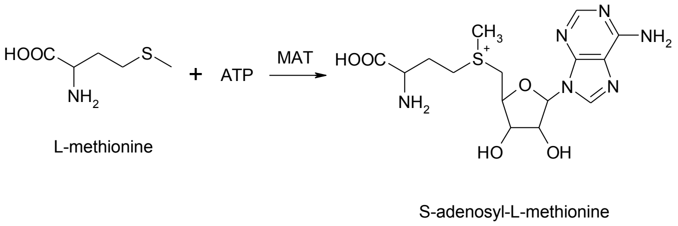
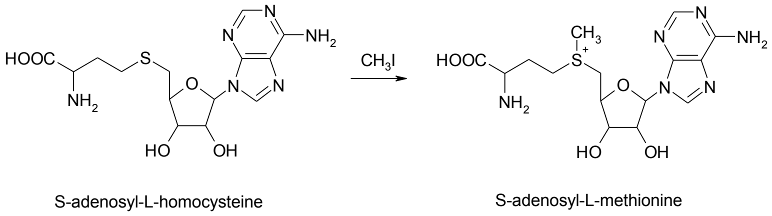
In this communication we present the enzymatic and chemical methods of synthesis of *S*-adenosyl-L-methionine (SAMe) – the major methyl group transfer agent in biological systems. In mammals, SAMe is produced from L-methionine and ATP in reaction catalyzed by methionine adenosyltransferase (MAT) – *scheme 1*. For mechanistic study of this reaction a labeled with ^{14}C isotopomers of L-methionine are needed. Therefore, we have developed the method of synthesis of these isotopomers using as substrates L-homocysteine and $^{14}CH_3I$. For needs of above synthesis the procedure of isolation and purification of MAT from porcine liver was eleborated.



Scheme 1. Enzymatic synthesis of *S*-adenosyl-L-methionine.

The optimal conditions of the chemical synthesis of S-adenosyl-L-methionine were developed. Also SAMe was obtained in the course of methylation of S-adenosyl-L-homocysteine (SAH) by CH_3I – *scheme 2*.



Scheme 2. Chemical synthesis of *S*-adenosyl-L-methionine.

The reactions mentioned above were controlled by TLC. The *S*-adenosyl-L-methionine was purified by adsorption and ion-exchange chromatography using Silica Gel 60 and ion exchangers: Amberlite CG-50 (H^+) or Dowex 50W X8 (H^+). It was also isolated from the reaction mixture by preparative TLC.

Medical application of organophosphorus compounds

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Organophosphorus compounds possess broad spectrum of application. This includes their use in some branches of industry as well as in medicine. Presented work describes various organophosphorus drugs and their mechanism of action.

Number of organophosphorus compounds have found application in medicine. Among these which have been marketed, one can notice cyclophosphamide, which have chemoterapeutic activity. It can be used to treat some types of cancer and autoimmune disorders.[1] Another example, fosinopril is used in hypertension treatment. It acts as angiotensin converting enzyme inhibitor.[2] Bisphosphonates also possess currently a wide application as drugs to treat osteoporosis because of their ability to prevent the loss of bone mass.[3] Aledronate and risedronate are representative examples of bisphosphonates in osteoporosis treatment. Bisphosphonates inhibit the digestion of bone by osteoclasts. These compounds are also used in chemotherapy of bone metastasis or multiple myeloma.

Such organophosphorus compounds as phosphonic, phosphonamidate or phosphinic analogues of amino acid or peptides possess a wide variety of promising physiological activities. They are believed to act as high energy hydrolytically stable tetrahedral transition state analogues of the reaction performed by various enzymes, causing inhibition of these proteins.[4] This approach appeared to be most successful in the case of metalloproteases, for which a wide variety of such inhibitors have been described. For example organophosphorus compounds such as phosphinic pseudodipeptides are considered to be used as anti-malarial drugs. They may block the activity of alanyl (EC 3.4.11.2) and leucine aminopeptidases (EC 3.4.11.1) of the human malaria parasite *Plasmodium falciparum*.

Diaryl esters of α-aminophosphonates are considered as inhibitors of serine proteases due to their capability of irreversible phosphonylation of the active site serine residue, what results with high potency of their action and selectivity.[5] Such enzymes as serine proteases have been correlated with many pathological states in living organisms including cancer growth, metastasis or diabetes.

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Characterization and corrosion properties of electrodeposited Ni-W, Fe-W and Co-W alloys

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Amorphous alloys of ferromagnetics with tungsten represent a group of materials with hightened mechanical strength and corrosion resistance. As such they are used in production of mainly ferrite cores for transformers and electrode materials.The purpose of presented research was to estimate the corrosion properties of alloys in salt water and their usefulness as protective coatings.

A solution of 3% NaCl in purified water was used as an electrolyte. Samples, varying in thickness, were previously electrodeposited on copper substrate. After conditioning of the test electrodes in the solution for 1 hour, Electrochemical Impendance Spectroscopy (EIS) measurements (Autolab PGSTAT 20, 10kHz – 1,0 mHz, 10 mV amplitude) were made twice for each sample, with an interval of 6 hours. Afterwards each sample was polarized with a sweep rate of 2 mVs^{-1}. Starting potential was defined as open circuit voltage (OCV) -0,1 V.

Achieved results point to Ni-W alloys having the best corrosion properties amongst the tested alloys, said properties increasing with prolonged exposition both in Ni-W and Co-W alloys.

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Raman spectroscopy of Si nanowires

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Nanotechnology as sophisticated technology demands advanced research techniques. Raman spectroscopy could become a standard method for the non-destructive characterization of nanomaterials. This technique allows to determine key features of nanomaterials, such as: size, doping degree, chemical composition and structure. Raman spectroscopy has been successfully used in research of silicon nanomaterials such as silicon nanowires [1].

Silicon nanowires are attractive due to the role of Si in the current semiconductor industry. Compared with the bulk silicon, nanowires have a lot of novel physical properties, such as optical emission and more efficient electronic transport [2].

Silicon nanowires used in this study were obtained by method based on the Vapour-Solid mechanism without utilisation of any catalyst. This method allows to obtain nanowires with the diameter less than 20 nm.

In this work, Raman spectroscopy was used to estimate silicon nanowires sizes. Typical red shift of first-order TO band as well as its broadening (comparing to spectrum of bulk Si) characteristic for Si nanoparticles and nanowires was observed as it was shown in figure 1. Nanowire size was estimated based on Raman band position according to the formula proposed by Piscanec et al [2].

Additionally an aspect of doping of Si nanowires will be shown. Influence of different dopants on vibrational properties of investigated nanowires will be discussed based on analysis of broad low frequency shoulder accompanying the first-order TO band of Si nanowires.

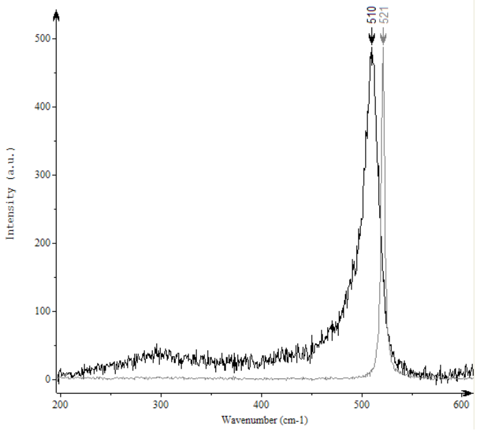

Figure 1. Raman spectra of bulk silicon (gray line) and Si nanowires (black line)

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New aliphatic-aromatic liquid crystalline polyimide

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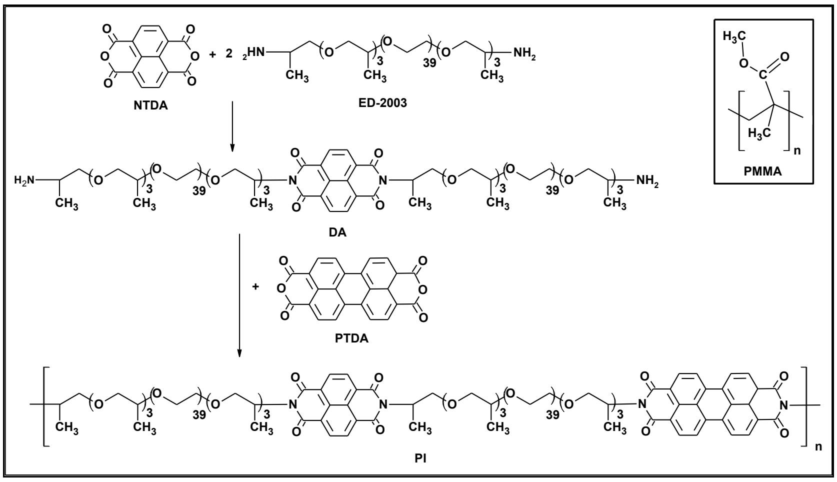
The unique combination of properties (high thermal stability, low dielectric constant, high breakdown voltage, good planarization, wear, radiation and chemical resistance, good adhesion properties, low thermal expansion and excellent mechanical properties) makes polyimides ideal for a variety of applications in many different industries, that is, microelectronics, microelectromechanical systems, aerospace, photoelectronics, alignment layers in liquid crystal displays, and for gas separation as membranes.[1, 2]

Were synthesized and tested a new both aliphatic-aromatic liquid crystalline diamine (DA) with naphthalene diimide moiety and polyimide (PI) with naphthalene and perylene diimide subunits. Their thermotropic liquid crystalline behavior was examined by the differential scanning calorimetry (DSC) and polarizing optical microscopy (POM). The thermal stability was evaluated by thermogravimetric analysis (TGA). The optical properties, that is, UV-Vis absorption and photoluminescence (PL) of obtained monomer and polyimide, were studied in solution and in solid state as a blend with inert poly(methyl methacrylate) (PMMA). The effect of solvent polarity, excitation wavelength and concentration of diamine and polyimide on emission properties was found. The electrochemical behavior of DA and PI was studied by cyclic voltammetry (CV) and differential pulse voltammetry (DPV). The electrical properties of DA and PI were investigated by current-voltage (*I-V*) measurements on ITO/compound/Al devices.

The first time to the best of our knowledge, polyimide containing in their structure both naphthalene and perylene diimides with liquid crystalline properties was descirbed[3].



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NEW *Tris*-ACE-α-CYCLODEXTRIN TRIPODS: FIRST RESULTS

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In the past decade, some seminal works describe the preparation and properties of new metallocyclodextrins molecular receptors.[1] These supramolecular architectures are potentially able to occur in various applications such as: selective complexing agents, biomimetic catalysts, or photo-active devices due to their coordination to metals properties (anions / cations) and complexation with small molecules. In this goal and to continue our research initially focused on 5,5 '-bipyridyl-α-cyclodextrins derivatives [2], [3], we describe here the preparation and first studies on new derivatives connected in the 6,6' position. By changing the location of connection on the heterocyclic unit, new properties of the cyclodextrin receptor emerged on metal coordination, redox and conformational equilibrium. During this work and to achieve an efficient preparation of substituted halomethylheteroaromatic units, a new method of synthesis [4], using the tetrachloro-diphénylglycoluril, as chlorine radical source was successfully used. Thus, bis-heterocycles as bipyrimidine, bithiazole, bipyrazine, bis-triazine, selectively halogenated in the position 6 or 6' position have been obtained in fairly good yields and could be directly grafted on the trisubstituted-ACE-α-cyclodextrin plateform by the Staudinger-Aza-Wittig (SAW) tandem reaction, allowing access to the desired molecular receptors in one-step only.

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Galvanic cells – evolution in time

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The history of cells is much longer than would be it seemed, and probably dates back to antiquity. Just before World War II during archaeological work conducted by a German team around Baghdad (territory of ancient Babylon) found strange discovery, coming from the third century BC - an clay pot, with copper cylinder and an iron rod inside. It was considered that this was probably one of the first galvanic cell.

Era of true galvanic cells came with the eighteenth century and the Galvani works involving impact electricity on processed frog legs. Alessandro Volta, the world's first building up a galvanic cell, did not realize that 200 years after his discovery, each person will be able to furnish his own, a small chemical cell. Further development of the Volta invention meant that a man can now produce electricity at any point on the Earth and in space.

The next step, in order to improve cell generating electricity, was to eliminate some inconveniences, which are revealed after some use of the cell. A disadvantage of this was collect on the copper electrode, hydrogen bubbles, which reduced the reactive surface. At the same time sludge of zinc sulphate precipitated on zinc plate. This resulted in a steady increase of the internal cell resistance and reduce the voltage at it's poles. The solution to this problem were addressed by the French chemist Georges Leclanche.

We are confronted with them every day - car, mobile phone, laptop. Often not even we see that are getting smaller, bigger, more reliable, and yet without them, all these high-tech devices would be dead. Let's get acquainted with their history and their prospects for future use.

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Capsaicin – spice up your life!

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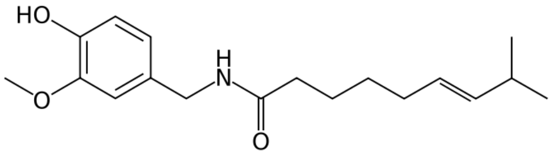
Capsaicin is the active component of chili peppers, which are plants belonging to the genus *Capsicum*. It is an irritant for mammals, including humans, and produces sensation of burning in any tissue with which it comes into contact. Capsaicin and several related compounds are called capsaicinoids and are produced as a secondary metabolite by chili peppers, probably as deterrents against certain herbivores and fungi.



capsaicin

Capsaicinoids can be acquired by chemical synthesis (nonivamide) or extracted from various peppers which greatly vary in their hotness and capsicinoid content.

The amount of capsicinoids has been traditionally measured organoleptically, but nowadays modern methods like HPLC and spectrophotometry are used.

Capsaicinoids have various interesting properties and are being used in food and pharmaceutical industries while having many other uses as well.

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Determination of detonation velocity of CHNO explosive compounds by means of multiple linear regression – an old method, but new results

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Velocity of detonation is one of the most important characteristic in description of explosive compounds. It is connected with other features of explosive materials such as the Chapman-Jouguet pressure, and it is a major factor in determining brisance of the explosive material, which is in turn a very important parameter for military application of explosives.

In our work, we utilized statistical approach (multiple linear regression method) to determine the correlation between velocity of detonation and explosive material density, chemical composition of explosive and detonation products, as it was the main purpose to develop a model capable of prediction of detonation velocity without taking into consideration any structural features. While it is obvious, that detonation velocity relies heavily on explosive material density, and therefore it is the most important parameter, the chemical composition is also important, since it express an oxygen balance, and the detonation products, as they express the amount of heat release, but in rather implicit manner. The training set for our regression model consisted of 34 CHNO explosives [1-3]. The decomposition equations for compounds with oxygen balance >-40% were determined using the Kistiakowsky-Wilson rules and for those with oxygen balance ≤-40% were determined using modified Kistiakowsky-Wilson set of rules [4]. As a result, we obtained an equation with $R^2 = 0.943$ and standard deviation of 2.65% from the experimental data for the training set.

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Molecular farming - plants as bioreactors for production of recombinant proteins.

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Plants have been utilized by humans since the dawn of civilization, supplying food, wood and therapeutics. Apart from animals, plants are the basic bioproduction system for valuable substances. In recent years with the rapid development in proteomics, the number of proteins being produced using recombinant techniques in plants was increasing constantly. Recombinant proteins produced in plants expression systems demonstrate potential applications as therapeutics, in diagnostics and in numerous branches of industry, e.g. as technical enzymes [1].

Molecular farming is the use of plants for production of heterologous proteins of great importance and value. Although these proteins are produced outside their natural source, they are functional, safe and nearly indiscernible from their natural equivalents [2]. Plants offer practical and safety benefits and generate lower production cost in comparison with the traditional expression systems like microbial or animal cells, or transgenic animals [3].

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Peptide bond synthesis in the aqueous milieu

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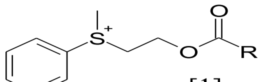
Peptide bond occurs in many natural compounds, drugs and biologically active substances. Therefore nowadays chemists are researching methods for the synthesis of this important moiety. A new challenge is the synthesis of peptides in water. These studies have been taken for two reasons. The first is the introduction of the rules of green chemistry and reducing consumption of organic solvents. The second - a modification of proteins, where the aqueous milieu is the best for the reaction, thanks to the greatest similarity to the natural milieu of proteins.

In order to perform peptide synthesis in water used coupling agents that are well water-soluble. Several groups of such compounds were described. These compounds are for an instance: the sillyl derivative of furanone (DPTF), p-dialkilosulfonophenols (HODASP • X$^-$)[2] or derivatives of triazine (DMT-NMM)[3].

To improve the solubility of amino acids in water instead of conventional protective groups such as Boc or Fmoc, which are hydrophobic, apply a group of high hydrophilicity. Examples include sulfur-containing groups as Pms [1], Sps [2], Msc or Esc[3][4].



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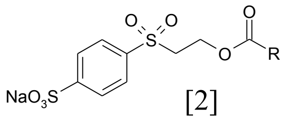

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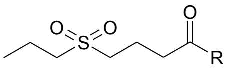

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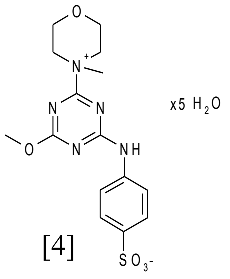
The Institute of Organic Chemistry at Technical University of Łódź synthesized[1] and examined the following triazine derivatives as condensing agents:



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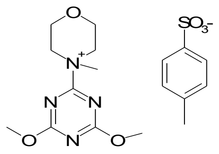

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Reactivity was checked trough synthesis of simple dipeptides in aqueous solutions of DMF or MeCN.

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Surface-Enhanced Raman Spectroscopy in detection of Neurotransmitters and Neuromodulators

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Neurons, the 'building blocks' of human central nervous system (CNS), communicate mostly by release of neurotransmitters and neuromodulators. The information may be transfrerred either directly to another cell or into the blood, what makes investiganting CNS activity by neurotransmitter molecular detection in body fluids and tissues possible.

In the view of growing ageing populations, there will be strong demand on new, efficient and simple neurodiagnostic methods[1]. Surface-Enhanced Raman Scattering (SERS), one of the most developing spectroscopic technique in recent years, has a great potential to become one. SERS effect, discovered *by Fleischmann et al.*[2] in 1974 is based on Raman scattering cross-section enhancement of molecules in proximity of roughened noble metal surface, typically Au and Ag. Dispite many advantages of SERS over fluorescence widely used in immunohistochemistry, due to higher sensitivity and specifity[3], insusceptibility to fluorescence-quenching agents[4] (i.e. oxygen) and sharper signals[5], there is only one recorded use of SERS in commercial biomolecular detection (Affymetrix). There are few SERS substrates on sale, moreover Raman and SERS spectra of many neurotransmitters, crucial for using SERS in molecular detection, have not been recorded and characterized yet.

In this work a general scheme of SERS-based neurotransmitter biosensor is briefly described. Raman and SERS spectra on electrodeposited Ag nanoparticles of some common neutransmitters: choline, acetylcholine and acetylthiocholine are presented and compared.

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The investigation of the microwaves on fatty acids' isomerisation

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The fatty acids play an important role in every cell of the body. They are are primary constituents of cell membranes. They are building material of phospholipids, mono-, di- and triacylglicerols. Essential fatty acids are used to generate certain intra-cellular hormone-like substances, which are responsible for regulating gene expression, cell signalling, inflammation and carcinogenesis, and also include anticarcinogenic factors.

In recent years there is continuous growing interest in application of an alternative heating system "microwave irradiation" in the organic synthesis and chemical process. When the reaction is carried out under microwaves usually these reaction are efficiently accelerated compared with conventional heating, due to the higher temperatures attained. Microwave reactions are also simple, inexpensive, very often these methods are solvent free and clean-up opportunities.

In this study, effect of microwave heating system on the fatty acids and their esters was investigated. Our results of research on the applications of microwave-assisted isomerization of linoleic acid to conjugated linoleic acid will also be presented.

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Low energy electrons and bromoderivatives of nucleobases.

A DFT study.

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Low energy electrons (LEE) are generated in huge amount during water radiolysis [1] and their genotoxic properties, i.e. the capability of producing single and double strand breaks (SSBs and DSBs) in DNA have been demonstrated in a number of studies [2,3,4]. The breakage of DNA strands becomes more efficient if halogen derivatives of nucleobases (Hal-NBs) are incorporated in the biomolecule. Thus, Hal-NBs may, in principle, be used as sensitizers in a future cancer radiotherapy.

However, before their clinical applications the mechanism of Hal-NBs degradation should be described and comprehend. It is known that electron-induced dehalogenation of Hal-NBs incorporated in DNA opens a radical route leading directly to strand breaks in the biopolymer [5]. Moreover, the research carried out on halouracils proved that 5-bromouracil rather than other halouracils was most sensitive on LEE's impact [6].

Therefore, in the current project we examined, at the B3LYP/6-31++G** level, the mechanism of electron-induced debromination of 8-bromoadenine (BrA), 5-bromocytosine (BrC), 8-bromoguanine (BrG) and 5-bromouracil (BrU). Geometry, thermodynamics and kinetics were evaluated in the gas phase and water solution. Our calculations show that BrA is the most electron-sensitive species (barrier-free breakage of the C8-Br bond) and the sensitivity of the studied bromoderivatives towards LEE's was found to be in the following order: BrA > BrG > BrC > BrU. These results suggest that BrA should be the molecule of choice for the future experimental and clinical studies.

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Structure, occurrence, isolation and the importance of phospholipids in nature and a variety of industries

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At first, in the presentation the structure of the most common phospholipids in egg yolks is discussed, followed by the presence of phospholipids and functions in nature and in a variety of industries, mainly food. In addition, the content of phospholipids in food products and the differences in fatty acid composition of soya lecithin and egg yolk were discussed and compared. Finally methods of isolating phospholipids from egg yolk on the basis of patent applications and publications were also discussed and compared.

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The Use of Resin in Elimination of Interferences from Surface Active Substances in Voltammetric Determination of Trace Amounts of Selected Elements

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Heavy metals belong to a class of pollutants that can produce undesirable effects, even though they might be present in minuscule quantities. In this group there are, among others, bismuth, cadmium and molybdenum. Therefore, a highly sensitive and simple method is necessary for determining the concentration of these heavy metals in environmental samples. Among the variety of techniques, electrochemical methods, mainly stripping voltammetry is preferred because of high speed of operation, minimum sample preparation, excellent sensitivity and precision. This technique is carried out in two steps. First step is based on adsorptive accumulation of a complex of the metal ion with an added specific ligand onto a hanging mercury drop electrode. The second step is an electrochemical desorption of the complex and a voltammetric scan to determine the amount of adsorbed metal ions.

Although voltammetric methods are simple and facilitate direct speciation analysis, they are vulnerable to numerous interferences arising mainly from the environmental sample matrix, such as organic matrix. The most common interfering compounds are surfactants. It is known that they are easily adsorbed at the HMDE surface and disturb the voltammetric signal of determinated metals. In this communication fast and sensitive adsorptive voltammetric methods for Bi (III), Cd (II) and Mo (VI) in the presence of high concentrations of surface active substances were elaborated. All kinds of surfactants such as anionic (SDS), cationic (CTAB) and nonionic (Triton X-100), were tested. In order to develop an elimination of interferences connected with the presence of these substances, the adsorptive properties of Amberlite XAD-7 resin was exploited. The most satisfactory results were obtained for determination of Cd (II) using cupferron as a complexing agent. In the proposed new procedure the presence of Amberlite XAD-7 resin totally eliminates interferences of all kind of surfactants even up to its concentration of 20 ppm. In the case of Bi (III), the addition of resin completely eliminates the unwanted negative influence of the cationic and anionic surfactants on bismuth peak heights, even 10 ppm of aforementioned surfactants do not affect the voltammetric signal. In the case of Triton X-100 the concentration of 5 ppm causes a decrease of the voltammetric signal to 50 % of its original value. For Mo (VI) the adsorptive accumulation was carried out using two complexing agents, cupferron and chloranilic acid. The addition of resin causes that inherency of even 50 ppm of Triton X-100 does not affect at all the voltammetric signal in the case of accumulation of Mo (VI) complex with cupferron. In the case of accumulation as Mo(VI) - chloranilic acid complex, 5 ppm of Triton X-100 does not affect the signal of Mo (VI). The addition of resin effectively diminishes interferences caused by anionic and cationic surfactants both in the case of accumulation of Mo(VI) as chloranilic acid and cupferron complexes. Procedures investigated in this study can be directly applied to analysis of natural water samples containing organic matrix without any prior separations.

Comparison of fatty acid composition of phospholipids from poultry yolks

Urszula Korzun, Agata Kołodziej, Witold Gładkowski

This research presents analysis of the composition of phospholipids in the phospholipid fractions isolated from egg yolks of different breeding birds: quail, ducks and geese. Phospholipids were used to isolate the fractionation of methanol and hexane. Phospholipid fractions were then purified in an ice bath for precipitation in the system hexane : acetone. Isolated phospholipids were dominated by acids and 18:1 16:0,18:0. The results were compared with the composition of fatty acids in phospholipids isolated from egg yolks.

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Microbiological transformation of 11α- and 17α-hydroxyprogesterone

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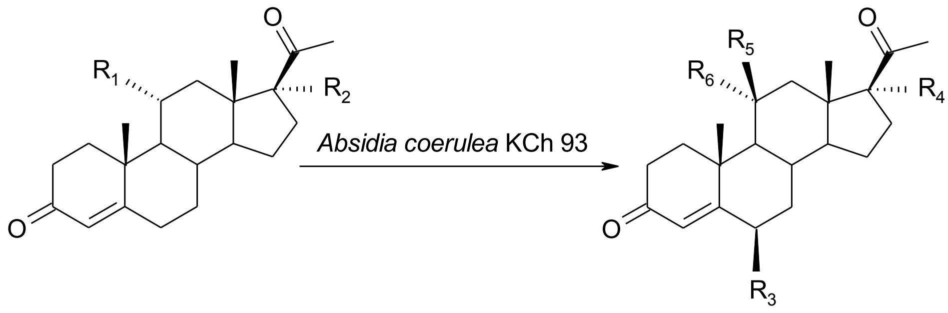
Bioconversion of steroids occurs under mild conditions (atmospheric pressure, room temperature). It is characterized by high regio- and stereoselectivity [1,2]. The current research in this area concentrates on searching for new compounds which are very difficult to achieve by chemical synthesis. The point of biotransformations is to find economical and environmentally less toxic methods of synthesis [3,4].

In this experiment microbiological transformation of 11α-hydroxyprogesterone (**2**) in the culture of *Absidia coerulea* KCh 93 has been carried out. As a result of this process one product was obtained (6β, 11α-dihydroxyprogesteron (**5**)). The result of biotransformation of 17α-hydroxyprogesterone (**1**) in the culture of the same strain two products were obtained in high yield: 11α and 11β,17α-dihydroxyprogesteron (**3** and **4**).



1	R_1=H	R_2=OH	**3**	R_3=H	R_4=OH	R_5=OH	R_6=H
2	R_1=OH	R_2=H	**4**	R_3=H	R_4=OH	R_5=H	R_6=OH
			5	R_3=OH	R_4=H	R_5=H	R_6=OH

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The Waters of Kozienicki Landscape Park

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Every year the Students` Scientific Group of Chemists of University of Łódź are organizing research camps, during which students examine the characteristics of surface waters. In 2007 and 2010 Students` Scientific Group of Chemists organized summer science camps in Garbatka, situated in Kozienicki Landscape Park.

The main purpose of the research was to establish the basic physical and chemical parameters determining the cleanliness class of river Zagożdżonka (left-bank tributary of the Vistula River) and the rivers feeding it: Brzeźniczka, Mirenka, Trupień and streams: Krępiec, Krypianka, Policzanka and Zwolenka.

The test results obtained during two camps will be presented and compared. I will also present the conclusions of the researches.

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Catalytic activity of $PdCl_2$ complexes with pyridines in nitrobenzene carbonylation

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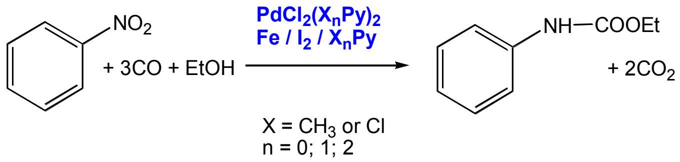
One-Pot Catalytic Synthesis of Carbamates



Over the last decades square planar palladium(II) complexes with nitrogen donor ligands have received much attention as catalysts for the carbonylations [1], polymerizations [2], and other reactions in synthetic organic chemistry [3].

There is a general agreement that catalytic activity of metal complexes with the ligands containing nitrogen depends on electron density of the palladium atom and a strategy to design (and to obtain) more active catalysts is based on incorporation of new, more electron donating ligands to manipulate the steric and electronic effects around the palladium center.

In our work we carried out several syntheses of square planar palladium(II) complexes of general structure $PdCl_2(X_nPy)_2$ (where: Py = pyridine; X_nPy = 2-MePy; 3-MePy; 4-MePy; 2,4-Me_2Py; 2,6-Me_2Py; 2-ClPy; 3-ClPy and 3,5-Cl_2Py) in order to study their activity as catalysts of nitrobenzene (NB) carbonylation – a process of industrial importance leading to production of ethyl N-phenylcarbamate (EPC). Electron withdrawing / electron donating properties of X_nPy ligands (described by experimentally determined acidity parameter pK_a) were correlated with activities of $PdCl_2(X_nPy)_2$ complexes expressed as yields and conversions of NB in carbonylation process in presence of catalytic system $PdCl_2(X_nPy)_2$ / Fe / I_2 / X_nPy. We observed that conversions of substrates and yields of EPC increase within increasing basicity of X_nPy ligand (for not sterically hindered X_nPy's). On the basis of current work and our previous studies a detailed mechanism of catalytic carbonylation of NB is proposed [4,5].

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Synthesis of biodegradable linear copolymers of L-lactide

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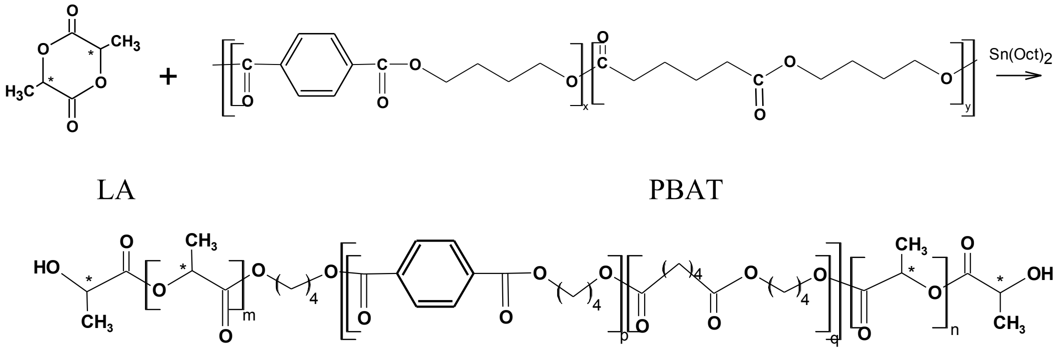
Poly(lactic acid) (PLA) is at present one of the most promising biodegradable polymers (biopolymers) and has been the subject of many papers over the last decade [1]. In order to extend the application of PLA, its properties are being modified by the incorporation into the structure of the polymer chain fragments from other biodegradable comonomers such as ε-caprolactone or cyclic carbonates.

The aim of this work was to develop suitable methods of synthesis of linear biodegradable copolyesters containing blocks of PLA. In order to obtain a linear structure of the copolymer we used aliphatic-aromatic copolyester poly(butylene adipate-co-terephthalate) (PBAT) as macroiniciator for the ring-opening polymerization (ROP) of lactide (LA). One of the advantages of this polymerization technique is that high molecular weight polymers can be produced and reactions can be taken to very high conversions [2]. In the synthesis we used stannous octanaoate $Sn(Oct)_2$ as a catalyst. Although there are available a variety of catalysts used for ROP, such as antimony compounds, zinc compounds and alkoxides, stannous octoate is preferred because it is approved by the FDA as a food stabilizer [3].



LA

PBAT

PLA-PBAT-PLA

Conditions for this reaction have been optimized. The highest molecular weight of the copolymer has been obtained at a temperature of 190°C and the reaction time of 3 h. Above this temperature, we observed the unwanted transesterification reaction. The formation of triblock copolymers was confirmed by NMR and DSC measurements.

The thesis was partially realized as a part of Innovative Economy project number POIG.01.01.02-10-025/09 BIOPOL entitled "Technology to produce biodegradable polyesters using renewable raw materials". The project was financially supported by European Union-European Fund of Regional Development.

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Biotransformation of 16-dehydropregnenolone in cultures selected strains

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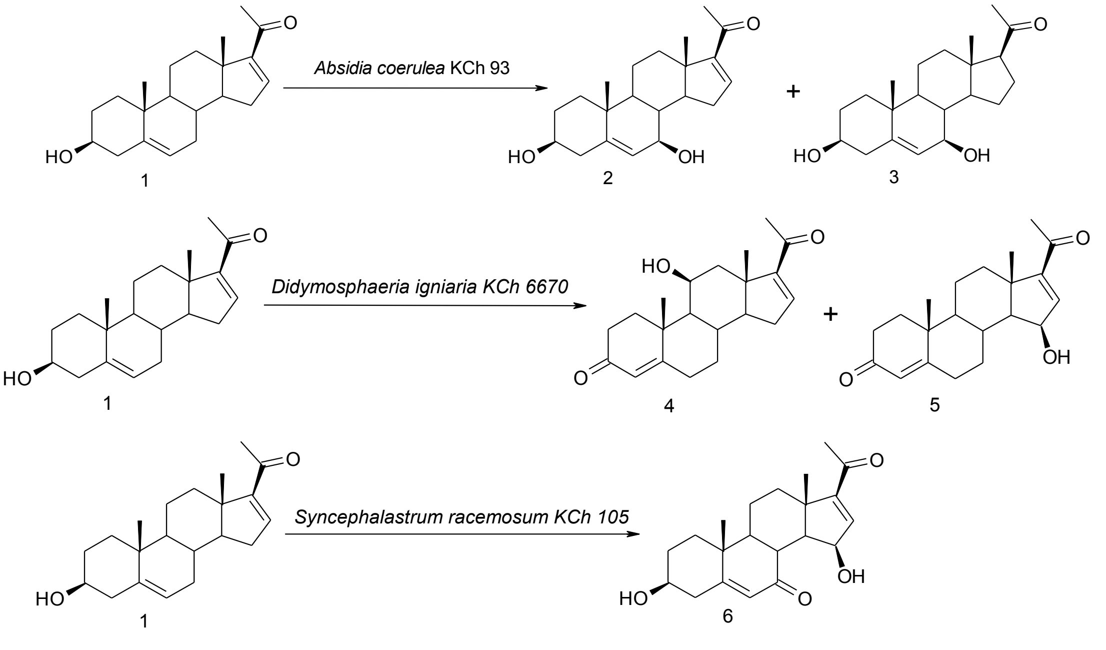
Microbiological transformation of steroid compounds in the last several years has been the subject of intense research [1]. The development of biotransformation has been based mainly on finding new enzyme systems. It turned out that the microorganisms which carry out hydroxylation most frequently were fungi, which transformed the substrate in different positions of the steroid skeleton. Such metabolites can potentially be used in the synthesis of other useful compounds in the pharmaceutical industry [2].

As a result of biotransformation of 16-dehydropregnenolone (**1**) conducted by the *Absidia coerulea* KCh 93 strain two products were obtained in which the hydroxyl group was introduced in the position of 7β (**2**). In the second case reduction of the double bond C_{15} - C_{16} occurred additionally (**3**). *Didymosphaeria igniaria* strain also transformed this substrate in to the two products, both resulting in oxidation of hydroxyl group at C_3. Hydroxylation at position 11β (**4**) in the first case and position 15β (**5**) in the second case also occurred. In the case of *Syncephalastrum racemosum* strain one product was obtained in which 15β hydroxylation and oxidation of carbon C7 took place simultaneously (**6**).



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Photoconductivity of 2,4,7-trinitrofluorenone and poly(N-vinylcarbazole)

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The photoconductor has to be capable of both photogenerating the charge carriers and transporting them through the bulk. Polymeric photoconductors have many positive characteristics such as wide spectral sensitivity, low cost, and architectural flexibility. Such materials, when properly doped, can exhibit high photogeneration efficiency, though in general they show relatively low charge carrier mobility. The polymeric photoconductors known thus far are polymers with a saturated backbone containing active chromophores as pendant groups or molecularly dispersed dopands. Poly(*N*-vinylcarbazole) (PVK) (Fig.1), sensitized by adding the electron acceptor 2,4,7-trinitrofluorenone (TNF) (Fig. 1), is the best known and most widely investigated polymeric charge-transfer (CT) complex system.

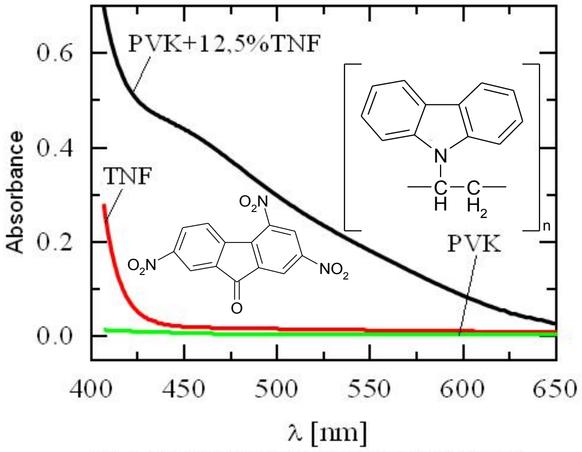

Fig. 1. Absorbance for PVK, PVK+TNF and TNF dissolved in dichloromethane thin (4 μm)

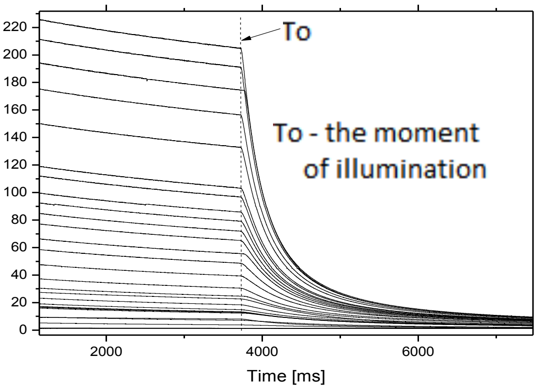

Fig. 2. The SPD curves for the PVK+TNF layers.

In this paper we present results of examination of surface voltage photodischarge in PVK+TNF CT system. The samples of PVK, and their CT complexes with TNF were prepared by dissolving them in dichloromethane and by casting them on chromium-plated metal supports at room temperature. A slow, limited evaporation rate yields highly transparent, homogeneous films of thickness in the range of 3 μm. Concentrations of TNF were 12,5 wt% in PVK, so that in all cases one TNF molecule was present for every 13 polymer mers. The films of PVK+TNF are brown–yellow in transmitted light. The absorption spectra of the solutions of PEVK, TNF, and PVK+TNF in dichloromethane are shown in Fig. 2. For the PVK+TNF system, one can recognize the CT band at around 450 nm (Fig. 1).

The photodischarge decays in the obtained nanocomposites were determined by means of Surface Potential Decay (SPD) method consisting in charging of the investigated film by corona discharge (in dark) and then in monitoring of speed of the surface potential decay induced by illumination of the film with light of desired wavelength and intensity. These measurements were performed for different initial negative surface potential. An HBO-200 mercury lamp with 430 nm interference filter was used as a light source. Typical surface potential decay curves for PVK+TNF films under illumination with blue light are shown in Fig. 2. These system shows remarkably dark decay and photodecays of the doped PVK samples are initially very quick. The potential decay rate, is proportional to the photogeneration quantum yield of PVK+TNF system.

Synthesis and characterization of modified glassy proton electrolytes which can be used in fuel cells

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In the area of fuel cells there are many system designs characterized by various working temperature, kind of membrane, used fuel etc. One of them is a fuel cell with proton exchange membrane (PEM), which is useful for many applications, but has several big disadvantages. Catalyst poisoning by CO and sulfur containing compounds is strong in low working temperature range, large noble metals containing catalysts load are needed to achieve expected current densities and, last but not the least, low operational temperature leads to the low efficiency of the residual heat utilization due to poor efficiency of the heat exchange process. Another type of fuel cell is PAFC (Phosphoric Acid Fuel Cell) which reduced problems from PEM, also suffers from some important drawbacks. The biggest are: aggressive electrolyte and limited minimal generated power, which reduce a number of small applications where they could be potentially used.

A solution for this problems can be found in fuel cell system design utilizing proton conductive glass electrolyte, which can work in higher temperatures than PEM (similar to PAFC) but is solid. It solves the problem of catalyst deactivation, and makes a possibility of effective cogeneration of heating power maintaining the features of small size and versatility of PEMFC. In addition this solid electrolyte is not chemically aggressive. Fuel cells with this kind of electrolyte can be used in a small home applications fed with reformed natural gas which are in long term inoperable in case of PEMFC due to the catalyst poisoning by sulfur compounds. The presented idea is related to the modification of the glass electrolyte with a nominal composition of 30% P_2O_5 and 70% SiO_2 (molar ratio), named as $30P_2O_5$–$70SiO_2$, prepared by the accelerated sol–gel process, in which, the precursors: tetraethyl-orthosilicate and trimethyl phosphate were partially hydrolyzed in the mixture of ethanol and water and then further hydrolyzed in the presence of formamide. This glass electrolyte can be modified by using some kind of polymer additives, which can cause some changes in mechanical properties of the glasses. In this report PVA (poly (vinyl alcohol)) is used. Due to this polymer, the glass electrolyte is more flexible and more mechanically stable.

FT-IR studies shows that PVA has no influence on progress of reaction, yield of product is same in both cases (with and without polymer)

On the other hand SEM testing is a proof that PVA doting decreases the number of cracks and fractures on surface in the resulting membrane.

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1,10-phenanthroline coordination compound containing zinc bromide

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Zinc is essential element for humans and is homeostatically regulated in the body. It plays an important role in protein synthesis and it is also a co-factor for many enzymes regulating cell growth and hormone levels, including regulation of gene transcription and growth factor metabolism. Zinc plays an important role in the formation and metabolism of mineralized tissues [1]. Skeletal muscle accounts for approximately 60% of the total body zinc content, and bone, with a zinc concentration of 100-200 mg/g, for approximately 30%[2]. The food sources rich in zinc are usually also rich in protein. Meat, poultry, dairy products, shellfish and whole-grain products are good sources of zinc [3].

1,10-Phenanthroline (phen) is a classic chelating bidentate ligand for transition metal ions that has played an important role in the development of coordination chemistry [4] and still continues to be of considerable interest as versatile starting material for organic, inorganic and supramolecular chemistry. Phen is a rigid planar, hydrophobic, electron-poor heteroaromatic system whose nitrogen atoms are placed to act cooperatively in cation binding. These structural features determine its coordination ability toward metal ions. The phen ligand behaves as a weak base in aqueous solution, its basicity is remarkably lower than aliphatic diamines, such as ethylenediamine [5]. Phen displays noticeable coordination ability for transition metal cations. In fact, the complexes with phen exhibit a larger entropic contribution to complex stabilization, mainly due to the hydrophobic nature of phen and to the consequent larger desolvation of metal cations upon complex formation. At the same time, the poorer s-donor ability of the heteroaromatic nitrogen atoms is compensated by the ability of phen to behave as p-acceptor [6,7]. In consequence, the complexes $[M(phen)_x]^{2+}$ in aqueous solution are generally stabilized by a favorable enthalpic contribution, accounting for the formation of a couple of strong coordination bonds [8].

The thermal decomposition of the investigated complex compound is a gradual process. According to TG and DTG curves, compound $[ZnBr_2(phen)_2]$ decomposes in 2 steps. First, the compound $[ZnBr_2(phen)_2]$ losses one phenanthroline molecule**.** This decomposition starts at about 105°C. After this stage, the complex compound is stable up to about 440°C. At this temperature the next phenanthroline begins to decompose and remaining zinc bromide starts to sublimate. This stage ends at temperature of about 830°C. Probably, the second stage consists of two steps overlapping in the TG and DTG curves.

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MTDLs (multi-target-directed ligands) as a drugs in Alzheimer disease

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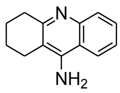
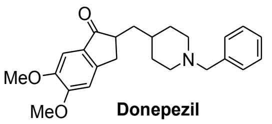
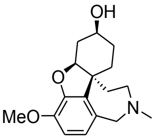
Alzheimer disease (AD) is the most common cause of dementia. This neurodegenerating disorder is a major problem for contemporary society. Current therapeutic approaches for the treatment of AD offer only limited and transient benefits to patients, with no attenuation of the further loss of neuronal cells in these conditions. None of the present drugs cure or even stop the development of this disease. Tacrine is the first drug approved by FDA (Food and Drug Administration) as an inhibitor of acetylocholinoesterase AChE (1993) and till today in a therapy only AChE inhibitors (donepezil, rivastigmine, galantamine, huperizine) and NMDA receptor antagonist (memantine) are used. Such compounds are not disease-modifying agents behaving only as cognition enhancers.



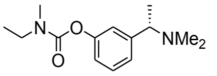
Tacrine



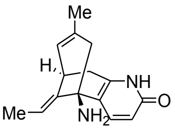
Donepezil



Galantamine



Riwastigmine



Huperizine A

AD has multifactorial origin and it's not surprising that the current drug design paradigm of one-drug-one-target may not be a sufficient model to develop treatment regiments for AD. Drugs hitting a single target are insufficient for the treatment of diseases like neurodegenerative disorders. That's why the doctors apply their patients multiple-medication therapy (MMT) also known as "cocktail" or "combination of drugs". MMT is composed of different drugs that combine different therapeutic mechanisms. In order to facilitate taking medications second approach might be used - multiple-compound medication (MCM) also called "single-pill combination". Medicinal research is constantly seeking to improve the efficiency of drugs. The third strategy is to combine one molecule pharmacophores of different drugs in the same structure to afford hybrid molecules. That's what the MTLDs (multi-target-directed ligands) means, hybrid drugs, which comprises the incorporation of two drug pharmacophores in one single molecule with the intention to exert dual drug action.

Already synthesized hybrids show that such coupling results in higher biological activity. This single compound may be able to hit multiple targets. Molecule contains inhibitor of AChE and butyrylcholinesterase (BChE) and for example calcium channel blocker, radical scavenger, may protect neurotransmitter system. After coupling the molecule acquires better properties. For example the inhibitor's activity increases, it can connect with different parts of the enzyme (peripheral and active binding sites).

There is no doubt, that we are entering an exciting new phase in the history of medicinal chemistry that requires a fundamental shift away from a 'one-compound-one-target' mind-set.

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Beginnings of nutrigenomics on the market. The case of proanthocyanidins

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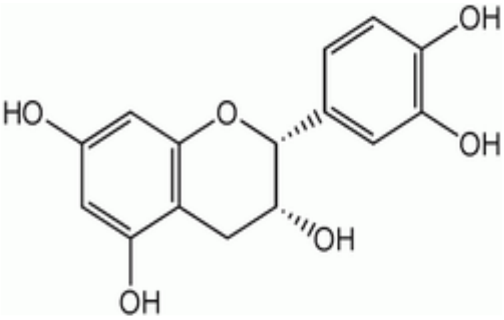
Nutrigenomics is a new branch of science that examine the effects of food components, present in our daily diet, on gene expression. It means that indirectly, by studying it, we could gain influence on our health.

One of the major ideas of nutrigenomics is to work out an individual, personal feeding strategy. By doing this it would be possible to control the expression of the certain genes and as a result the achievement of potential health benefits. Although the idea is noble and could save many lives, the research on nutrigenomics is still developing and it is in the early experimental phase.

Currently it is possible to come across many small companies that are offering diet supplements, basing on nutrigenomics assumptions. Those companies often base on non confirmed effects of chemical compounds and try to create a special „nutrigenomic" diet, with no knowledge of our human genome. The example of this practice may by the food supplements that contain proanthocyanidins and supposedly influence the expression of certain gens in our genome.

Proanthocyanidins are polymer chains of flavonoids such as catechins. Proanthocyanidins have strong anti-oxidant properties and in right doses they generaly have good influence on our health. Proanthocyanidins probably have moderate impact on gen expresion, but it is not know which genes are activated by them.

Currently researchers are trying to conclude whether proanthocyanidins are initiators or inhibitors of cellular apoptosis.



Pic.: example of repeating unit of proanthocyanidins

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Diastereoselective photocyclization of 2,3-dibenzylidenesuccinic acid derivatives

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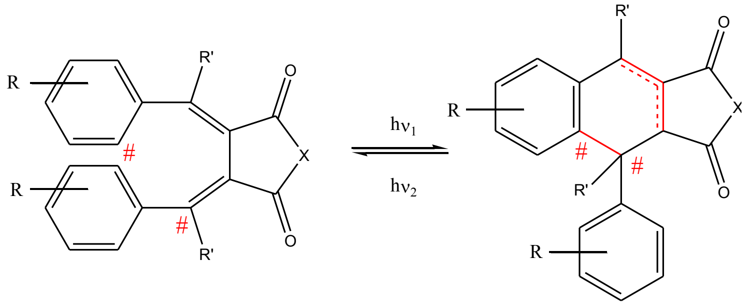
Lignans analogues - 2,3-dibenzylidenesuccinic acid derivatives, may undergo a UV light-driven cyclization leading to a mixture of 1-aryl-dihydronaphtalenes isomers. Those compounds are axially chiral. We introduced a chiral substituent on the nitrogen atom (X=N) or a chiral motif (X) in the structure and we expect to observe a chiral induction during the photochemical cyclizations.



R=H, OCH_3
X- chiral substituent
R'=H, CH_3

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Biotransformations and anitbacterial activity of iodolactone with metoxyphenyl ring

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Since the beginning of the last century halogenated organic hydrocarbons have been extensively applied in industry, agriculture, medicine, and daily life. Numbers of those compounds have wide spectrum of biological activity including anticancer [1, 2], antibacterial [3, 4] and antifeedant [5] activity. For those reasons they are applied as an antibiotics (clindamycin, flumequine), anti-inflammatory agents, analgesics (triamcinolone, diclofenac) and polymers (teflon, polyvinyl chloride). Common use is connected with large scale of production of those compounds and involves some problems with biodegradation of halogenoorganic pollutants.

Microbial dehalogenation is one of the most important steps in biodegradations of halogenated organic compounds. The key enzymes responsible for removing halogen atom from a compound are called dehalogenases [6].

Here will be presented chemical synthesis and evaluation of antibacterial activity of novel □-iodo-□-laktone with metoxyphenyl ring. The results of biotransformations by wild strains of filamentous fungi will be also described. In that process the novel □-iodo-□-laktone was dehalogenated and the □-hydroxy-□-laktone was obtained as a product.

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Optimization of the oligocarbonate diols synthesis

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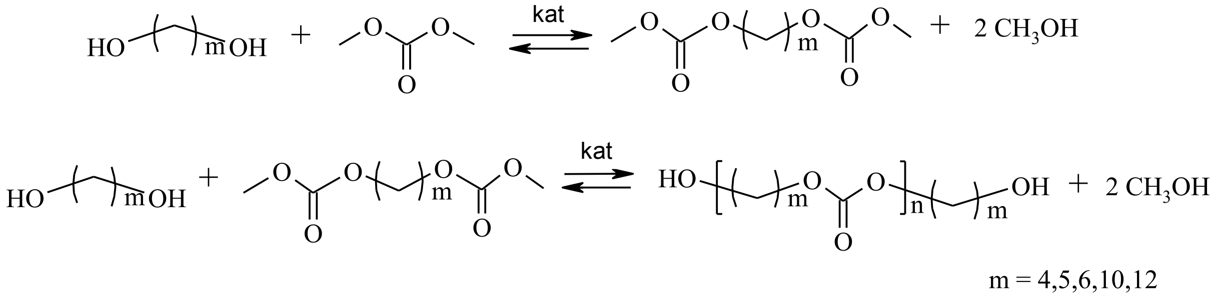
Methods of preparation of aliphatic oligocarbonate diols include, among others, condensation of a diol with phosgene, or a copolymerization of oxirane with carbon dioxide in the presence of organo-zinc compounds as catalysts [1]. A more efficient method of synthesis of these compounds is a polycondensation of five-membered alkylene carbonates with α, ω-diols [2]. However, the main disadvantage of this method is a partial decarboxylation leading to the formation of a copolymer containing carbonate as well as ether linkages.

The most promising method of obtaining aliphatic oligocarbonate diols is the reaction of glycolysis of dialkyl carbonate (dimethyl or diethyl carbonate) with diols [3]. However, the difficulties in obtaining the desired molecular weight of the polymer occur.

Taking this into account, we performed a two-step synthesis of oligocarbonate diols based on dimethylcarbonate (DMC) and linear terminal diols containing 4, 5, 6, 10 and 12 carbon atoms in a hydrocarbon chain.

In the first stage of the synthesis the bis(methylcarbonate)alkylene was obtained in a reaction of a diol with 10-molar excess of DMC. Oligocarbonate diols were synthesized in the second step in the polycondensation of the obtained bis(methylcarbonate)alkylene with a diol in an appropriate molar ratio. The catalyst used in both reactions was potassium carbonate.



Obtained products were characterized by a molecular weight within the limits of 1600-5500 and did not have ether linkages in their structure. They were characterized by IR and ^{1}HNMR spectra, GPC and DSC analysis and by viscometric measurement.

Oligocarbonate diols might be used as macroinitiators in the synthesis of polylactide (PLA) or as soft segments in poly(carbonate-urethane)s.

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Preparation of pyrolytic carbons from polymer precursors

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Li-ion batteries are important components of the portable, computing and telecommunication equipment used by modern society. Consumers are in constant demand for thinner and lighter batteries with high capacity. Their increasing use at the present time, pushes to developing new and improved electrode materials for lithium ion batteries that would lead to dramatically higher energy capacity and longer cycle life. [1]

Battery negative electrode is made of porous carbon or graphite while positive electrode of transition metal oxides (cobalt, manganese or nickel). Conductive carbon layer (CCL) designed to the anode layers are usually obtained by pyrolysis of organic compounds or polymers. [2]

This work is related to preparation and characterization of carbon coated particles of anode material which forms composite electrode for lithium-ion battery. The carbonaceous material for the study was obtained from copolymer composed of: N-vinyloformamid (NVF) and acrylamide (AAM). Copolymers were obtained by radical polymerization. Precursors of anode materials (SiO_2 and SnO_2) were coated with water-soluble copolymers as a source of carbon. The resulting precursors were converted into a highly conductive composites during pyrolysis and carboreduction. The conductive carbon layers (CCL) were characterized by Raman spectra and electrical conductivity measurements.

Acknowledgement

This work was supported by the Polish Ministry of Science and Higher Education under research grant No. N N209 088638.

The part of the measurements was carried out with the equipment purchased thanks to the financial support of the European Regional Development Fund in the framework of the Polish Innovation Economy Operational Program (contract no. POIG.02.01.00-12-023/08).

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Radiation synthesis of nanogels derived from microemulsion

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Hydrogels, three-dimensional polymeric networks with the spatial structure and water trapped inside, plays nowadays an increasingly important role. They are for example used in medicine, industry and technology. With the development of the new technologies, methods of nanogels synthesis were developed. Nanogels are crosslinked macromolecules with nanometer size.

One of the synthetic routes, involves the use of reverse micelles - spherical aggregates formed by some surfactants in organic non-polar solvents. Due to unique phenomenon of self-assembly of surfactant molecules, free space is being formed, that could be filled with an aqueous solution of polymer.

The aim of this study is to produce and characterize the polymer nanogels. 0.1 molar solution of bis (2-ethylhexyl) sodium sulfosuccinate (known under the trade name AOT) in n-heptane was used. The first stage of the work was to optimize the method of preparation of reverse micelles and then to examine their size and stability depending on molar ratio of water to surfactant in the solvent, method of mixing water with the AOT solution and the time at which the microemulsion was stored. Then first attempts to synthesize pH and temperature responsive nanogels based on poly(acrylic acid) and poly(vinyl methyl ether) have been done.

The work was financed in part by the National Centre for Research and Development (NCBiR), Poland, grant number N R05 0073 06/2009 and International Atomic Energy Agency CRP No. 15473

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Archaeological glass analysis by means of LA ICP MS

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The knowledge about the elemental composition of genuine glass, made by a human in the past, can support the investigation of its age, provenance and production technology. Since the long-lasting influence of the environmental conditions on the deposited glasses could have provoked its corrosion, the changes of the archaeological glass surface composition, in comparison to the bulk, need to be taken into account. Therefore, in archaeometric researches, usually only the bulk glass composition is of interest. However, the knowledge about the composition of the corroded surface of the glass bring important information on the mechanism and final effects of glass corrosion phenomena, that can help to improve restoration and conservation methods for the objects that belong to the museum collections.

The elemental composition of archaeological glasses can be determined by several instrumental techniques, but the preferences are made to these which enable fast, multi-elemental and sensitive direct analysis of solid samples of various shapes and dimensions in atmospheric pressure without any previous pretreatment of an object. The possibility of distinctive analysis of the composition of surface versus bulk matter is of great importance. A non-destructive character of the measurements should be also retain, namely because of the great cultural and historical value of the objects.

The analytical technique which match closely to the above description is Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA ICP MS). In this presentation the possibilities and limitations of LA ICP MS for the investigation of elemental composition of archaeological glass will be presented on the example of the analysis of glass beads coming from various archaeological excavations in Poland. The results obtained with the use of nanosecond (λ=193, 266 nm) and femtosecond (λ=800 nm) lasers and different micro-sampling techniques will be compared. The LA ICP MS results will be evaluated with regard to the results obtained, for the same set of samples, by means of the commonly used method in glass analysis – Electron Probe Microanalysis (EPMA).

SELECTED PROPERTIES OF SPELT STARCH ILLUMINATED WITH ULTRAVIOLET AND LINEARLY POLARISED VISIBLE LIGHT

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Starch from spelt wheat *(Triticum spelta)* was illuminated by ultraviolet and linearly polarised visible light (>500 nm) for 5, 15, 25 and 50 hours. Each spelt starch sample was characterized by measurement of the following physicochemical properties: average molecular weight (M_w), radius of gyration (R_g) of polysaccharide chains, chain lenght distribution of amylopectin structural units and crystalline structure. Molecular weight (M_w), radii of gyration (R_g) were measured by high performance size exclusion chromatography, coupled with multi-angle laser light scattering and refractive index detectors (HPSEC-MALLS-RI). Changes in average molecular weight and radii of gyration were different for starch illuminated with ultraviolet and visible light. Illumination with ultraviolet induced different depolymerisation/repolymerisation reactions than for samples illuminated with visible polarised light. We observed that the illumination led to more changes in amylose fraction for starch illuminated with visible light. The chain lenght distribution of amylopectin structural units of native and illuminated starches was characterized by the hydrolysis with isoamylase from *Pseudomonas amyloderamosa*. Additionally we measured X-ray diffraction spectra for spelt native starch and after illumination.

New anthracene derivatives for optoelectronic materials

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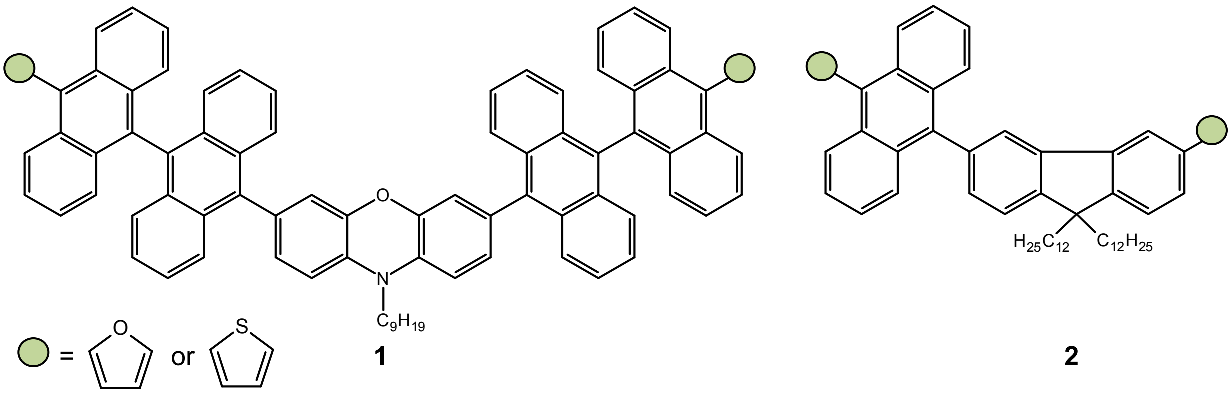
The future of organic electronics is now the realization of low-cost, flexible and easy-to-process optoelectronic devices among other organic light emitting diodes (OLEDs) for full-color displays. In such devices the active layers are composed of semiconducting low-weight materials or polymers, which properties can be easily tune by incorporating an electron donating/withdrawing molecules into polymer backbone.[1,2]

Even if many emitting materials have been designed and utilized in the fabrication of OLEDs, there is a lack of the blue color emitters with high performance. They are difficult to obtain as they require lower band gap and are more versatile.[3] The "donor-acceptor" type polymers possessing anthracene moiety, which is considered to be suitable for producing high efficiency and stable blue-light-emission, seem to be particularly interesting for that application.[2,4]

Symmetric and asymmetric anthracene monomers **1** and **2** were synthesized by a direct Suzuki and Still cross-coupling reactions with the employment of a palladium compounds as catalysts, Scheme 1.



Scheme 1. Chemical segments of novel branched anthracene co-monomers

Synthesis of new anthracene derivatives will be presented and their potential application for optoelectronic devices will be discussed.

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New anti-cancer drugs analogues for the modification of multifunctional nanocarriers

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Nanotechnology appears to dominate contemporary science. In nanotechnology world sees a huge potential which could bring benefits in drug development, water decontamination, information and communication technologies, and the production of stronger, lighter materials. According to U.S. government estimates, the nanotech economy will be worth $1 trillion by 2012[1].

Drug activity depends not only on direct effects caused by this drug in a precise place but also it depends on how the drug reaches and then leaves this place out. Scientists think nanotechnology could help with drug delivery and precision targeting by using metal particles[2].

The way drug is given, will it be orally, intravenously or intramuscularly etc, is very important. Medications given orally find their way in the liver where they may be involved in some enzymatic reactions, and this could completely deactivate them. Drugs injected straight to the bloodstream should have optimal half- life and reach the right tissues, cells and be able to penetrate through the membrane. Using gold nanoparticles stabilized with drug we could change its transport through the bloodstream, changes its half-life, improve precision of medication delivery.

In my work I focus on chemical synthesis of mercapto-functionalized organic molecules (mercaptopurine, antrachinone and flutamide derivatives) also synthesis and modifications of nano-vehicles for anti-cancer drug targeting and delivery.

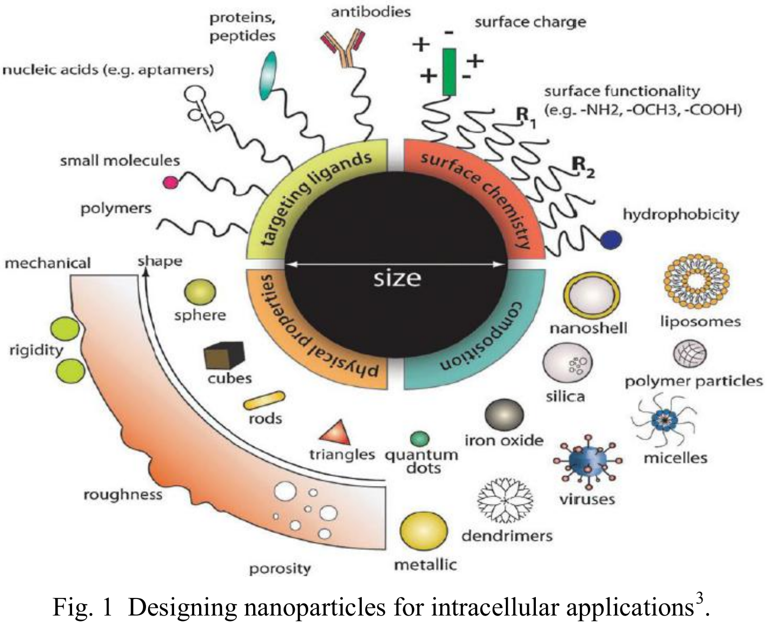

Fig. 1 Designing nanoparticles for intracellular applications[3].

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Chemometric in analysis of fluorescence fingerprints

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Chemometrics uses mathematic and statistic tools to extract relevant information from chemical data [1]. Chemometric techniques can be used to model complex and multivariate chemical data containing concentration profiles, spectra, etc. obtained from different analytical techniques. In this work we focus on popularise applications of chemometrics to fluorescence fingerprints.

Fluorescence spectroscopy is sensitive, non-destructive and low cost analytical technique. Using this technique excitation and emission spectra for examined samples are register [2]. Excitation and emission fluorescence spectra can be collected simultaneously and are called fluorescence landscapes. They can be treated as chemical fingerprints. Due to attractive fluorescence spectroscopy properties, its fingerprints are used for instance to describe food products [3], biological samples [4], monitor chemical processes [5], drug control [5], etc.

We applied chemometrics tools to analyze fluorescence fingerprints of yoghurt [7]. Among many chemometric applications there were exploration (principal component anaysis, PCA), calibration (partial least squares regression, PLS) and discrimination (discriminant partial least squares, D-PLS) analysis preformed on given data.

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„Blondzik, tipsik i solara - o środkach i zabiegach upiększających z chemicznego punktu widzenia"

Osypiuk Alicja

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Cosmetics is a name derived from the Greek word kosmeo-embellishes or kosmetikos-beautifying. Thus, cosmetics is the art of beautification. Legacy of the ancients is not just a word, neither a series of guidelines for the cultivation of the art of beauty. Even the ancients sought to achieve order and harmony, using available materials performed combs, necklaces, and Ointments used for decorating the body.

Despite the passing of time desire to keep and improve the beauty of the imperfections of human nature have not changed. Today, as never before it plays an unprecedented role in the appearance of a properly functioning human society. Now it is not enough to be healthy and posess a neat appearance. Humanity began to look for innovation, with the goal of attracting attention to a specific unit of the environment. Every day people brake new barriers - tattoos on the knobs of the eyes and hair extension treatments are becoming a symbol of our generation.

The message prepared by me introduce some beauty treatments and resources needed to implement them. Since the topic is very extensive I will confine myself to the most popular methods for both women and men. This presenation will contain information about solarium, hair extension treatments and teeth whitening.

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Microcontact Printing (μCP) of fluorescent proteins using porous PDMS stamps

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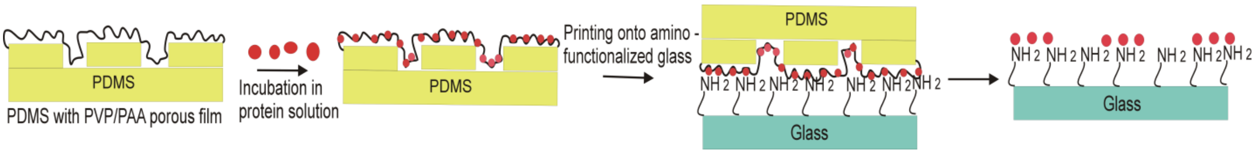
Pattern fabrication is an important issue in many fields of science ranging from microelectronics, nanotechnology to biological sensing microarrays production. One of the methods used in surface patterning is soft lithography technique - microconatact printing (μCP) [1]. It is very simple and efficient method of surface structuring which allows to create even tens nanometers small patterns.

In presented experiment PDMS stamps modified with porous PAA [poly(acrylic acid)] /PVP[poly(2-vinylpyridine)] [2] film were used to investigate efficiency of microcontact printing of two fluorescent proteins (His-DsRed and HIgG-Fc-FITC) onto amino functionalized glass substrate. It was proved that porous structure acts as an ink reservoir while printing so the multiple printing from one stamp without reinking is possible. Then the influence of molecular weight of PVP and time of post base treatment on morphology of micropores in the film and printing results was studied.



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Chemically Capped Spliced Leader RNAs - a usefull tool for studies on Function of the Nematode Spliced Leader

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Translation initiation of most eukaryotic mRNAs is mediated by a cap-dependent mechanism. During the initiation step of translation, the cap is specifically recognized by eIF4E (eukaryotic initiation factor 4E), the smallest subunit of a larger complex, eIF4F, which also consist of a RNA helicase, eIF4A, and a scaffolding protein, eIF4G. Recognition of the cap by eIF4E and ribosome recruitment through eIF4G is a rate-limiting step of translation. The cap present at 5' end eukaryotic mRNAs contains 7-methylguanosine linked via a 5',5'- triphosphate bridge to the first transcribed nucleotide (MMG-cap, m^7GpppG). In nematodes however, two different mRNAs co-exist in cell. In addition to mRNAs with the typical MMG cap, about 70% of RNAs possess an atypical, hypermethylated form of the cap with two additional methyl groups at the N2 position (TMG-cap, $m_3^{2,2,7}GpppG$). This atypical cap is added with a 22 nt conserved splice leader sequence (SL) to pre-mRNA during spliced leader *trans*-splicing to form the mature 5' end of the mRNA. In general, eukaryotic eIF4E proteins are unable to effectively recognize and bind the TMG cap. However, the parasitic nematode Ascaris suum efficiently translates TMG capped RNAs. Studies have shown that the 22 nt nematode SL sequence significantly enhances translation of $m_3^{2,2,7}G$-capped RNAs in nematodes, but has little effect on the translation of m^7G-capped messages. Efficient translation of $m_3^{2,2,7}G$-capped RNAs requires specific nucleotides and structural elements within spliced leader sequence including a stem loop that contains a 3 bp stem immediately downstream of the cap.The molecular mechanism through which the SL enhances translation of TMG-capped mRNAs remains unknown. Based on modeling of the SL stem-loop, we propose a model that suggests 1) the N2 methyl groups of the TMG cap interact with bases in the SL RNA stabilizating the stem and perhaps eIF4E bound to the $m_3^{2,2,7}G$-spliced leader RNA and 2) that the SL stem loop interacts with eIF4E leading to conformational changes that influence the eIF4E/eIF4G interaction and thereby enhance ribosomal requirement. In order to test this model and better understand the interaction between Ascaris eIF4E and $m_3^{2,2,7}G$-spliced leader RNAs, m^7G- and $m_3^{2,2,7}G$-capped spliced leader RNAs have been synthesized for use in several experimental analyses. 5' phosphorylated 22 nt nucleotide SL RNAs were chemically capped with either an m^7G- or $m_3^{2,2,7}G$-cap and purified using HPLC. Wild-type and mutant SL oligonucleotides, capped with 7-methylguanosine or N^2,N^2,7-trimethylguanosine will be used for NMR solution structural studies of the SL RNA and for eIF4E:SL RNA x-ray crystallography to test our model of the SL RNA stem loop and its interaction with eIF4E.

X-ray Photoelectron Spectroscopic Studies of Carbon Fiber Surfaces

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It is believed that X-ray photoelectron spectroscopy is the most powerful technique to investigate the surface chemistry of carbon fibers. This type of analysis reveals the composition from a depth of 2-20 layers (100Å) and the electronic state of the surface region of the sample. XPS is extremely versatile method, because beside information about concentration of particular element, it also shows the concentration of each functional group. It is possible thanks to the process of delconwoution. The carbon peaks, which can be observed in the binding energy range from 280 to 295 eV, can be attributed to several functional groups. It has to be pointed out, that sometimes authors assign different value of binding energies to the same functional groups, as it is presented in Table 1. Peak C1s is usually deconvoluted on four or five peaks: i) the representant graphitic carbon, ii) carbon bonded phenolic or alcoholic hydroxyls or ether oxygens, iii) carbonyl or quinone groups, iv) carboxyl or ester groups, and one more v) carbon present in carbonate groups and adsorbed CO and CO_2. O1s spectrum is fitted to three component peaks: peak I (531.2-531.6 eV) which corresponds to ketone, lactone and carbonyl group, peak II (532.-533.4) to hydroxyl and ether groups and peak III (534.6-535.4 eV), which is usually of low intensity due to chemisorbed oxygen and some absorbed water.

Table 1. Comparison of C1s peak deconvolution proposed by different authors.

	C-C	C-OH,C-OR	C=O	COOH, COOR	CO_3^{2-}, CO_2	C-N
C.U. Pittman	286.6	286.1-286.3	287.3-287.6	288.4-288.9	290.4-290.8	-
Z. Xu	284.7-284.9	285.5-285.8	286.7-286.8	288.7-288.8	-	-
K.J. Huttinger	284.7	286.1	287.6	288.6	-	-
P.M.A. Sherwood	284.6	286.1-286.2	286.4-286.6	289.1-289.4	290.5-290.9	-
J. Liu et al.	284.8-284.9	286.0-286.4	287.1-287.3	289.0-289.4	-	-
N. Dilsiz	285.0	286.3-286.5	287.3-287.6	288.6-2889	290.3	-
Z. Zhang	284.2-284.3	286.3-286.6	288.0	289.5-289.7	-	285.7

In my presentation I show how we made a deconvolution of C1s, O1s and N1s peaks of unoxidized and oxidized intermodulus strength carbon fibers.

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The phenomenon of electroporation of lipid membranes

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Every living organism is built from cells, of which an inherent element is a cell membrane letting these cells exist in the environment. The complexity of biological membranes makes it virtually impossible to draw detailed physical conclusions from studies of these membranes and simplification is therefore required. Since the realization that lipid bilayers comprise the fundamental structure of all biological membranes, they have been the subject of numerous experimental studies [2]. As a result, membrane models of variable complexity and destination have emerged, some aiming at elucidating structural details of the bilayer membrane and others striving to mimic its functions. Development of the science showed that both biological membranes and lipid bilayers used as model membranes have a lot of unusual electric properties. One of them is ability to electroporation.

Electroporation of bilayer lipid membranes is a reversible phenomenon relying on the sudden decrease of the resistance of the membrane under the influence of the applied constant-intensity current [1]. Generally, this membrane resistance fall is being justified with the presence of hydrophilic pore in lipid bilayer, enabling the flow of molecules or ions through the membrane [2]. The hydrophilic pore appears as a result of reorientation of the lipids in the membrane under the influence of the electric field caused by the flowing current. Occurrences happening in individual stages of the electroporation are still not known completely, however, the general outline of the whole process one can already qualify. The first stage is the creation of volume fluctuations and defects in the structure of the membrane which precede the uprising of hydrophilic pore [1,4]. Next stage is a reorientation of lipids in the membrane leading to the occurring of hydrophilic pore [2,3]. An ending stage, appearing after the disappearance of the electric field, is reconstructing by the membrane its constant structure and return lipids to their home positions, called the relaxation of electroporation [1].

The phenomenon of electroporation can be examined and triggered by the charge pulse and current clamp methods [2]. These methods differ between themselves mainly in the value of the applied current intensity and the time that current influence on the membrane. Course of some stages of the electroporation process also differs slightly.

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Influence of organic dyes on sonochemical degradation of DNA. The way to sonodynamic cancer therapy

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Ultrasound is a mechanical wave of a frequency in the range 20 kHz – 10 MHz and velocity in liquids of about 1000 – 1600 m/s, which translates into the wavelength range of 10^{-6} to 10^{-2} m. So this kind of wave is not able to couple the energy levels in molecules directly.

The chemical effects of ultrasound in liquids are induced by acoustic cavitation process, i.e. creation of gas bubbles and their fast oscillation or implosion. During an adiabatic compression gas in the bubble can be heated to extremely high temperatures. This may cause pyrolysis of dissolved substances and free radical generation. Macromolecules can also become damaged by mechanical stress around collapsing cavitation bubbles.

It has been postulated that presence of specific substances can enhance the action of ultrasound on tumor cells (sonodynamic effect), in an apparently similar way as photosensitizes enhance the light-induced tumor cell damage (photodynamic effect being the basis of photodynamic cancer therapy). The application range of sonodynamic therapy could potentially be much broader than photodynamic therapy, since ultrasound can penetrate the tissues much better than light does. However, the mechanism of sonodynamic effect is not yet well understood.

Many substances used in photodynamic cancer therapy can be excited by ultrasound as well. One of them is porphyrin, which is able to interact with double helix of DNA, thus dramatically increasing tumor cells killing factor *in vitro* as well as *in vivo*. In this work we have studied the influence of this and some other organic compounds on sonochemical degradation of deoxyribonucleic acid. Using agarose and polyacrylamide gel electrophoresis, efficiency of double stand breaks of DNA in the presence of few compounds like bengal rose, dimethylformamide and 5-fluorouracil was determined and compared with the action of ultrasound, under identical conditions, on DNA alone.

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Application of europium and terbium complexes to build fiber-optic sensors of UV radiation

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In the twentieth century, researchers have discovered that the concentration of ozone, responsible for protecting our planet from UV radiation, in the atmosphere decreased significantly. The intensity of this harmful radiation is continuously measured and monitored by sensors, such as electrical sensors. Fiber optic sensors represent an alternative to the pneumatic and electrical sensors, and many of the properties of optical transmission system meets the requirements of an ideal. Light is safe agent in penetrating the center point of measurement. Optical fibers are constructed from relatively cheap materials, and as dielectric tracks are not subject to interference, the influence of external fields, overvoltage's, are much easier to install than copper cables due to their small size and weight. The core of the fiber is made of two layers, one inside is made of silica glass, which undamp ultraviolet radiation, a second one, external, includes a phosphor. UV-phosphor particles present in the active layer emit light with a wavelength longer than the length of incident light. The generated signal is transmitted over fiber draining into the detector.

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Ab-initio systematic analysis of stacking interactions in benzene-benzene, benzene-pyridine and pyridine-pyridine supramolecular compounds

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Stacking interactions or π-π interactions are one of the most common noncovalent interactions (together with hydrogen and halogen bonds) found in both natural and anthropogenic supramolecular systems. These interactions play a very important role in stereoselectivity of organic reactions [1], they are crucial for assembly in biological systems [2] and they also contribute to many areas of science such as medical chemistry [3] and nanotechnology [4]. Thus, the study of their role in both model and real systems has outstanding significance.

Although lots of theoretical calculations have been made in this field, there is a lack of systematic analysis of π-π interactions in real systems. This knowledge can be significantly useful in understating the limits of stacking interactions application in the stabilization of nucleic acids or designing drugs. Thus, the systematic analysis of π-π interactions in benzene-benzene, benzene-pyridine and pyridine-pyridine systems was performed and it is presented. The Gaussian03 software was used and the 6-311++G(3df,2p) basis set was applied to Hartree-Fock calculations followed by a Moller-Plesset correlation energy correction [5] truncated at second-order [6]. To determine the contribution of interactions dispersion energy the all calculations were also made with usage of the B3LYP functional [7]. In all cases the Basis set superposition error corrections were carried out using the counterpoise method [8].

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Excited-State Intramolecular Proton Transfer in aryl-imidazole molecules with chromophore modifications

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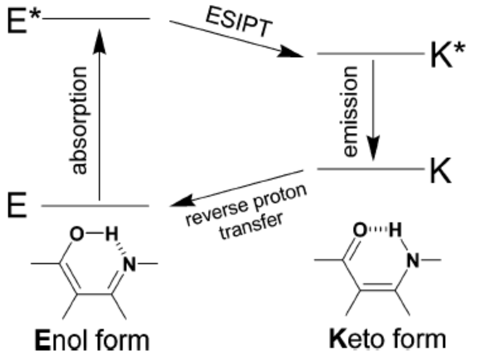
Aryl-imidazole derivatives exhibit interesting photoluminescence and chemiluminescence properties. They are potential chemosensors because of their piezochromism, photochromism and thermochromism in the solid state and in the solution. However, only few reports described 2,4,5-triphenylimidazole as fluorophore in cation chemosensor.

Chemosensor can be used to detect metal cations in environment, food and biological systems with the advantages of simplicity, high selectivity and sensitivity. Development of a new chemosensor has therefore attracted great interest.

My task is to examine the relationship of absorption and emission properties of derivatives and analogues of arylimidazoles. In particular, synthesis the compound which exhibits ESIPT.

Excited state intramolecular proton transfer (ESIPT) phenomena have been investigated in the past decades due to the practical applications of ESIPT exhibiting molecules as laser dyes, photostabilizers, fluorescent probes in biology and light-emitting materials for electroluminescent devices. ESIPT typically occurs in aromatic molecules having a phenolic hydroxy group with an intramolecular hydrogen bond to the nearby hetero atom of the same chromophore. Compound with ESIPT have Large Stokes shift and will be have a double fluorescence depending on the nature of the molecular and external factors such as solvent and temperature.



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Synthesis of cyclic analogues of tryptophan by the Pictet-Spengler condensation of chiral aminoaldehydes with β^2- or β^3-*homo*-Trp derivatives

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Cyclic analogues of tryptophan which introduce local constraints reduce the flexibility of the indol moiety are very valuable tools to probe the bioactive conformation of the peptide ligands. The Pictet-Spengler reaction [1] has been one of the possibilities to prepare such analogues, with freezed the indol moiety in tryptophan, containing 1,2,3,4-tetrahydro-β-carboline skeleton. The heterocyclic skeleton of 1,2,3,4-tetrahydro-β-carbolines possesses multiple sites for functionization, therefore they are an ideal choice for the design of pharmacophore-based libraries in drug discovery, through generation of a large member of structurally diverse compounds.

β-Amino acids represent an important class of biologically relevant molecules. Oligomers composed of β-amino acids can form predictable secondary structures stable to metabolic transformations and they can mimic α-peptides in peptide-protein interactions. For this reasons β-amino acids are very usefull for peptidomimetics design.

We report the synthesis of β^3- and β^2-*homo*-tryptophan and their derivatives as components to Pictet-Spengler reactions and diastereoselectivity studies of Pictet-Spengler condensation of L- and D-α-aminoaldehydes as carbonyl components with β^2- or β^3-*h*Trp methyl esters and N-terminal β^3-*h*Trp dipeptides as arylethylamine substrates.

The synthesis of L-β^3-*homo*-tryptophan was accomplished by Arndt-Eistert homologation of L-α-tryptophan [2]. Optically active L-β^2-*homo*-tryptophan was synthesized with the use of (+)-2,10-camphorsultam as chiral auxiliary [3]. Cyclizations of different tryptophan derivatives with L- and D-α-aminoaldehydes were performed in the presence of TFA and at low temperature (-40°C) to avoid racemization of chiral aminoaldehydes.

Pictet-Spengler condensation of L- and D-α-aminoaldehydes as carbonyl components with β^3-*h*Trp methyl esters and dipeptides with N-terminal β^3-*h*Trp as arylethylamine substrates lead to 1,3-disubstituted 1,2,3,4-tetrahydro-β-carbolines, a new stereogenic center was created and the mixture of *cis/trans* products was obtained. The reactions was studied in terms of double stereodifferentiation. The influence of the carboxyl terminus of β^3-*h*Trp on the ratio of *cis/trans* products was also investigated. The conformations of cyclic products were studied by 2NMR ROESY spectra.

During the Pictet-Spengler reaction with the use of L-β^2-*homo*-Trp-OCH_3 a new 7-membered ring was created. It is possible to form two different diastereoisomers. The stereoselectivity of these reactions is still under investigation.

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Hybridization of ligands as a way of generating combinatorial libraries of drug candidates

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Computational methods and their application in the process of drug design is a central theme in chemoinformatics. Virtual screening techniques are widely used in the process of searching drug candidates and thanks to them we can evaluate large libraries of chemical compounds. VS methods are divided into two main groups – those that rely on knowledge about the protein target (structure-based VS) and those ones that are based on the information of known actives (ligand-based VS). [1,2]

Structure databases that undergo the process of virtual screening may come from commercially available resources or they may be generated in combinatorial way. We generated a combinatorial library of 5-HT6 ligands by hybridization of known actives using BREED technique. [3] Then the multistep virtual screening protocol (Lipinski's Rule of Five, Veber's Filter, Physicochemical property filter, ADMET filter, Pharmacophore filter, Docking) was applied and the best compounds were selected and ordered to determine their affinity towards 5-HT6 receptor.[4]

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DFT calculations of CO_2 - zeolite interactions: adsorption and molecular dynamics simulations

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Crude oil, coal and natural gas are still the most significant sources of energy and their consumption is dynamically rising. There is no serious alternative to conventional energy sources at the moment, so it is predicted, that consumption of fossil fuels will increase.

Carbon dioxide emission is a consequence of combustion processes, where use of fossil resources has main contribution. Apart from having negative effect on the climate, carbon dioxide is a useless waste. At the moment, there is no technology for effective conversion of CO_2 into useful and highly demanded products in order to utilize large amounts of CO_2.

Many solutions for carbon dioxide utilization have been proposed, including: underground and underwater storage, CO_2 reforming of methane, electrochemical reduction, conversion to carbon monoxide and methanol. An interesting concept is conversion of carbon dioxide into fuel-like hydrocarbons, that could be used as fuel components. This would enable production of fuels and saving of fossil resources.

This work is focused on studying interactions between CO_2 molecule and modified zeolite structures. The scope of the study includes docking simulations with self-developed tool and molecular dynamics using DFT method. This allowed to characterize the influence of the presence of cations on interactions between CO2 molecule and zeolite structure.

Models used in the simulations were created by modification of DOH zeolite structure. Two selected Si atoms were replaced with two Al atoms and, for charge compensation, a +2 cation was introduced (Cu^{2+}, Zn^{2+}, Pd^{2+}, Ni^{2+})

The simulation results show that, the presence of a cation in the zeolite structure has important influence on adsorption energy. The structures, that contain cation are able to adsorb CO_2 stronger.

Furthermore, the smaller is the distance between CO_2 molecule and cation, the lower is the adsorption energy. This means that the adsorption is stronger close to the cation. This effect has interesting consequences in MD results - CO_2 molecule, when close to cation, is "locked" in one position, whereas CO_2 far from cation can make a rotation. In this way, cation can be described as adsorption active center. Adsorption energy magnitudes are typical for chemisorption (~1eV).

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Transformation of quinine and quinidine to β-amino acid derivatives – potential catalysts of asymmetric synthesis

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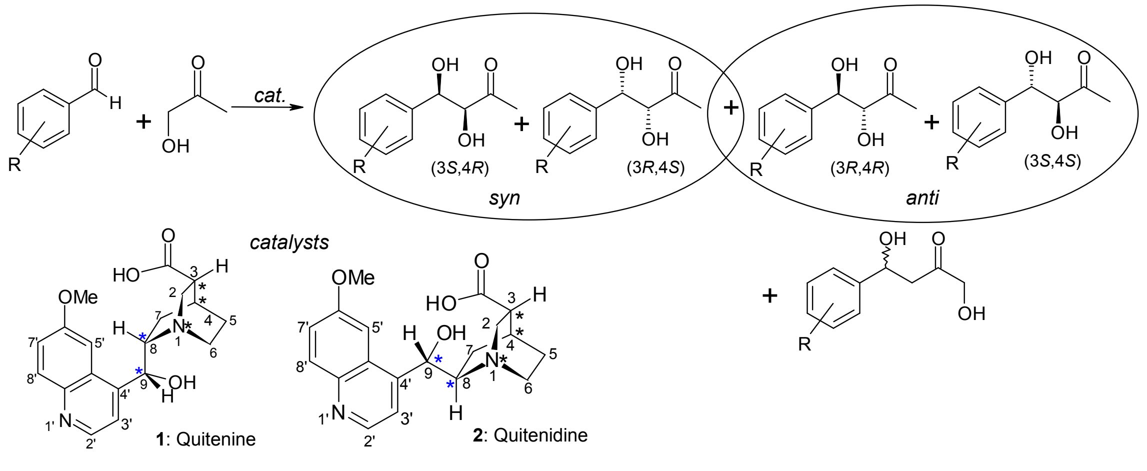
Quinine and quinidine, natural *Cinchona* bark alkaloids, are known as antimalarial and anti-arrhythmic agents. In the last thirty years, these alkaloids using have been targeted in the asymmetric syntheses area.

Cinchona alkaloids and their derivatives are used as optically active bases in the separation of racemic organic acids and as modifiers of metal catalysts. They also can play roles of organocatalysts in asymmetric synthesis or act as ligands complexes catalyzed an enantiodifferation process during one or two bond formation, including a olefins dihydroxylation reaction (Sharpless). *Cinchona* alkaloids transformed to chiral quaternary salts as asymmetric phase-transfer catalysts (eg. O'Donell type syntheses) and bonded with various types of polymers are the most interesting directions of applications.

In our experiments, we transformed the quinine and quinidine into quitenine **1** and quitenidine **2** and then to their salts and complexes with transition metals, and next we examined the activity of these systems as catalysts for an asymmetric aldol reaction of substituted benzaldehydes with hydroxyacetone (HA). Regioselectivity, diastereoselectivity and enantioselectivity can be investigated depending on catalysts and reaction conditions.



Our first results show the expected regioselectivity towards the 1,2-diols, which were separated by column chromatography. Diastereoselectivity (*syn*/*anti* ratio) of the products obtained with using the pairs of catalysts (quitenine vs quitenidine and their derivatives), were determined on the basis of ^{1}H NMR. The enantioselectivity (ee) were measured by HPLC analysis on a chiral phase.

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Synthesis and Characterization of CdSe Quantum Dots

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Quantum dots (QDs) are nanometer-scale semiconductor crystals whose charge carriers are confined in all spatial dimensions. Confinement of electron-hole pair takes effect in unusual optical properties that highly depends on single crystal size. Broad absorption and narrow emission spectra, photostability and long fluorescent lifetime after excitation gives QDs wide range of potential applications [1, 2]. One of most significant perspectives for quantum dots is their use medical imaging. Optical properties of QDs allow simultaneous excitation of different coloured nanocrystals using single wavelength [2].

In this study CdSe nanocrystals were synthesized using CdO, elemental Se, oleic acid and trioctylphosphine by kinetic growth, with 1-octadecene as a solvent [3, 4]. Absorption, emission and fluorescence lifetime of obtained colloidal QDs were measured. Moreover, influence of synthesis parameters on nanocrystal sizes was investigated.

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The investigation of $Fe(CN)_6^{3-/4-}$ system on 4-mercaptopyridine self assembled monolayers on gold.

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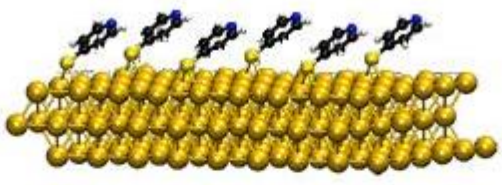
Nowadays, one of the most interesting issues around the nanotechnology are researches which are concentrated on self organization of molecules on metal surfaces. Thin monolayers of organic compounds with high level of self-organization are formed by spontaneous ordering of molecules on substrate surface. These monolayers are particularly easily formed by absorption of sulfur onto gold surface, which is the result of particularly high affinity of these elements. This property was used in order to obtain monolayers of 4-mercaptopyridine (4-mpy) on the conductive gold surface.



4-mercaptopyridine on gold surface

Self assembled monolayers of 4-mpy were prepared by immersing the electrode- cleaned gold substrate in 10^{-3} mol/l of 4-mpy ethanolic solution over 24 hour. Then, the investigations of protons connection to the modified surface were carried out. To determine such surface protonation constant, the electrochemical titration method was used.

This technique consists of performing series of cyclic voltammograms of calibrated redox system $Fe(CN)_6^{3-} / Fe(CN)_6^{4-}$ at different values of pH, controlled by Britton- Robinson buffers. The cyclic voltammetric measurements were performed with AUTOLAB PGSTAT - 128N, in the system of three electrodes, where the working electrode was modified surface of gold, Ag/AgCl electrode was the reference and Pt wire was the counter one.

The obtained protonation constant was compared to the literature data.

Anthocyanins, carotenoids, chlorophyll - health hidden in colors

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Anthocyanins, carotenoids or chlorophyll are nothing else than organic compounds but most of all they are plant pigments. Due to this they are out of the ordinary against a background of other chemical compounds. Those pigments give the plants a unique color (red, yellow, orange, green, etc.), ensuring the attractiveness of fruits and vegetables for consumers. But what really is hidden in fruits and vegetables?

How do these pigments affect their pro medical properties? Is the cabbage really empty? Answers to these and many other questions are revealed in my presentation.

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Properties of elastomeric nanocomposites containing montmorillonite (MMT)

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Nowadays, interest in nanomaterials is still growing. One of a kind of nanomaterials are nanocomposites, which have a particularly good functional properties. We have a lot of hope that these properties will be even better when we make a composite with layered aluminosilicate minerals, in example: kaolinite, montmorillonite, etc.

Some of aims of our examination were to confront characteristic of elastomer, elastomer with montmorillonite and elastomer with modified montmorillonite. We wanted to check how properties of that nanocomposites depend on type of used fillers.

Application of layered aluminosilicates as fillers is beneficial on account of the safety of obtaining nanocomposites. At their synthesis, usage of aluminosilicates avoids danger, that is connected with direct dosage of nanoparticles, which the influence on the human organism isn't known.

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Direct melt/solid polycondensation of L-lactic acid to poly(L-lactic acid) with high molecular weight

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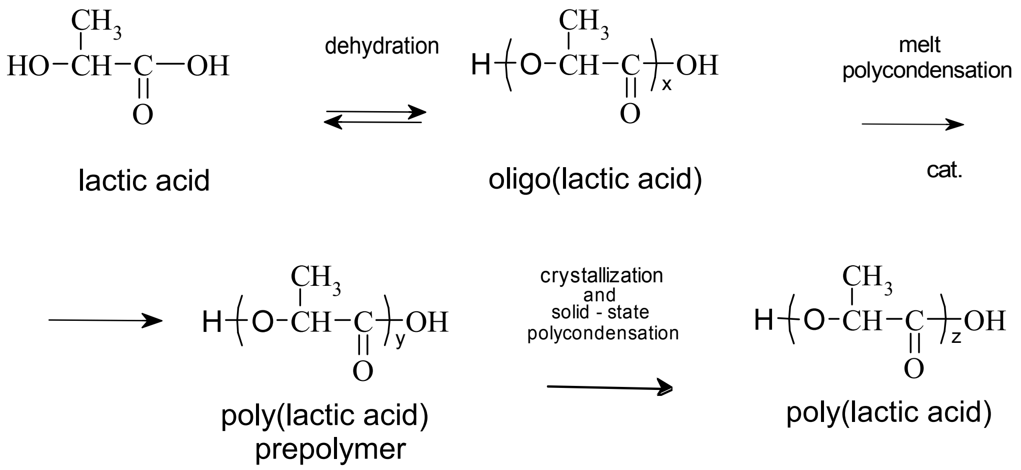
Poly(L-lactide) (PLLA) has usually been prepared by ring-opening polymerization of L-lactide. Recently, it has become accepted that the polycondensation of L-lactic acid (LA) can also give PLLA with a significantly high molecular weight.

In our study we succeeded in preparing poly(L-lactic acid) with high molecular weight (around 100000 Da) from LA by the melt/solid polycondensation method, in high yield and in a relatively short reaction time. Initially a prepolymer of PLLA was prepared by direct melt polycondensation of LA by using binary catalyst system which consisted of tin (II) chloride dihydrate activated by acids proton from p-toluenesulphonic acid as the co-catalyst. This catalyst system was effective in conducting the polycondensation without racemization of the resultant polymer, whose molecular weight reached about 40000 Da. Obtained melt-polycondensate of LA was than crystallized by heat-treatment around 105 °C and subsequently subjected to solid-state polycondensation at temperature above glass transition yet below melting point of PLLA [11]. The reaction occurs between the terminal groups in the amorphous phase of semicrystalline polymer. Due to the relatively low temperature of the process, side reactions and thermal degradation of the product are limited.



During our research we also examined the effect of the presence of talc and silica nanoparticles and also crystallization time on solid state polycondensation, crystalinity and molecular weight of PLLA. It was found that when the amount of talc or silica was already below 1 wt% the intrinsic viscosity and molecular weight of the final product were larger than the polymer without additives (1.1 dl/g, 116000 Da and 0.76 dl/g, 67000 Da, respectively). In the case of polymers with nucleating agent, the degree of crystallinity was higher (35%) than pure PLLA (24%) after the same crystallization time according to the theoretical heat of fusion (203.4 J/g) of the ideal PLLA crystals. Moreover, these products, in comparison to pure polymer, attained a higher value of molecular weight in shorter SSP time and were characterized by brighter color.

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Carbon dioxide in the MTG technology – Fuel of the Future

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Carbon dioxide - a colorless, odorless gas. Gas which, in recent years there have been problems with too much in the atmosphere, and the consequence of a rise in "greenhouse effect" causing climate change. This question is also raised during the discussion on the use of traditional fossil fuels such as oil or coal. Through a team of researchers led by Lublin Professor Dobiesław Nazimek from the Department of Chemistry, Maria Curie-Sklodowska University in Lublin, were able to develop a method of processing carbon dioxide in the organic fuel.

Thanks to the work on synthetic photosynthesis, there is the possibility of cheap remake of carbon dioxide into relatively complex hydrocarbons, and then to methanol, which have undergone heat treatment and synthesis of the MTG technology and leads to a 108-octane synthetic gasoline that does not contain nitrogen or sulfur compounds.

The study showed that the MTG reaction is highly exothermic, but the total heating effect is highly dependent on the selectivity of the reaction. However, in order to obtain a cheap synthetic gasoline or diesel fuel, cheap material for its production has to be found. Selective oxidation of methane in the direction of methanol is considered one of the greatest challenges of a modern catalysis.

So far, the experiments used laboratory-pure gases. Now work is underway on the gases in which impurities are present. It is estimated that after implementation of the method on an industrial scale, it allows to obtain cheaper gasoline by about a quarter. According to estimates by Professor Nazimek if his method was used in the largest industrial plants in the country, Poland could produce approximately 21 million tons of fuel annually. For comparison, during the year we consume about 6 million tons of gasoline. Moreover, production of fuel from carbon dioxide, can make us independent from the supply of Russian oil.

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Solvent effects on enzymatic deamination of L-alanine

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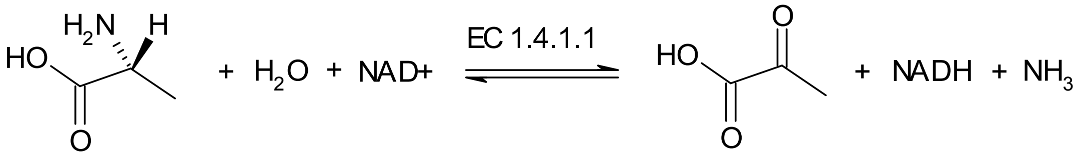
Enzymatic reaction of deamination of L-alanine (L-Ala) to pyruvic acid is catalyzed by L-alanine dehydrogenase (ADH, EC 1.4.1.1). The reaction proceeds according to the scheme [1]:



ADH is a key enzyme in the catabolism of L-Ala, because pyruvic acid which is the product of deamination is converted into carbon dioxide and coenzyme A [2]. Moreover the enzyme shows stereospecificity and catalyzes the elimination of *pro-R* proton from the second position of L-Ala [1]. The reaction proceeds at room temperature in carbonate buffer medium at pH 10. ADH enzyme shows catalytic activity in the presence of cofactor NAD^+ [3]. Despite many reports in literature, mechanism of converting L-Ala into pyruvic acid is not fully known and understood. To study the mechanism the solvent isotope effects method (SIE) was used. It is based on a comparison of kinetic parameters in Michaelis equation determined for the deamination reaction in the protonated and fully deuterated reaction media. The determination of numerical values of SIE is necessary to explain better the reaction mechanism.

This work was supported by the grant BST- 153123.

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Multicomponent aliphatic-aromatic copolyesters

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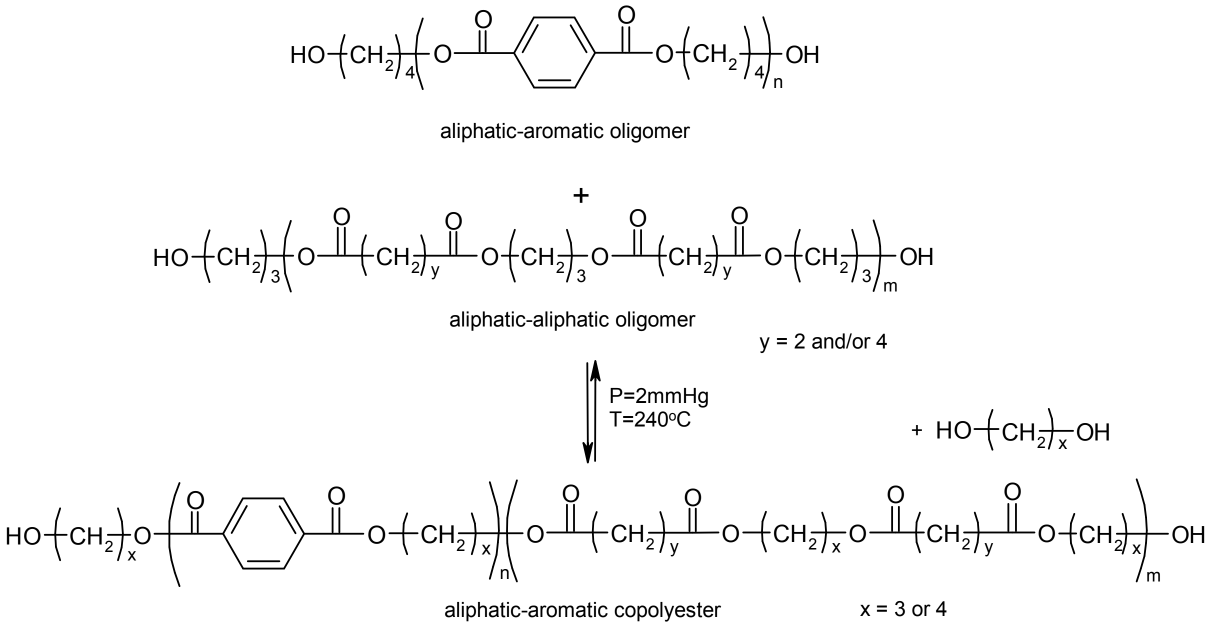
Purpose of this work was investigation on the synthesis of multicomponent aliphatic-aromatic copolyesters that combine good mechanical properties of aromatic polyesters and biodegrability of aliphatic polyesters. Synthesized polymers are expected to be widely used in packaging industry, as well as polymeric plasticizers for high-crystallinity polymers such as: poly(lactic acid).

The copolyesters were prepared by the two-stage melt polycondensation method of prior synthesized oligomers. Two oligomers were obtained from dimethyl terephthalate and 1,4-butanediol as well as adipic acid, succinic acid and 1,3-propanediol, respectively. The reaction was carried out under an nitrogen atmosphere at 190-230 °C. In the second stage the pressure was reduced (2 mmHg) in order to facilitate the removal of the diols excess (Scheme).



In our work the effect of diol to acid molar ratio, catalyst type, aromatic segments content on molecular weight, glass transition temperature (T_g) and mechanical properties of synthesized polyesters was studied. Hydrolytic degradation of copolyesters was measured in bufer solution under different pH = 2.2, 7.4, 10.0 and biodegradation was monitored at pH = 7.4 in the presence of different enzymes. It was found that copolyesters exhibit good mechanical properties (tensile strenght 4-17 MPa, and elongation on break up to 410%), and relatively low T_g.

Synthesis of platinum(II)-tachykinin peptides complexes for potential antitumour applications

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The most powerful and useful anticancer drugs belong to cisplatin derivatives. *Cis*-diamminedichloroplatinum(II) analogs are responsible for the inhibition of DNA transcription what leads to cell death. After binding to double DNA strand cisplatin disrupt base-pairing guanine to cytosine cross-links which lead to unwinding of the DNA. As a result cisplatin works against both types of cells, destroying cancer and normal type ones. Therefore, more selective delivery system of platinum ion to cancer cells is still needed. Based on the evidence that various neuropeptide receptors are present on different human cancer cell membranes in higher concentration, comparing to normal tissues, we proposed to use peptide ligands of such receptors as prospective selective carriers of platinum ions to cancer cells.

Tachykinin NK_1 receptors ligands could serve as such carriers. The most important member of tachykinin family, substance P (SP) is an endogenous ligand to NK_1 receptors. SP regulates biological functions also some of related to cancer, such as transmission of pain information, angiogenesis and tumor cell migration [1]. Applying antagonists of NK_1 receptor may contribute to improved drug selectivity, the same decrease toxicity.

Our aim is to synthesize platinum (II) complexes with analogues of substance P receptors' antagonists as an address part of our molecule. Such compounds could serve as carriers for platinum ions. As a part responsible for complexation we use amino acids that are able to form coordination bonds with metal ion (histidine, methionine, serine, cysteine, threonine). These amino acids are coupled to N-terminal sequence of pharmacophore peptide.

SEARCH FOR NEW TUBERCULOSTATICS. AN X-RAY STUDY

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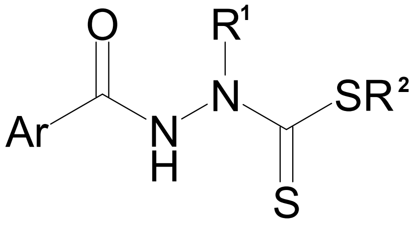
The increasing resistance of *Mycobacterium tuberculosis* to existing agents and the resulting spread of the pathogen, in both developed and developing countries, makes the search for new tuberculostatics an important issue.

The studied compounds (CM-3, CM-5) were obtained by Foks and coworkers at Department of Organic Chemistry, Medical University of Gdańsk as derivatives of aroyldithiocarbazonic acids (Scheme), showing tuberculostatic activity [1,2]. It was suggested that general planarity of the molecules could be prerequisite for activity [3] in this chemical class.



Compound	**Ar**	**R^1**	**R^2**
CM-3	3,4-Cl_2-Ph	Me	Me
CM-5	3,4-Cl_2-Ph	Me	n-Bu

The crystals suitable for X-ray experiment were obtained by slow evaporation of the solvent from the ethanol solution.

The molecules of CM-3 and CM-5 demonstrated significant twist at N—N bond due to spatial repulsion introduced by Me (R^1) group. It isin accord with our hypothesis (above), because the compounds are not active against *Mycobacterium tuberculosis.* In both crystals the molecules from infinite chains (C(4)) through intermolecular hydrogen-bonds N-H...O, common for amides. The chains run parallel to the [100] direction.

This study was supported by the Ministry of Science and Higher Education under the project No. N204 111735.

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Foldability of peptides derived from N-terminal beta-hairpins of 1E0L protein (WW domain)

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Substantial knowledge has been accumulated about the mechanism of the formation of the α-helical structure [1-3]. However, much less is known about the formation of the β-type structures which is indispensable to understand better the protein folding process. Research on the determinants of β-hairpin-structure formation also has a practical aspect, because the peptides forming spontaneously β-hairpins in solutions very often aggregate into amyloid fibrils, a phenomenon directly connected with Alzheimer's, Parkinson's, Creutzfeld –Jacob's, and many other neurodegenerative diseases.

It has been shown that some short protein fragments can fold in aqueous solution into conformations with shape similar to that they assume in the parent protein even though they lack fine details such as hydrogen-bonding network [4]. Thus, these fragments may play an important role as nucleation centers in initiating protein folding through local interactions [5,6].

The conformational studies and potentiometric titration studies of fragments of the 1E0L protein are presented. The sequences of peptides are as follow:

The peptide fragments of 1E0L protein	Peptide sequences
7-23	Ac-Glu-Trp-Thr-Glu-Tyr-Lys-Thr-Ala-Asp-Gly-Lys-Thr-Tyr-Tyr-Tyr-Asn-Asn-NH_2
11-19	Ac-Tyr-Lys-Thr-Ala-Asp-Gly-Lys-Thr-Tyr-NH_2
12-18	Ac- Lys-Thr-Ala-Asp-Gly-Lys-Thr- NH_2

The conformational studies of three peptides showed that the shape of these peptides seems to depend on the size of the charged side chains at the ends and that the bent shape of the alanine sequence is formed to enable screening of this nonpolar sequence from the solvent by sufficiently short charged side chains.

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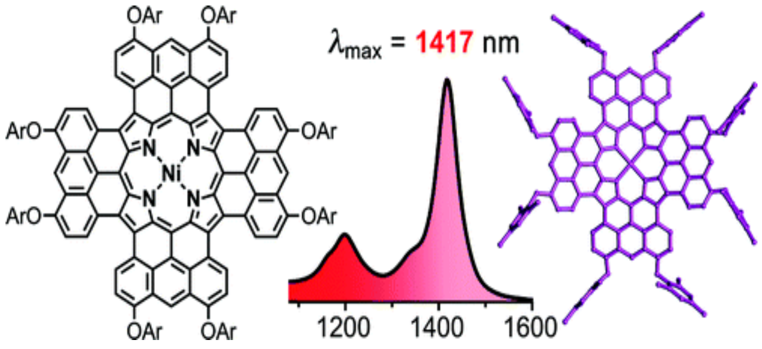
Novel fused porphyrin with aromarics moiety obtained by intermolecular oxidation - synthesis and optical properties

Marek K. Węcławski



Fused porphyrins are synthsized by oxidative ring closure Rusing $FeCl_3$or $Sc(OTf)_3$/DDQ . Elongation of porphyrin system cause significant change in optical and electronic properities which, makes them promising candidates for functional materials . These compounds are interesting for applications In the Fields of organic semiconductors, photosensitiziers, photovoltaics and nonlinear optics.

Neutral aminopeptidases - the role, function and transition state inhibitors

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Aminopeptidases are a group of enzyme that perform various functions in eukaryotic and prokaryotic cells. Their activity has been detected in many mammalian tissues and organs, in plants and in single cell organisms, what is attributed to their broad substrate specificity. They catalyze the removal of amino acids from the N-terminus of a peptide or protein [1,2]. Several aminopeptidases play a vital role in biological processes such as hormone level regulation, control of cell proliferation, inflammatory and immunological responses, antigens and neuropeptides, blood pressure control and angiogenesis. An elevated concentration of these enzymes in human organism has been indicated in such diseases as cancer, leukemia, cystic fibrosis, eyes lens cataract and other [1,3,4]. Counterpart enzymes expressed by single cell organisms are mostly responsible for proteolysis and nutrition delivery [5].

In these cases, blocking the activity of these enzymes might appear profitable in development of new generations of potent drugs. The design of new effective and selective inhibitors of the aminopeptidases is a subject of intensive studies.

Transition state analogs is an interesting class of inhibitors that mimic the highly energetic transition state of reaction catalyzed by enzyme.

Here, we present the role, function and transition state inhibitors of three main neutral metallo-aminopeptidases, as perspective targets in therapeutic intervention against devastating human diseases.

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Selective oxidation of ammonia to nitrogen and water vapour over mixed metal oxides obtained from hydrotalcites

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The ammonia slipstream after DeNOx-SCR [1], the purification of reformats for fuel-cell applications [2] and another chemical processes are plagued with ammonia-containing exhaust gas. Selective catalytic oxidation of ammonia to nitrogen and water at low temperatures (NH_3-SCO) would be suitable method for removal of ammonia from oxygen-containing flue gases. Several catalysts were proposed for the NH_3 oxidation. Among them, oxide system containing copper and/or iron were reported to be active and selective catalysts for this process [3].

Hydrotalcite-like materials with the various molar Mg/Cu/Fe ratios (2/0/1, 2/0.25/1, 2/0.5/1, 2/0.75/1, 2/1/1) were used as precursors of catalysts for the selective oxidation of NH_3. The samples were prepared by the coprecipitation method using aqueous solutions of corresponding metal nitrates and a solution of NaOH as a precipitating agent. The pH was maintained of 11.0 (8.0 for Mg-Cu hydrotalcite) by dropwise NaOH addition. The precursors were calcined at 600°C in order to obtain catalytically materials. XRD, XRF, BET, NH_3-TPD and H_2-TPRed techniques were used for characterization of calcined and non-calcined hydrotalcite-like materials. Additionally, calcined samples were tested as catalysts for the NH_3-SCO process. The measurements were performed in a flow microreactor system equipped with a QMS detector. Temperature programmed methods and catalytic tests with various space velocity were used to study reaction mechanism.

Metal mixed oxides have been found to be active and selective catalysts of ammonia oxidation, however their performance strongly depends of the composition of the samples. The highest activity and selectivity to N_2 were observed for the sample with the Mg/Cu/Fe ratio of 2/0.5/1 (Fig. 1.).

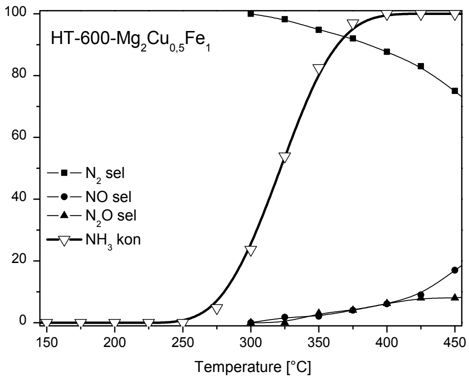

Fig. 1. Example of the results of catalytic tests for sample of calcined hydrotalcite

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Bioactive hydrogel dressings containing angiogenesis – stimulating factor

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Hydrogels are two-component systems, consisting of a spatial network of interconnected chains of hydrophilic polymers and water that fills the pores of the network. Due to numerous advantages, hydrogels are of great use, especially in medicine and pharmacy. They are used for the production of contact lenses, the encapsulation of cells, as carriers of drugs and, above all, as dressings for treating difficult to heal wounds.

Numerous studies have shown that a moist environment provided during the treatment of chronic wounds accelerates the healing process compared with traditional dressings applied. These conditions fulfill the hydrogel dressings. They protect delicate tissues from the effects of mechanical forces and the influence of the external environment, while considerably reducing the risk of infection. Also protect nerve fibers from over–stimulation, pain and trauma during using or changing the dressing. Hydrogel dressings are used in local treatment of wounds of different etiology such as pressure sores, leg ulcers, diabetic foot ulcers, fistula and cancer wounds. Currently, research on the synthesis of a new generation of hydrogel dressings containing biologically active substances, which in addition to the protective function, include funding for and stimulate natural healing processes in the wound are performed.

In this work radiation synthesis of hydrogel dressings, containing polyvinylpyrrolidone - PVP, poli(ethylene glycol) – PEG, agar and various concentrations of biologically active substance, was used. Active substance introduced into the dressings accelerates the healing of wounds. This compound acts as an activator of angiogenesis, mediates the formation of new blood vessels by stimulating endothelial cells. The prepared polymer compositions of the active substance were irradiated in an electron accelerator (Electronics ELU-6) with dose of 25 kGy (50 Hz, 4 μs, 6 MeV). Release kinetics of active substance from the hydrogel dressings by high performance liquid chromatography – HPLC and gel swelling kinetics by the gravimetric method were investigated. The equilibrium swelling degree of hydrogels and gel fraction content were determined.

The work has been financed by the National Centre for Research and Development (NCBiR), Poland, grant number N R05 0073 06/2009.

Synthetic preparation of proton conducting glasses for hydrogen fuel cell applications

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A new class of proton conducting glass membranes for hydrogen fuel cell applications is developed. These glasses are designed to yield high proton conductivities could be potentially applied as an electrolytes in H2/O2 fuel cell. The sol–gel method was used to prepare the SiO_2-P_2O_5–TiO_2 glasses with high proton conductivities and chemical stability[1]. In bulk of electrolytes are still present -OH groups able to proton conducting process. Glasses were prepared by the reaction of the tetraethoxysilane (TEOS), trimethylphosphate (TMP) and tetraethoxy titanium (TEOT) with the polymeric additive poly(ethylene oxide) PEO which possess attributes of surfactant and flocculants. To reach better wettability and mechanical properties. The chemical stability of these glasses increases significantly upon the addition of TiO_2 and PEO. The obtained glasses were less porous comparison with the pristine glassy electrolytes based only on SiO_2–P_2O_5 amorphous structure. The structural formation and higher reaction yield were confirmed by the FTIR analysis. XRD results for annealed sol–gel samples indicated mainly the presence of a vitreous (amorphous) phase, which could be correlated with SEM images where no crystal boundaries were observed[2]. TG and DTA data shows weight loss associated to an endothermic effect for the evaporation of water and liquid organic phase.

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PCR Synthesis of Double Stranded DNA Labeled with 5BrdU. A Step Towards Finding a Bromonucleoside for Clinical trials

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5-Halouracils are analogues of thymine in which the methyl group of thymine has been replaced with a halogen atom. Incorporation of 5-bromouridine (5BrdU[1]) into DNA makes it sensitive to UV and ionizing radiation, which opens up a prospective route for the clinical usage of 5-bromouridine and other halonucleosides. 5BrdU radiosensitizes genomic DNA to single and double strand breaks and also to inter cross-links , the impairments that lead to chromosomal aberrations, a decreased rate of DNA repair processes of lethal damage and eventually to cell death.

In the present work the polymerase chain reaction (PCR) protocol, which enables a long DNA fragment (resembling DNA synthesized in the cell in the presence of halonucleosides) to be completely substituted with 5BrdU, was optimized. Using HPLC coupled to enzymatic digestion, it was demonstrated that the actual amounts of native nucleosides and 5BrdU correspond very well to those calculated from the sequence of PCR products. The synthesized DNA is photosensitive to photons of 300 nm.

HPLC analysis demonstrated that the photolysis of labeled PCR products leads to a significant decrease in the 5BrdU signal and the simultaneous occurrence of a uridine peak. Agarose gel electrophoresis shows the development of double strand breaks, and polyacrylamide gel electrophoresis suggests that single and double strand breaks are formed as a result of UV irradiation.

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MODELLING OF SOLVENT EFFECT ON NITROGEN NMR CHEMICAL SHIFTS IN THIAZOLES AND THIADIAZOLES

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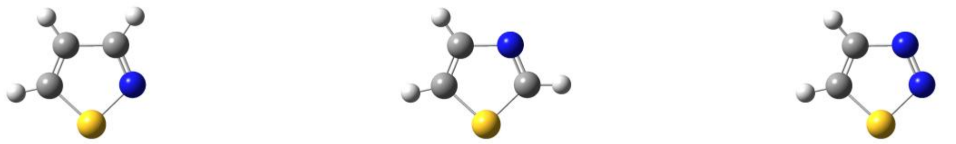
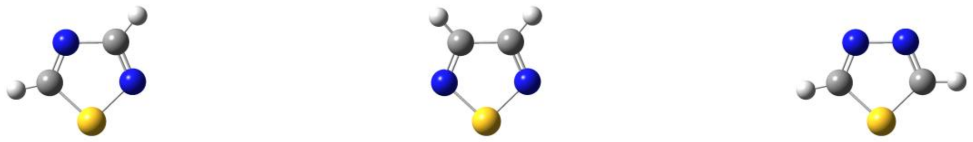
Thiazoles and thiadiazoles are five- membered heterocyclic compounds containing a sulphur atom and one (thiazoles) or two (thiadiazoles) nitrogen atom(s) (see Fig. 1). In this work the solvent effect on the ^{14}N NMR spectra for these molecules dissolved in twelve solvents were investigated. In order to model solvent effect, we used the COSMO (*Conductor-Like Screening Model*) approach. Moreover, in the case of protic solvents the ESM model (*Explicit Solvation Model*) and the hybrid model (COSMO+ESM) were employed.



1,2 - thiazole 1,3 - thiazole 1,2,3 - thiadiazole



1,2,4 - thiadiazole 1,2,5 - thiadiazole 1,3,4 - thiadiazole

Fig. 1 Thiazole and thiadiazole molecules

The theoretical values of the nitrogen magnetic shielding constants were obtained at the DFT-GIAO level. In this work, 26 different DFT potentials were examined. The theoretical data were compared with experimental ones [1].

All calculations were performed with the PQS *ab initio* package [2].

References:

1. M. Witanowski, W. Sicinska, Z. Biedrzycka, Z. Grabowski and G. A. Webb, *J. Chem. Soc. Perkin Trans.* 2, 619, (1996)
2. PQS version 3.3, Parallel Quantum Solutions, 2013 Green Acres Road, Fayetteville, Arkansas 72703

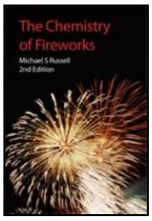
List of Participantes

Notes

Notes

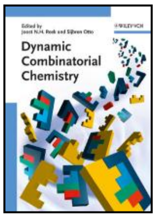
Looking forward to seeing you at the Winter Symposium!

ACADEMIC BOOKS and LITERATURE



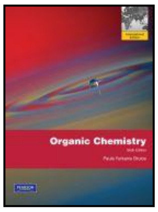
Chemistry of Fireworks
M. S. Russel
Royal Society of Chemistry, 2009

This book, a fully revised, extended and updated second edition explores the chemistry and physics behind the art of pyrotechnics.



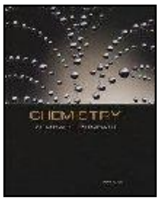
Dynamic Combinatorial Chemistry
R. N. Joost, O. Sijbren
Wiley-VCH, 2010

This long–awaited first book on this exciting new field in organic and supramolecular chemistry.



Organic Chemistry
P. Y. Bruice
Pearson Education, 2010

Bruice balances coverage of traditional topics with bioorganic chemistry to show how organic chemistry is related to biological systems and to our daily lives.



Chemistry, International Edition
S. S. Zumdahl
Cengage Learning, 2010

This book allows the reader to learn chemistry basics quickly and easily by emphasizing a thoughtful approach built on problem solving.

Green Analytical Chemistry
M. Guardia, S. Armenta
Elsevier, 2010

This reference work offers a structured compilation of theoretical concepts and experimental procedures leading to green or sustainable analytical methods.

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