International Year of
CHEMISTRY
2011

Seventh National Conference on Chemistry

International Conference on Green Technologies and Environmental Protection

26–29 May 2011, Sofia, Bulgaria

Book of Abstracts

СХБ
1901

110th Anniversary
of Union of Chemists in Bulgaria

Seventh National Conference on Chemistry
International Conference on Green Technologies and Environmental Protection
26–29 May 2011, Sofia, Bulgaria
Venue: University of Chemical Technology and Metallurgy

This event is dedicated to the110th anniversary of the Union of Chemists in Bulgaria

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Seventh National Conference on Chemistry

International Conference on Green Technologies and Environmental Protection

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110th Anniversary
of Union of Chemists in Bulgaria

Seventh National Conference on Chemistry and International Conference on Green Technologies and Environmental Protection, Book of Abstracts

Sofia 2011

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Schedule

Thursday, 26 May

09:00–18:00 Registration (**Room 210**)
Asen Zlatarov Hall
16:00–16:30 Opening session
16:30–17:15 Plenary lecture P1
17:15–18:00 Plenary lecture P2
18:00–18:30 Presentation by Medical Technics Engineering Ltd.

19:00–21:00 **Welcome reception at University of Chemical Technology and Metallurgy**

Friday, 27 May

Asen Zlatarov Hall
09:00–09:45 Plenary lecture P3
09:45–10:15 Coffee break
10:15–12:45 Session 1 Symposium 7
12:45–14:00 Lunch
14:00–16:00 Session 1 Symposium 7
16:00–16:30 Coffee break
16:30–17:30 Session 1 Symposium 7
17:30–19:30 Symposium 7 Poster presentations

Hall 424
10:15–12:45 Session 2 Symposium 8
12:45–14:00 Lunch
14:00–16:00 Session 2 Symposium 8
16:00–16:30 Coffee break
16:30–18:30 Symposium 8 Poster presentations

Hall 431
10:15–11:30 Session 3 Symposium 4
11:30–12:45 Symposium 4 Poster presentations
12:45–14:00 Lunch
14:00–15:30 Session 5 Symposium 1
15:30–17:30 Symposium 1 Poster presentations

Hall 439
10:15–11:45 Session 4 Symposium 5
11:45–12:45 Symposium 5 Poster presentations
12:45–14:00 Lunch
14:00–15:30 Session 6 Symposia 9 and 11
15:30–16:30 Symposia 9 & 11 Poster presentations
20:00–23:00 **Conference dinner**

Saturday, 28 May

Asen Zlatarov Hall
09:00–10:00 Session 7 Symposium 6
10:00–10:30 Coffee break
10:30–11:15 Session 7 Symposium 6
11:15–12:45 Symposium 6 Poster presentations
12:45–14:00 Lunch
14:00–16:00 **Round table discussion**

Hall 424
09:00–10:00 Session 8 Symposium 3
10:00–10:30 Coffee break
10:30–12:30 Symposium 3 Poster presentations

Hall 431
09:00–10:00 Session 9 Symposium 2
10:00–10:30 Coffee break
10:30–12:45 Session 9 Symposium 2
12:45–14:00 Lunch
14:00–16:00 Symposium 2 Poster presentations

Hall 439
09:00–10:00 Session 10 Symposium 10
10:00–10:30 Coffee break
10:30–10:45 Session 10 Symposium 10
10:45–12:00 Symposium 10 Poster presentations

16:30–18:30 **Excursion**

Sunday, 29 May

Asen Zlatarov Hall
10:00–10:45 Plenary lecture P4
10:45–11:15 Closing session

Programme
(as of 1 May 2011)

Thursday, 26 May 2011

Room 210

9:00	18:00	**Registration**	

Asen Zlatarov Hall

16:00	16:30	**Opening session**	
16:30	17:15	P1-Plenary lecture: From alchemy to green and sustainable chemistry	Pr. A. Lattes France
17:15	18:00	P2-Plenary lecture: Breaking bonds to order a dream still alive?	J. P. Mittal India
18:00	18:30	Bruker optics innovations in FT-IR and Raman spectroscopy	M. Huber Germany
19:00	21.00	**Welcome reception at University of Chemical Technology and Metallurgy**	

Friday, 27 May 2011

Asen Zlatarov Hall

9:00	9:45	P3-Plenary lecture: Studies on development and biodegradation of novel UV cured films	R. K. Soni India
9:45	10:15	**Coffee break**	

Session 1 Symposium 7: Chemistry and environmental protection

10:15	10:45	7-K1-Keynote lecture: Enzymes for green chemistry and environmental quality	C. Junghanns, P. Demarche, R. R. Nair, S. N. Agathos Belgium
10:45	11:15	7-K2-Keynote lecture: Dust reduction by fuel additives	R. D. Kaushik India
11:15	11:45	7-K3-Keynote lecture: Green chemistry and sugars: a fruitful mixing for new amphiphilic molecules (or surfactants)	I. Rico-Lattes France
11:45	12:15	7-K4-Keynote lecture: Development of agro-derived green epoxy resin	A. P. Gupta, V. Kumar, A. Dev India
12:15	12:45	7-K5-Keynote lecture: Organized molecular systems as reaction media for green chemistry	Pr. A. Lattes France
12:45	14:00	**Lunch**	

14:00	14:30	7-K6-Keynote lecture: A comparative study of R12, R134a, and mixture of R290 and R600a in a domestic refrigerator	A. K. Ahluwalia India
14:30	14:45	7-O1. Studies on fungal biodegradation of lactic acid based rubber sheets	S. Soam India
14:45	15:00	7-O2. Characterization of oil palm empty fruit bunch (OPEFB) as a source of biomaterial	M. A. Abdullah, M. S. Nazir, B. A.Wahjoedi Malaysia
15:00	15:15	7-O3. Enhancement of solubilization of polycyclic aromatic hydrocarbons by gemini conventional mixed surfactant systems	Kabir-ud-Din India
15:15	15:30	7-O4. Bio-energy crop sugarcane developed through tissue culture technique for sustainable environment	K. Sengar India
15:30	15:45	7-O5. Biogas recovery from waste organic materials: a comparative experimental study	V. Beschkov, I. Angelov, P. Petrova Bulgaria
15:45	16:00	7-O6. Removal of chromium from water with the help of aromatic amide prepared by pet waste	A. Gupta India
16:00	16:30	**Coffee break**	
16:30	16:45	7-O7. Investigations of radon exhalation rates, natural environmental radioactivity, and radiation exposure from Indian commercial granites	M. Mishra, R. G. Sonkawade, R. Prasad, S. A. H. Naqvi, V. K. Rastogi India
16:45	17:00	7-O8. *Jatropha curcas*: sources of bioenergy for environmental protection	R. S. Sengar, R. Chaudhary India
17:00	17:15	7-O9. The psychochemistry of pollutants: effects of chemicals on human behaviour	P. K. Sharma India
17:15	17:30	7-O10. Development of integrated bioenergy devices for improvement of quality of life of poor people	A. M. Omer United Kingdom
17:30	19:30	**Poster presentations (7-P1-P17)**	

Hall 424

Session 2 Symposium 8: Polymers (plastics, rubbers, chemical fibres, cellulose)

10:15	10:45	8-K1-Keynote lecture: A novel route of synthesis and characterization of bisaminoethyl terephthalamide from polyethylene terephthalate (PET) waste	R. K. Soni, S. Singh India
10:45	11:00	8-O1. Study on physical modification of isotactic polypropylene using LLDPE	Yo. Denev, G. Denev, B. Bogdanov, A. Popov Bulgaria
11:00	11:15	8-O2. Electrospun poly(ε-caprolactone)/ascorbyl palmitate nanofibrous materials	D. Paneva, N. Manolova, M. Argirova, I. Rashkov Bulgaria
11:15	11:30	8-O3. Recent advances in the synthesis and properties of functionalized fluoropolymers as engineering materials	G. Kostov Bulgaria
11:30	11:45	8-O4. Photozyme-stimulated pesticide photodegradation	V. Toncheva, A. Sotirov, G. Georgiev Bulgaria

11:45	12:00	8-O5. In vitro bioactivity of collagen/calcium phosphate silicate hybrids in the presence of glutaric aldehyde and chondroitin sulphate	L. Radev, V. Hristov, T. Vladkova Bulgaria
12:00	12:15	8-O6. Polymers from renewable resources: eco-friendly building materials	P. C. Thapliyal India
12:15	12:30	8-O7. The influence of high-density polyethylene added to ionic thermoplastic elastomer compounds based on maleinized ethylene-propylene terpolymer rubber	M. D. Stelescu Romania
12:30	12:45	8-O8. Predictive modelling and experimental measurement of biodegradable packaging films derived from renewable resources	A. P. Gupta, M. Sharma India
12:45	14:00	**Lunch**	
14:00	14:15	8-O9. Quaternized chitosan-based electrospun nanofibrous materials with antitumour activity	M. Ignatova, N. Manolova, R. Toshkova, E. Gardeva, L. Yossifova, M. Alexandrov, I. Rashkov Bulgaria
14:15	14:30	8-O10. Monomer participation in the equilibrium between active and dormant propagation radical states of ATRP	G. S. Georgiev Bulgaria
14:30	14:45	8-O11. Functionalization of polycaprolactone using glycidyl methacrylate in supercritical carbon dioxide for polycaprolactone-starch blend	M. Iqbal, C. Mensen, Q. Xian, A. A. Broekhuis, F. Picchioni Netherlands
14:45	15:00	8-O12. Impact of zinc oxide on the UV absorbance and mechanical properties of UV cured films	R. K. Soni, M. Teotia India
15:00	15:15	8-O13. Synthesis of *n*-(dichlorophenyl)maleimides and thermostable copolymers on the their basis	V. Konsulov, K. Gurova, Z. Grozeva, Y. Tacheva, K. Tachev Bulgaria
15:15	15:30	8-O14. Adaptive chemistry. 3. Bayesian approach to dynamer adaptive ability	G. S. Georgiev Bulgaria
15:30	15:45	8-O15. Electrospinning of poly(L-lactide) and poly(L-lactide)/PEG in the presence of some bioactive substances	A. Toncheva, M. Spasova, D. Paneva, N. Manolova, I. Rashkov Bulgaria
15:45	16:00	8-O16. Studies on development of biodegradable formulation of natural rubber latex	S. N. Mishra, R. K. Soni India
16:00	16:30	**Coffee break**	
16:30	18:30	**Poster presentations (8-P1-P19)**	

Hall 431

Session 3 Symposium 4: Analytical chemistry

10:15	10:45	4-K1-Keynote lecture: Advances in on-line separation and miniaturization in flow injection analysis	S. D. Kolev Australia
10:45	11:00	4-O1. Development of methods for trace element determination in accordance with Green chemistry principles	V. Kmetov, V. Stefanova, K. Simitchiev, D. Georgieva, N. Kovachev, A. Canals Bulgaria, Spain

11:00	11:15	4-O2. Kinetic-spectrophotometric determination of *p*-toluidine based upon its oxidation by periodate catalysed by MnII	P. Singh India
11:15	11:30	4-O3. NMR crystallography: the new application of combined theoretical and spectroscopic approach to structural description in the solid state	A. Ahmedova, V. Antonov, M. Nedyalkova, M. Mitewa Bulgaria+
11:30	12:45	**Poster presentations (4-P1-P6)**	
12:45	14:00	**Lunch**	

Session 5 Symposium 1: Physical chemistry and electrochemistry

14:00	14:15	1-O1. Synthesis and phase composition of nanosized ferrimagnetic particles in iron-containing silicate glasses	R. Harizanova, I. Gugov, C. Rüssel, D. Tatchev, V. Singh Raghuwanshi, A. Hoell Bulgaria, Germany
14:15	14:30	1-O2. Physicochemical characterization of As-Se-Ag glassy materials	V. Ilcheva, P. Petkov, T. Petkova Bulgaria
14:30	14:45	1-O3. Air gas-diffusion electrodes for operation in saline electrolytes	J. Milusheva, S. Hristov, R. Boukoureshtlieva Bulgaria
14:45	15:00	1-O4. Anodic behaviour of electrodeposited molybdenum oxides in neutral electrolyte	M. Petrova, M. Bojinov, I. Gadjov Bulgaria
15:00	15:15	1-O5. Self-assembly of protein monolayers on thin gold films electrodeposited on graphite: a potential for biosensing environmental pollutants	N. Dimcheva, E. Horozova, Tz. Godjevargova, M. Chuleva, D. Georgieva Bulgaria
15:15	15:30	1-O6. Corrosion inhibition of mild steel in acidic solution by plant extract of Lantana camara	H. C. Sharma, S. Kumar, J. Sharma, S. P. Mathur India
15:30	17:30	**Poster presentations (1-P1-P18)**	

Hall 439

Session 4 Symposium 5: Catalysis

10:15	10:45	5-K1-Keynote lecture: Recent progress in the catalytic petrochemical processes	L. A. Petrov Kingdom of Saudi Arabia
10:45	11:00	5-O1. Comparative texture study of dried and reduced Ni/silica gel catalyst precursors for vegetable oil hydrogenation	D. Nikolova, J. Krstić, L. Spasov, D. Simeonov, D. Lončarević, M. Gabrovska, D. Jovanović Bulgaria, Serbia
11:00	11:15	5-O2. Effect of silver modification on component interaction in Mg-Ni/SiO_2 precursors of vegetable oil hydrogenation catalysts	M. Gabrovska, J. Krstić, D. Nikolova, P. Tzvetkov, M. Shopska, D. Lončarević, D. Jovanović Bulgaria, Serbia
11:15	11:30	5-O3. Dry reforming of methane over PrO_x-Al_2O_3 supported Pt catalysts	I. Tankov, S. Andonova, K. Arishtirova, B. Pawelec, J. L. G. Fierro, S. Damyanova Bulgaria, Spain

11:30	11:45	5-O4. Study of nanosized ferrite materials prepared by co-precipitation method	Z. Cherkezova-Zheleva, N. Velinov, K. Koleva, B. Kunev, V. Kojuharov, I. Mitov Bulgaria
11:45	12:45	**Poster presentations (5-P1-P7)**	
12:45	14:00	**Lunch**	

Session 6 Symposium 9: Chemical technologies and Symposium 11: Chemical education

14:00	14:30	9-K1-Keynote lecture: Application of nanotechnologies and nanomaterials	G. Vissokov Bulgaria
14:30	14:45	9-O1. Plasma chemical synthesis of multicomponent nanopowders, their characteristics, and processing	J. Grabis Latvia
14:45	15:00	9-O2. Electronic polarizability, optical properties and chemical bonding of oxide glasses	V. Dimitrov, T. Komatsu Bulgaria, Japan
15:00	15:15	9-O3. Contemporary possibility for utilization of waste vulcanisates	M. Dimov, Yo. Tasheva, P. Petkov Bulgaria
15:15	15:30	9-O4. Production of mineral fertilisers in Bulgaria and their contribution to sustainable development	K. Petkov, Z. Kirova, I. Dombalov, Y. Pelovski, M. Nikolova, V. Georgiev Bulgaria
15:30	16:30	**Poster presentations (9-P1-P2 and 11-P1-P3)**	
20:00	23:00	**Conference dinner**	

Saturday, 28 May 2011

Asen Zlatarov Hall

Session 7 Symposium 6: Chemical engineering

9:00	9:30	6-K1-Keynote lecture: Theoretical problems in chemical engineering	C. B. Boyadjiev Bulgaria
9:30	10:00	6-K2-Keynote lecture: New technology for purification of flue gas from sulphur dioxide	N. Kolev, L. Ljutzkanov, D. Kolev, D. Dzhonova-Atanasova, E. Razkazova-Velkova Bulgaria
10:00	10:30	**Coffee break**	
10:30	10:45	6-O1. Numerical analysis of local field distribution in multi-phase composites	I. Saykova, I. Hinkov, R. Blajev Bulgaria
10:45	11:00	6-O2. Potentials of CFD characterization in ‘green’ production of exopolysaccharides	S. D. Vlaev, M. Martinov, R. Popov Bulgaria
11:00	11:15	6-O3. Heavy metal adsorption in fluidized bed: experimental and modelling	E. Hristova, I. Tsibranska Bulgaria
11:15	12:45	**Poster presentations (6-P1-P25)**	
12:45	14:00	**Lunch**	
14:00	16:00	**Round table discussion: Chemistry for green technologies**	

Hall 424

Session 8 Symposium 3: Inorganic chemistry

9:00	9:30	3-K1-Keynote lecture: ‘M’A(S) NMR	A. Samoson Estonia, United Kingdom
9:30	9:45	3-O1. Rare earths chemistry: scientific, technological and production activities and thin films deposition at the Department of Inorganic Chemistry of Sofia University	M. Milanova, N. Minkova, A. Terziev, M. Getsova, G. Tzvetkov, N. Petrova, M. Uzunova-Bujnova, S. Anastasova-Ivanova, J. Zaharieva, R. Kralchevska, R. Todorovska, D. Todorovsky Bulgaria
9:45	10:00	3-O2. *p*-Tert-butylcalix[4]arene tetrakis(N,N-dimethylacetamide) as a second ligand in the complexation of trivalent lanthanoids with thenoyltrifluoroacetone in solution and investigation of a solid Eu(III) complex	M. Atanassova, N. Vassilev, Z. Mizimakoski, I. Dukov Bulgaria
10:00	10:30	**Coffee break**	
10:30	12:30	**Poster presentations (3-P1-P18)**	

Hall 431

Session 9 Symposium 2: Organic chemistry

9:00	9:30	2-K1-Keynote lecture: FTIR and FT-Raman spectra of 2-amino-5-bromobenzonitrile: a DFT study	M. Sharma, M. Amalnathan, I. H. Joe, R. K. Soni, M. A. Palafox, V. K. Rastogi India
9:30	9:45	2-O1. Synthetic and *in-vitro* studies of some azetidin-2-ones as potential antifungal agents	A. K. Halve India
9:45	10:00	2-O2. Synthesis and IR spectral analysis of N-acetyl-methyl amides of some amino acids	A. Chapkanov, T. Dzimbova Bulgaria
10:00	10:30	**Coffee break**	
10:30	10:45	2-O3. Effect of coffee on growth pattern and production biology of Milk thistle (*Sillybum marianum*)	P. R. Tah, S. Saxena, A. K. Goyal Australia, India
10:45	11:00	2-O4. Prospects of eco-friendly *Jatropha curcas* plants as a medicinal use	R. Chaudhary, R. S. Sengar India
11:00	11:15	2-O5. Synthetic and antimicrobial studies of some thiosemicarbazones	A. K. Halve, J. K. Gupta India
11:15	11:30	2-O6. Synthetic and electrochemical studies on some potential bioactive sulphonamide analogues	R. Jain, A. K. Halve, R. Kathal India
11:30	11:45	2-O7. Therapeutic evaluation of 1-(2-{2-hydroxy-5-[phenyldiazenyl]phenyl}-4-oxo-1,3-thiazolidin-3-yl)-3-phenylthiourea	A. K. Halve, Amitkankoriya India
11:45	12:00	2-O8. Effect of cationic surfactant on the kinetics of interaction of $[Ni(II)\text{-}Gly\text{-}Tyr]^{+}$ with ninhydrin	M. Akram, D. Kumar, Kabir-ud-Din India
12:00	12:15	2-O9. Synthesis of 2-(aryl mercurithio)-5-phenyl 1,3,4-thiadiazoles	S. Agarwal, S. Verma India

12:15	12:30	2-O10. Synthesis and spectral studies of Ni(II) and Cu(II) complexes with a new azamacrocyclic ligand	Anupma India
12:30	12:45	2-O11. Complexes of nickel(ii) , copper(ii) with 2-carboxybenzaldehyde(thiosemicarbazone): synthesis, spectral analyses and antibacterial studies	Vandana, S. Chandra India
12:45	14:00	**Lunch**	
14:00	16:00	**Poster presentations (2-P1-P12)**	

Hall 439

Session 10 Symposium 10: Oil processing, petrochemistry and organic synthesis

9:00	9:30	10-K1-Keynote lecture: Feed properties impact on a fluid catalytic cracking unit: key issues in a diesel market	D. Stratiev, I. Shishkova Bulgaria
9:30	9:45	10-O1. Synthesis and photophysical properties of fluorescence sensing diester-terminated 1,8-naphthalimide	N. I. Georgiev, V. B. Bojinov Bulgaria
9:45	10:00	10-O2. Dependence of FCC catalyst selectivity on feed hydrotreatment	I. Shishkova, D. Stratiev, K. Stanulov Bulgaria
10:00	10:30	**Coffee break**	
10:30	10:45	10-O3. A novel PET-based fluorescent sensor for protons and transition metal ions	N. Marinova, V. Bojinov Bulgaria
10:45	12:00	**Poster presentations (10-P1-P5)**	

16:30	18:30	**Excursion: Sofia sightseeing**

Sunday, 29 May 2011

Asen Zlatarov Hall

10:00	10:45	P4-Plenary lecture: Archaeometry: the field for application of chemical analysis	I. Kuleff Bulgaria
10:45	11:15	**Closing session**	

Abstracts

P1. From alchemy to green and sustainable chemistry

Pr. A. Lattes

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Alchemy is one of the most evocative subjects in the history of science. The very word fills the mind with images both vivid and mysterious. Not only did alchemy make important contributions to the development of modern science, but it also fired the popular imagination so strongly that images of the alchemist and his art pervaded literature, theatre, painting, and music. The more celebrated goals of alchemy, such as the transmutation of base metals into gold, still tease and tantalize, even when we know quite well of their impossibility. The cloak of secrecy with which alchemists enshrouded their knowledge and activities often serves, like a whisper, better to attract our curiosity than to elude it.

Yet for all the notoriety that alchemy has gained, the topic remains complex, puzzling, and widely misunderstood.

– How is alchemy related to chemistry?
– What did alchemists really do in their laboratories?
– On what materials did they operate and to what ends?
– How were alchemists perceived by the public?
– Is alchemy magic, science of some of both?
– Do the secrecy and mystery of alchemy hide real contributions to human knowledge or merely camouflage the idle dreams (or worse, the frauds) of foolish people?

Modern chemistry started at the end of the 18th century, with Lavoisier works. Organic synthesis was highly developed for the first time during the next century and the 20th century. At the beginning of the 21st century, chemistry must respond to three major societal needs: furnish new products and improve existing ones, contribute substantially to economic activities, preserve the environment, the common part of these three sectors being the sustainable development domain.

Europe imposes on industry the constraining rules set forth in the proposed REACH regulation. To respond as effectively as possible to the concern for sustainable development, green- or sustainable chemistry appeared at the beginning of the 1990s. Green chemistry is the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances. The scope of action of this concept is broad and applies to all the sectors where chemistry plays any role. Examples are numerous in energy, transportation, medicine, textiles, agriculture, etc.

P2. Breaking bonds to order a dream still alive?

J. P. Mittal

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This lecture deals with the possibilities of conducting the bond selective chemistry with the help of tunable intense infrared lasers giving the opportunity for chemists a bond/mode selective chemistry, hence minimizing the wasteful side products. Examples from our current research will be given of using photons as a reagent.

P3. Studies on development and biodegradation of novel UV cured films

R. K. Soni

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Plastics are synthetic polyesters having a wide range of applications in household, agriculture, and architecture. Careless disposal of plastic bags chock drains, blocks the porosity of the soil, and causes problems for ground water recharge. In the present work, an attempt has been made to develop biodegradable films using UV curable resins compounded with a new resin derived from lactic acid, and other monomers. The copolymer of lactic acid, maleic anhydride, and ethylene glycol was synthesized and characterized by using spectroscopic techniques (IR, etc.) and other analytical techniques. The synthesized resins have been used for the development of UV curable formulations in different proportions. Cast films formed with these formulations were tested for their biodegradability under both soil and water. It was concluded that the addition of lactic acid based resin enhances the biodegradability of UV cured films

P4. Archaeometry: the field for application of chemical analysis

I. Kuleff

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Archaeometry as an investigation field was born more than 215 years ago, when the German chemist and pharmacist Martin-Heinrich Klaprot carried out the first chemical analysis of archaeological findings made of bronze and glass. While most of the famous chemists, physicists, and mineralogists in the 19th century took part in studies of archaeological findings, the real archaeometry practically started after the end of World War II.

In this report, some of the archaeometric investigations carried out during recent years in Bulgaria will be presented. These investigations allowed determination of the chemical composition of pottery, archaeological glasses, different metals (copper, bronze, lead, and gold), etc. Various analytical methods, such as INAA, ICP-AES, ED-XRF, and ICP-MS have been applied. In many cases, it was possible to determine the geographical and geochemical place of origin of the raw materials used by the ancient masters to produce the archaeological objects. Thus, new knowledge about the level of technology for processing of the raw materials (ore, clay, sand, plant ashes, etc.) in ancient times has been acquired. This knowledge gives new understanding of the life of ancient people that is the aim of archaeological investigations.

1-O1. Synthesis and phase composition of nanosized ferrimagnetic particles in iron-containing silicate glasses

R. Harizanova [1], I. Gugov [1], C. Rüssel [2], D. Tatchev [3], V. S. Raghuwanshi [4], A. Hoell [4]

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Oxide glasses and glass-ceramics containing 3d-metals are of both theoretical and practical interest due to their electrical and magnetic properties. In case ferrimagnetic nanocrystals are formed, depending on phase composition, size and volume fraction of the formed particles, they can be applied as parts of ferrofluids in magnetic resonance imaging systems and in biomagnetic sensors for detection of different chemical and biochemical substances.

The present investigation is aimed at synthesizing magnetic nanosized crystals in glasses from the $Na_2O/MnO/SiO_2/Fe_2O_3$ system prepared using a conventional glass-melting technique. The phase composition and microstructure of the obtained glass-ceramics were studied by X-ray diffraction and electron microscopy. Anomalous small-angle X-ray scattering was used to gain information about chemical composition and element distribution in the formed nanocrystals as well as to estimate their size distribution.

1-O2. Physicochemical characterization of As-Se-Ag glassy materials

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Multicomponent chalcogenide glasses occupy a significant place in the group of amorphous materials due to possible application in semiconductor technique and optoelectronics. The unique properties of these materials are caused by structure disorder and by prospect to modify their behaviour by variation of composition. Their potential application involves optical storage media, optical elements, electrolytes for solid-state batteries, and sensitive media in sensor systems for liquid and gas analysis. Introduction of metal atoms like silver into the chalcogenide matrix is often used to vary the glass properties in a desired direction.

We present results of physicochemical characterization of chalcogenide glasses from the As-Se-Ag system as a function of silver content.

Glasses of different concentration of silver were synthesized by a melt-quenching method. Variations of basic physicochemical characteristics were investigated and discussed. Experimentally derived parameters were compared with theoretically calculated one and elucidated in terms of the Phillips-Thorpe theory.

1-O3. Air gas-diffusion electrodes for operation in saline electrolytes

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Air gas-diffusion electrodes for reduction of oxygen from the air are commonly used as cathodes in metal-air systems and fuel cells with alkaline electrolytes.

Air gas-diffusion electrodes are also used in electrochemical cells operating with neutral electrolytes: magnesium-air cells, aluminium-air batteries, and microbial fuel cells.

The electrodes, which are subject of this study, consisted of two layers: hydrophobic layer (gas side) and the active layer (solution side). One of the most important tasks in the development of air gas-diffusion electrodes is to find proper catalysts for the electrochemical reduction of oxygen, which ensures high electrochemical characteristics and long exploitation time of the electrodes. Various non-platinum catalysts, introduced into the active carbon, were studied: pyrolyzed CoTMPP, VS50–CoTMPP–700, ACCoNi, and AC with 4% silver. Transport limitations that occur in catalyst beds were evaluated by ΔE ($E_{oxygen} - E_{air}$) *vs*. current density (i) analysis. Optimal values of the parameters of the overall structure of the electrodes and an optimal composition (weight ratio of active carbon to catalyst) of the catalyst were found.

The experiments were performed in NaCl aqueous solution at room temperature.

1-O4. Anodic behaviour of electrodeposited molybdenum oxides in neutral electrolyte

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Electrodeposition of molybdenum oxide films on Zn-coated Al substrates from an ammonia heptamolybdate electrolyte with pH 8 was carried out. Careful regulation of the deposition parameters enables to acquire mixed valence, thin and dense MoO_x coatings. These films exhibit good electric, photoelectric, and electrochemical properties and can be applied in the field of catalysis, selective solar absorption, and gas sensing. The chemical composition of the obtained molybdenum oxide films was characterized by X-ray photoelectron spectroscopy (XPS). The phase composition of oxides deposited at different current densities was assessed by X-ray diffraction. Based on the obtained results, hypotheses about electrodeposition kinetics and identity of the produced molybdenum oxides were advanced. The anodic behaviour of the oxides was characterized by voltammetry and impedance spectroscopy in a borate buffer solution (pH 7), and the anodically modified films were also characterized by XPS. Analysis of the electrochemical and surface analytical data on these films shows that the layers exhibit good electronic and ionic conductivity and have a typical composition of $MoO_x(OH)_y$.

These results made it possible to elaborate a kinetic model of the processes and to estimate the values of the kinetic and transport parameters by a quantitative comparison between model predictions and electrochemical and surface analytical data. The proposed model will enable a deterministic optimization of the coatings for a wide range of specific applications.

1-O5. Self-assembly of protein monolayers on thin gold films electrodeposited on graphite: a potential for biosensing environmental pollutants

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Thin gold layers were electrodeposited on spectroscopic graphite through brief electrolysis from acidic solutions of $HAuCl_4$. The surface topology of the gold-modified graphite was examined by atomic-force microscopy. After a suitable electrochemical pretreatment, the obtained gold-plated graphites were further used as solid matrices to immobilize two proteins – myoglobin and acetylcholine esterase enzyme *via* a self-assembly process. It was found that self-assembled monolayers failed to form on non-pretreated Au-modified graphite.

The so-produced enzyme electrodes were characterized by a variety of electrochemical methods: cyclic voltammetry, pulse techniques, and constant-potential amperometry in both the absence and presence of their enzyme substrates. Results confirmed that the immobilized proteins retained their catalytic activity to a large extent, which is electrochemically detectable. The immobilized acetylcholine esterase enzyme showed high catalytic activity upon hydrolysis of its typical substrate – acetyl-thiocholine that decreased on addition of dissolved organophosphorus insecticides. The immobilized myoglobin was proven capable to electrochemically reduce thrichloroacetic acid in neutral aqueous solutions at negative potentials.

These findings demonstrate a potential for designing electrochemical biosensors to monitor environmental pollutants like organophosphorus pesticides and polychlorinated hydrocarbons.

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1-O6. Corrosion inhibition of mild steel in acidic solution by plant extract of Lantana camara

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Corrosion inhibition performance of mild steel in acid solution containing different concentration of plant extract of Lantana camara have been investigated using mass loss and thermometric techniques. Inhibition efficiencies of these compounds have been evaluated at different acid strength. The inhibition efficiency increases with inhibitor concentration and decreases with strength of acid.

1-P1. Role of out-of-plane deformations in the photochemistry of DNA and RNA bases: comparison between 6-azauracil and uracil

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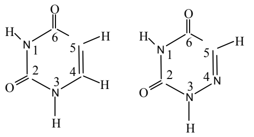
We performed a comparative theoretical study of the relaxation mechanisms of the excited states of uracil and its nitrogen analogue, 6-azauracil, at CASSCF and CASPT2 levels. There was a good agreement between the calculated vertical excitation energies and the experimental UV absorption maxima for both compounds. A low-lying conical intersection between the S_0 and S_1 states was found for uracil and 6-azauracil. The geometries of these conical intersections involve C=C twisting of uracil and C=N twisting of 6-azauracil. The conical intersection of uracil is accessible from the Franck-Condon region of the $^1\pi\pi^*$ state *via* a barrierless reaction path, while the conical intersection of 6-azauracil is not. We suggest that the deactivation of the excited electronic state of 6-azauracil takes place *via* intersystem crossing to triplet states. This conclusion is in agreement with the observed phosphorescence quantum yield of 6-azauracil, which is much higher than that of uracil. Our computational investigations indicate that the $S_1 \rightarrow T_1$ relaxation in 6-azauracil involves C=O elongation and possibly other pathways.



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Canonical structures of uracil and 6-azauracil

1-P2. Pulse electrolysis for water splitting

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Over the last decade, the problem of the greenhouse effect and the pollution has been acquiring greater importance for the progress of the mankind. That stimulated an extensive search for alternative environmentally-friendly fuel sources. Since 2003, as a viable alternative, hydrogen technologies have been included in the framework programmes of the European Commission. In October 2008, these technologies have been labelled ‘one of Europe’s leading new strategic energy technologies of the future’ with ample financial support for the next six years.

In spite of the sizable efforts in this domain, two of the main elements of hydrogen economy that still await a viable solution are storage and transport of hydrogen. A possible solution to these issues could be the increase of hydrogen generation efficiency, which would allow for its production on site when needed. In that sense, no storage or transport of fuel is required. Pulse electrolysis, widely used in the field of electrodeposition and electrochemical surface treatment, appears to be a new promising method of high efficient water splitting. Some authors prove the concept in certain conditions using ultra-short pulses.

The use of pulse electrolysis for water splitting allows for non-faradic processes to take place in the system that are supposed to increase the apparent efficiency of the process over 100%. This phenomenon is of great fundamental scientific interest, thus one of the main goals of the investigation is to elucidate the mechanism of the processes underlying it.

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1-P3. Drainage of foam films from mixed solutions of bovine serum albumin and *n*-dodecyl-β-D-maltoside

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New data on foam film drainage from mixed aqueous solutions of key components – non-ionic surfactant '*n*-dodecyl-β-D-maltoside' ($C_{12}G_2$) and globular protein 'bovine serum albumin' (BSA) are presented. The capability of proteins to control the surface charge only by pH changes of the medium makes them preferential stabilizers especially in cases when fine tuning of stability is needed without changing surfactant type or surfactant and electrolyte concentration. In modern technologies and in highly specified biotechnological products proteins are used in combination with low molecular surfactants in order to change their hydrophobicity and to reduce the cost of the detergent mixture. Hydrophobicity is of prime importance for protein surface activity. The interaction between proteins and low molecular surfactants very often changes protein hydrophobicity.

The aim of the present study was to investigate experimentally the drainage of protein/surfactant foam films formed under different experimental conditions (surfactant concentration, pH of medium, film radius) and to compare it with that of the individual components. It was found that films from mixed protein-surfactant solutions even with very small radius (< 0.05 mm) exhibit an irregular drainage, which is not in accordance with theory suggested for foam films from low molecular nonionic surfactants.

1-P4. Thermal stability of cerium selenites and solubility of the systems CeO_2-SeO_2-H_2O and Ce_2O_3-SeO_2-H_2O at 100°C

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The three-component systems CeO_2-SeO_2-H_2O and Ce_2O_3-SeO_2-H_2O were studied at 100°C. Relevant solubility isotherms were drawn by the Schreinemakers' method. One solid phase of anhydrous cerium(IV) selenite $Ce(SeO_3)_2$ was obtained in the former system in the studied concentration range. With the latter system, anhydrous cerium(III) selenite $Ce_2(SeO_3)_3$ and cerium(III)hydrogen selenite $CeH(SeO_3)_2$ were formed using 1.52–15.25 and 15.25–61.35 mass.% of SeO_2, respectively. The obtained phases in the systems were characterized by chemical analysis, X-ray diffraction, and thermogravimetric analysis.

The thermal stability and decomposition kinetics of anhydrous cerium(III) selenite under non-isothermal condition of heating were studied by means of derivatograph. It was found that the selenite began to decompose at about 600°C, the maximum decomposition rate being at 765°C, which is compatible to a strong endothermic peak on the DTA curve. At 810°C $Ce_2(SeO_3)_3$ was decomposed completely to solid phase Ce_2O_3. Several kinetic models were applied to study the kinetics and the mechanism of decomposition of anhydrous cerium(III) selenite. Among the experimental data the best linear dependence was obtained by the apparent Coats-Redfern calculation procedure using a mechanism non-invoking equation with $n = 1$. On this basis, values of the activation energy, E_A, pre-exponential factor in the Arrhenius equation, A, and changes of entropy, $\Delta S^{\neq}$, enthalpy, $\Delta H^{\neq}$, and Gibbs free energy, ΔG, were calculated for an activated complex from the reagent.

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1-P5. Comparative study on compactness of various chalcogenide glasses

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Bulk samples from the systems Ge-Se-Ga, Ge-Se-In, Ge-Te-Ga, and Ge-Te-In were synthesized *via* direct mono temperature method in closed volume. Synthesis was conducted at a constant heating rate of 8.3×10^{-2} K/s. The final step of the glass preparation procedure was the so-called 'melt-quenching' – fast soaking of the melted alloy into freezing water. The cooling rate was about 1.6×10^{2} K/s.

Several physicochemical properties as density, compactness, molar volume, number of atoms per bond and overall average bond energy of the synthesized chalcogenide glasses were determined and their composition dependences were investigated.

A comparative investigation of the composition-compactness dependence of the prepared chalcogenide glasses was conducted.

The influence of chalcogen elements Se and Te on the compactness of the bulk samples was studied. On increasing the selenium and tellurium content, the compactness rose and specifically with the element of smaller atomic radius, selenium, this increase was bigger. Additionally, the influence of metal components Ga and In, alloyed in Ge-Se and Ge-Te systems, on sample compactness was investigated. Addition of Ga and In caused the compactness to rise and the increase was bigger again with the element of smaller atomic radius, namely Ga. On adding gallium and indium the atomic bond lengths became shorter which led to a smaller average atomic radius and, thus, to an increase in compactness.

1-P6. Physicochemical properties of $(GeTe4)_{1-x}In_x$ and $(GeTe5)_{1-x}In_x$ glasses

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Bulk glasses from the $(GeTe_4)_{1-x}In_x$ and $(GeTe_5)_{1-x}In_x$ systems with $0\leq x\leq 20$ were synthesized by melt-quenching technique. Bulk samples were investigated to determine the composition dependence of some selected physical properties.

Glasses were obtained by mono temperature synthesis in evacuated ampoules using standard melt-quenching technique. Elemental raw materials of high purity Ge (99.99%), Te (99.999%), and In (99.99%) were carefully weighed. The raw materials were transferred into quartz ampoules that were then sealed under vacuum. Samples in evacuated quartz ampoules were heated to 1000 K at a heating rate of 8.33 K/s. The temperature was maintained constant at 450°C (melting temperature of Te) for one hour and at 1000 K for three hours. The melted samples were quenched in water at a rate of 1.63 K/s.

The obtained glasses had a grey-black colour with shining surface and glassy fracture.

Basic physicochemical properties of the samples, such as density, ρ, molar volume, V_m, and compactness, δ, were determined.

Samples densities were determined by the pycnometer method.

The average coordination number (Z), constraints per atom (NCO), and the radial (Na) and axial (Nb) bond strengths were calculated.

1-P7. Composite materials based on immiscible glasses and iron spinel nanoparticles

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New composite materials were produced by incorporation technique. Phase-separated TeO_2-B_2O_3-Fe_2O_3 glasses were used as matrices in which iron spinel nanoparticles were included.

The structural evolution in the glasses was studied by TEM and EPMA in advance in order to select compositions of convenient sizes and distribution of the immiscibility nano- and micro formations.

Three different types of iron containing nanosized particles (Fe_3O_4, $CoFe_2O_4$, and $CuFe_2O_4$) were obtained by co-precipitation method in alkali medium. Their shape and size were detected by HRTEM.

Scanning electron microscopy and EDAX investigations of nanocomposites thermally treated and cooled in the presence or absence of external magnetic field were performed. It was established that the magnetic field stimulates the orientation of the heterogeneous formations of the composites. The prepared products are promising magnetic materials.

1-P8. Temperature dependence of dielectric characteristics of doped bismuth titanate ceramics

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Bismuth-titanate ceramics with additives were obtained by melt quenching combined with additional heat treatment. The phase composition of selected samples in the systems Bi_2O_3-TiO_2-SiO_2, Bi_2O_3-TiO_2-Nd_2O_3, and Bi_2O_3-TiO_2-SiO_2-Nd_2O_3 was determined by X-ray diffraction (XRD) analysis. The microstructure was observed by scanning electron microscopy (SEM). Energy dispersive spectroscopy (EDS) was applied to identify the distribution of microcrystals in the matrix. The XRD data showed that the main crystalline phases in the ceramics were Bi_2O_3, Bi_2SiO_5, and $Bi_4Ti_3O_{12}$. SEM and EDS analyses illustrated a microstructure of various crystal morphology and different crystal composition. The main electrical characteristics of the glass-ceramic materials were measured as a function of temperature. All the investigated samples were dielectric materials with conductivity between 10^{-9} and 10^{-13} $(\Omega\ \mathrm{cm})^{-1}$, capacitance between 10^{-11} and 10^{-12} F, and dielectric losses tgδ between 0.02 and 0.1. A correlation was established for the synthesis method applied, the thermal history, and the microstructure and the dielectric parameters of the studied materials.

1-P9. Crystallization kinetics of chalcohalide glasses from the $GeSe_2$-Ag_2Se-AgI system

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The thermal properties of chalcohalide glasses from the $GeSe_2$-Ag_2Se-AgI system were determined by differential thermal analysis at heating rates of 10, 15, 25, and 35 K/min. Using the obtained results, sample activation energies were calculated by two independent models, developed by Kissinger and Augis & Bennett. The activation energy values varied in a wide range from 38 to 132 kJ/mol. A correlation between sample activation energy and sample composition was found and discussed.

1-P10. Dissolution kinetics of chalcogenide glasses from the $GeSe_2$-In_2Te_3-GeTe system

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Samples of the $GeSe_2$-In_2Te_3-GeTe system were synthesized and shaped in the form of parallelepiped. Then they were dissolved in 20% KOH and heated up to 298, 323, 348, and 363 K. By the obtained weight differences the dissolution rate of the samples was determined. The activation energy of the dissolution process was determined by the Arrhenius equation. An investigation of the dissolution rate behaviour depending on solvent concentration was also performed. A correlation between the determined properties and glass composition was established and discussed.

1-P11. Carbon-based composite electrodes for hybrid battery-capacitor devices

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Nanoporous activated carbons and nanosized electrochemically active $Li_4Ti_5O_{12}$ powder were synthesized and characterized. Two types of electrodes for supercapacitors were fabricated: pure carbon electrodes and composite electrodes containing activated carbon and $Li_4Ti_5O_{12}$ oxide in different proportions. Asymmetric supercapacitors, composed by activated carbon as a negative electrode, and composite activated carbon/ $Li_4Ti_5O_{12}$ oxide, as a positive electrode in organic electrolyte $LiPF_6$ – DMC/EC, were assembled and electrochemically tested. Capacitance values up to 160 F/g and current rate up to 600 mA/g were obtained with good cyclability (over 3000 cycles) of the hybrid lithium battery, a capacitor device thus being developed.

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1-P12. First stages of growth of nanoporous oxides on titanium in organic fluoride containing electrolyte

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Nanostructured oxides on titanium metal have been extensively investigated due to a variety of applications related to valuable chemical and physical properties, including mechanical and thermal resistance, low electrical conductivity, chemical inertness, permeability, and biocompatibility. Anodic oxidation has proven to be the most promising route for the growth of self-ordering nanoporous and nanotubular arrays on Ti, the best results so far being obtained in ethylene glycol (EG) based electrolytes with a fluoride and small amounts of water added.

In the present paper, emphasis is put on investigation of the initial stages of barrier film growth and dissolution on Ti in EG electrolyte with 0.015–0.20 M NH_4F using electrochemical and surface analytical techniques. Steady-state current-potential curves and electrochemical impedance spectra as depending on potential in the range –0.1/5.0 V *vs.* silver chloride reference electrode were registered. In addition, chemical composition of the oxides formed at 0.1 to 1.5 V in electrolytes containing 0.06 and 0.20 M NH_4F was estimated by X-ray photoelectron spectroscopy (XPS).

Preliminary treatment of the impedance spectra allowed estimating the barrier layer thickness and the ion migration rate coefficient as depending on applied potential and fluoride content of the electrolyte. XPS analysis revealed the presence of a non-stoichiometric oxide containing mainly Ti^{4+} and a certain amount of Ti^{3+}, with a significant degree of hydroxylation. Using a dual layer model, estimates of the total thickness of the oxide from XPS data are also presented. On the overall, the effect of added fluoride leads to a higher efficiency of film formation (higher current densities and higher film thickness at constant potential), which is in complete accordance with findings of other authors for thick nanoporous oxides. A kinetic model of the process to quantitatively interpret the electrochemical and surface analytical results is currently being elaborated.

1-P13. Quantitative studies of anodic antimony oxide formation and dissolution in oxalic acid electrolytes

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Voltage-time curves obtained during galvanostatic anodization of antimony in oxalic acid solutions exhibited different shapes in dependence of current density and/or electrolyte concentration used. Variously long induction periods appeared at current densities equal to or lower than 1×10^{-3} A/cm^3 and at electrolyte concentrations equal to or higher than 0.05 M. The shapes of the voltage-time curves and the lengths of the induction periods show a poor reproducibility. Data on charge passed during the induction periods as well as on breakdown voltage and frequency and amplitude of the voltage oscillations were acquired. An ICP method was applied for quantitative studies of anodic film dissolution in dependence of the charge passed during anodization.

1-P14. Initial stages of anodic oxidation of aluminium in neutral fluoride electrolytes

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In recent years the formation of nanoporous oxide films on aluminium and other valve metals has attracted increasing attention due to their application in various technical fields. These self-ordering films grow relatively thick and thus can be used for sensors, catalysts, solar and battery cells of enhanced photocatalytic and photovoltaic activity. Furthermore, their characteristics, e.g. pore diameter and thickness are easily controlled by the anodic oxidation parameters. A number of substances can be incorporated within their pores, which allows obtaining new functional nanomaterials that possess unique magnetic, semiconducting, and electronic properties. Recently, it has been demonstrated that neutral electrolytes containing fluoride ions are suitable for formation of self-ordered alumina templates. The presence of fluoride ions is supposed to initiate the nucleation and growth of nanoporous anodic alumina. However, little is known about the initial stages of the template formation process, involving Al dissolution, barrier film growth, and nanopore initiation.

In the present work, emphasis is put on the investigation of the initial stages of anodic oxidation of Al in 0.5 M $(NH4)_2SO_4$ + 0.05–0.1 M NH_4F using cyclic voltammetry and electrochemical impedance spectroscopy. Voltammetric results indicate a change in the mechanism of oxidation in the range of sweep rates, 20–50 mV/s, probably related to an increase of the film growth fraction of the current with sweep rate. Electrochemical impedance spectra were in qualitative agreement with data of previous authors on sulphuric acid solutions, which demonstrate an analogy among the processes of Al dissolution, barrier film formation, and nanopore initiation in acidic and neutral electrolytes. Preliminary interpretation of the impedance spectra allowed estimating the barrier layer thickness and the ion migration rate coefficient as depending on potential and fluoride content. In order to elaborate a quantitative model of the electrochemical behaviour of Al in neutral sulphate-fluoride solutions, compositional data on the oxides obtained are required.

1-P15. Characterization of amorphous phosphate coatings onto carbon steel surfaces

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This study continues an investigation of the preparation and characterization of amorphous phosphate coatings on carbon steel surfaces obtained in solutions of a new product, KAF-09 OF, developed at this university.

Gravimetric, electrochemical, and physical methods (XRD, TEM, XPS, and AFM) were used to determine the influence of pH (2÷6), temperature (20÷80°C), and agitation (0÷2000 min^{-1}) on mass/thickness, composition, and structure of the coatings as well as on the passivation characteristics of the phosphating solutions having different pH, concentration, and temperature.

It was established that the coatings were of greatest mass/thickness at pH 2.0 for all the studied temperatures. Raising the temperature from 20 up to 80°C caused a two- to threefold increase of mass/thickness for the pH (2.0–6.0) applied. pH enhancement and agitation speed led to a higher tendency to anode passivity of the steel. The physical methods applied in this study were reliable to indicate composition, type of probable compound, and structure and roughness of the obtained phosphate coatings. The phosphate films were X-ray amorphous, with indefinite habit and very well expressive relief. The coatings contained basic elements such as oxygen, phosphorus, iron, molybdenum, calcium, which are probably combined as phosphate and oxide compounds.

The new phosphating product, KAF-09 OF, has successfully been employed in several Bulgarian companies for preliminary treatment to promote paint adhesion and corrosion resistance of painted articles.

1-P16. A study on the kinetics of copper cementation onto magnetic particles

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Batch experiments on copper cementation from aqueous solutions on iron spheres have been performed. The main efforts were stressed on the establishment of optimal conditions for copper removal depending on iron particle surface, mixing intensity in the vessel, optimal pH, etc. A kinetic equation has been developed with analysis of the experimental conditions on model parameters.

1-P17. Kinetic dependences of cellulase adsorption on pulp

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The enzymatic hydrolysis of cellulose is a complex heterogeneous process including cellulase adsorption on the cellulose surface as initial step. The kinetic characteristics of the process are determined by the adsorption step regularities. The aim of this work is to study the kinetics of enzyme complex cellulose adsorption on bleached and unbleached pulp.

Cellulase NS50013 enzyme, product of Novozymes AS, having activity of 700 EGU/g was added as 2% referred to the pulp mass. The temperature was varied within 40° and the pH was kept at 5.1, while the reaction time was varied within 30 min. Enzyme adsorption was studied by measuring the residual protein content using the colorimetric Bradford micromethod.

The adsorption kinetics of cellulase on bleached and unbleached kraft pulp was described by exponential kinetic equation. This equation was found providing good interpretation of cellulase behaviour on pulp surface. Values of the activation energy and the pre-exponential factor were estimated. The activation energy was constant during the adsorption process, but the pre-exponential factor decreased thus diminishing the rate of the process. The rate of enzyme adsorption decreased on increasing lignin amount in the pulp.

1-P18. Study of the adsorption equilibrium in the cellulase-pulp system

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Cellulase enzymes are polyproteins with catalytic function to cellulose hydrolysis. The aim of this work is to study the adsorption of cellulase on the surface of bleached and unbleached kraft pulp and to establish the thermodynamic parameters of the process.

The effect of various experimental parameters, such as lignin content, initial and equilibrium enzyme concentration, contact time, and temperature was investigated. Cellulase NS50013 enzyme, product of Novozymes AS, having activity of 700 EGU/g was added as 1, 2, 3, and 4% referred to the pulp mass. The temperature was varied within 40° and the pH was kept at its optimal value, while the reaction time was varied within 20 min. Enzyme adsorption was studied by measuring the residual protein content using the colorimetric Bradford micromethod.

The model of non-homogeneous surface was applied to describe the adsorption equilibrium in the bleached and unbleached pulp-cellulase system. The lignin and the hemicellulase deteriorate the cellulase adsorbability. It was established that the values of the equilibrium constant increase with temperature increase. Thermodynamic parameters of the process, such as changes of Gibbs free energy, ΔG^0, enthalpy, ΔH^0, and entropy, ΔS^0, were calculated. The process investigated was found to proceed spontaneously although it was endothermic and the entropy change was positive. Thus, it was concluded that the entropy factor was determining.

2-K1. FTIR and FT-Raman spectra of 2-amino-5-bromobenzonitrile: a DFT study

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The idea of combining theoretical and experimental results for predicting vibrational wavenumbers is not new, and a variety of different approaches have been suggested. The calculations have been mainly carried out by using density functional methods (DFT) because they provide a very good overall description of medium-size molecules. Moreover, for the wavenumber calculations they appear more accurate than HF and MP2, and at lower computational cost.

Benzonitrile (BN) and its derivatives have important applications. From the spectroscopy point of view, a considerable number of publications about benzonitrile and its mono- and di-substituted derivatives have appeared in literature. However, neither a theoretical nor a complete experimental vibrational analysis of 2-amino-5-bromobenzonitrile molecule has been reported yet. Therefore, the present investigation was performed for the first time to study the vibrational spectra of this molecule and the full identification of all the normal modes. The density functional computations have been performed to support our frequency assignment. As DFT method the Becke's three-parameter exchange functional (B3) in combination with the correlation function of Lee, Yang and Parr (LYP) was selected. The basis set 6-31G** was used because it gives fairly good results. The most important findings of the present work are as follows:

The equilibrium geometry and the harmonic wavenumbers for 2-amino-5-bromobenzonitrile molecule have been determined, analysed and compared with experimental data for the first time by B3LYP DFT method. The results obtained appear to be the most accurate today.

The amino group produces higher change on the geometric parameters of the benzonitrile structure than the bromine atom. The weak interaction of amino hydrogen with the bromine atom reduces the pyramidalization of the amino group. The amino group also produces a slight non-planarity of the ring.

2-O1. Synthetic and *in-vitro* studies of some azetidin-2-ones as potential antifungal agents

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Human fungal infections have increased dramatically in the last two decades due to the growing number of immune compromised hosts, such as AIDS patients or those undergoing anticancer chemotherapy or transplantation. Since many drugs available in the market cause side effects or quickly develop resistance, they are ineffective against new types of fungi. Therefore, there is a general consensus that new antifungal compounds are urgently required for fungal infections. Azetidin-2-ones have acted as an important pharmacophore in the field of antimicrobials and considered as a key component of many biologically active compounds.

The present communication reports the synthesis of a new series of N-[3-chloro-2-(4-hydroxy-3-methoxy)-4-oxoazetidin-1-yl]-N'-phenylpropenamide by cyclization of 3-[2-(4-hydroxy-3-methoxybenzylidene)hydrazinyl]-3-oxo-N-phenylpropanamide through typical process. Structural identification was done by elemental analysis and spectroscopic data. The synthesized compounds were screened *in-vitro* against five fungal pathogens, i.e. *C. albicanes*, *A. fumigatus*, *C. neoformans*, *A. niger*, and *P. italecum* using disc diffusion assay. The compounds exhibited considerable inhibition against tested pathogens.

2-O2. Synthesis and IR spectral analysis of N-acetyl-methyl amides of some amino acids

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Nature has continuously provided humanity with a broad and structurally diverse arsenal of bioactive compounds that have been utilized as new drugs or as lead structures for the development of novel synthetically derived analogues. Ordinarily free amino groups of N-terminal residues in polypeptide chains are blocked in some instances by acetyl groups. The N-acetyl derivatives of α-amino acids represent interesting compounds because of their wide spectrum of action. Some of the L-proline and L-glutamine N-acetyl derivatives have importance in medicines because they are used as biologically active supplements. N-acetyl-4-hydroxy-L-proline was found to have analgesic and anti-inflammatory actions.

The purpose of the present work was to develop an efficient and simple method of synthesis of N-acetyl derivatives of α-amino acids (L-valine, L-prolinem and L-cystein) and use IR spectral analysis for their characterization. Conventional and linear-dichroic infrared (IR-LD) spectral analyses of oriented solid samples as a nematic liquid crystal suspension of amino acids L-valine (L-val) and L-proline (L-Pro) as zwiterionic structure and intermediate compounds were carried out. Based on the spectroscopic data IR characteristic bands of the zwitterions of amino acids accompanied with transition moment directions were assigned. Comparison and assignment of the solid-state IR spectra of all the systems studied were made using the statement that pure amino acids stabilize H_3N^+–, R–COO^- (L-Val) and H_2N^+–, R–COO– (L-Pro) zwitterions with characteristic IR spectral bands of –NH_3^+, –NH_2^+, and COO^- groups, O=C(amide), amide I($\nu_{C=O}$), amide II(δ_{NH}) of the HN–C=O fragment. The spectroscopic data enabled assignment the IR characteristic bands of the investigated compounds accompanied by structural prediction.

2-O3. Effect of coffee on growth pattern and production biology of Milk thistle (*Sillybum marianum*)

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Sillybum is mentioned as a thistle-like medicinal plant as early as Pliny and in Dioscorides' Materia Medica. Initially 50 seeds were sown of Milk thistle (*Sillybum marianum*) crop in four different pettry dish with soil T1, T2, T3, and T4 on same date 25th Jan 09 under lab condition and the effect of coffee in three different parts per million (ppm) solutions such as 300, 400, and 500 ppm was studied on the growth pattern and production biology at various stages of development. The main treatments comprised of three different pettry dishes on same date 25 Jan 2009 Viz. T1, T2, T3, and T4 sub-treatment included spray of parts per million (ppm) solutions of coffee such as 300 ppm (T2), 400 ppm (T3), 500 ppm (T4) and control (T1). The treatment repeated continuously seedling at regular intervals of 5 days. Control (T1) was sprayed with water. According to the above statements, the best result was shown in control (T1) according to treated plants and the result was not shown in the case of T2 where 300 ppm coffee was sprayed. In addition, the result came out that the 300 ppm solution of coffee was not sufficient for growth of Milk thistle. However, the above quantity of coffee according to 400 ppm and 500 ppm solution of coffee will be better for Milk thistle (*Sillybum marianum*).

2-O4. Prospects of eco-friendly *Jatropha curcas* plants as a medicinal use

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Jatropha curcas arise from Greek word ‘Jatros’, which means a ‘doctor’ and ‘trophe’ means ‘nutrition’. *Jatropha curcas* is a stress-resistant perennial plant growing on marginal soils. This plant is widespread throughout arid and semiarid tropical regions of the world and has been used as a traditional folk medicine in many countries. Jatropha can be planted on any kind of soil. In the recent years, Jatropha has become famous primarily for the production of biodiesel; besides this, it has several medicinal applications, too. Most parts of this plant are used for the treatment of various human and veterinary ailments. The white latex serves as a disinfectant in mouth infections in children. The latex of Jatropha contains alkaloids including Jatrophine, Jatropham and curcain with anti-cancerous properties. It is also used externally against skin diseases, piles, and sores among the domestic livestock. The leaves contain apigenin, vitexin, and isovitexin, etc., which along with other factors enable them to be used against malaria, rheumatic and muscular pains. Antibiotic activity of Jatropha has been observed against organisms including Staphylococcus aureus and Escherichia coli. There are some chemical compounds including curcin (an alkaloid) in its seeds that make it unfit for common human consumption. The roots are known to contain an antidote against snake venom. The root extract also helps to check bleeding from gums. The soap prepared from Jatropha oil is efficient against buttons. Many of these traditional medicinal properties of *Jatropha curcas* need to be investigated in depth for the marketable therapeutic products vis-à-vis the toxicological effects thereof. *Jatropha curcas* belongs to the family *Euphorbiaceae* and is thus closely related to other important cultivated plants like rubber tree and castor. The average seed weight varied from 0.53 to 0.74 g and kernel weight as proportion of raw seed weight was from 61 to 66%. The contents of crude protein, lipid, and ash of kernels from raw seeds were 27–30%, 55–62% and 3.7–5.2%, respectively. The levels of antinutrients in meal from the raw seeds were: trypsin inhibitor activity (14.6–28.7 mg trypsin inhibited/g), lectin (25.6–52.2 unit; one unit is the reverse of minimum amount of mg meal/ml assay which produced haemagglutination), saponins (1.9–2.3% as diosgenin equivalent) and phytate (8.4–10%). Phorbol esters in kernels from raw seeds were not detected in four samples and in other three samples, it ranged from 0.01 to 0.02 mg/g as phorbol-12-myristate-13-acetate equivalent. Roasting of seeds inactivated almost 100% of trypsin inhibitor activity. Although lectin activity reduced on roasting, it was still present in high amounts. Saponins, phytate and phorbol esters were not affected by roasting.

2-O5. Synthetic and antimicrobial studies of some thiosemicarbazones

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Thiosemicarbazones exhibit various biological activities and have attracted considerable pharmaceutical interest. They have been evaluated over the last 50 years as antibacterial, antifungal, antiviral, antitubercular, antitumour, and anticancer therapeutics. Studies were conducted on compounds bearing –N=N–, –N–C=S, and –CH=N– as pharmacophore. 5-[(3-Substituted phenyl)diazenyl] 2-hydroxybenzaldehyde and N-(3-substituted phenyl) thiosemicarbazones were synthesised by the condensation of 2-hydroxy 5-(substituted phenyl azo) benzaldehydes and thiosemicarbazides. Purity of compounds was ascertained by column chromatography and structures were assigned based on elemental analysis and spectral data. The synthesized compounds were screened for antimicrobial activities using disc diffusion technique against two bacterial pathogens viz. *S. aureus* and *E. coli* and two fungal pathogens, namely *C. albicanes* and *A. niger*. Chloramphenicol and fluconazole were used as standard drug, respectively. The compounds exhibited moderate activity.

2-O6. Synthetic and electrochemical studies on some potential bioactive sulphonamide analogues

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Sulphonamides are the most widely employed antibacterial agents in human and veterinary medicines for prophylactic and therapeutic purpose. Despite being the major achievements of chemotherapy, the pharmaceutically active variants of sulphonamides have their potential toxicological effects. Investigations have documented the widespread presence of trace amounts of sulpha drugs in ground water resources, plants, and animal by-products. When these synthetic chemicals degrade in the environment, they act as the agents of subtle change when environmental health perspectives are concerned. These pharmaceuticals in the environment are to be investigated keeping in view the sources, fate, effects, and risks of their presence.

This work reports the synthesis of 4-[({2-hydroxy-5-[2-(substituted methyl phenyl) diazen-1-yl]phenyl} methylidine)amino]-N-(5-methyl-1,2-oxazol-3-yl)benzene-1-sulphonamide by the condensation of 2-hydroxy-5-[2-(4-methylphenyl)diazen-1-yl]benzaldehyde with sulphamethoxazole. Formation of azomethines have been confirmed by elemental analysis and spectral data. Differential pulse polarography was employed to study the comparative redox patterns of the synthesized compounds. The polarographic and coulometric data on the redox behaviour of the compounds suggest the reductive cleavage of the azo and imine pharmacophores.

2-O7. Therapeutic evaluation of 1-(2-{2-hydroxy-5-[phenyldiazenyl]phenyl}-4-oxo-1,3-thiazolidin-3-yl)-3-phenylthiourea

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Pathogens immune response to exiting pharmaceuticals has risen dramatically in the last few decades due to the structural modifications, genomic mutations and biochemical alterations acquired by the microorganisms. Since many drugs available in the market cause side effects or face quickly developed resistance by the pathogens, there is a general consensus that new antifungal compounds are urgently required for conquering these microbes. From literature, biologically active thiosemicarbazone derivatives include 1,3,4-thiadiazoles as antibacterial and antifungal agents. A considerable number of thiosemicarbazone derivatives have been reported as intermediates for the synthesis of 5-membered compounds with potential bioactivity.

The present work explains the synthesis, fungal sensitivity evaluation of new 1-(2-{2-hydroxy-5-[phenyldiazenyl]phenyl}-4-oxo-1,3-thiazolidin-3-yl)-3-phenylthiourea (4), obtained by the reaction of 2-hydroxy-5-(phenyldiazen-1-yl)benzaldehyde (1) and N-phenylhydrazine carbothioamide (2) through 2-{2-hydroxy-5-[phenyldiazen-1-yl]benzylidene}-N-phenylhydrazine carbothioamide (3) followed by the treatment of mercaptoacetic acid with zinc chloride. All the compounds were tested for sensitivity against a panel of fungal organisms using disc diffusion method. Some of the compounds show high sensitivity. These active compounds were further examined for MIC determination against the similar panel of fungi through broth dilution assay.

2-O8. Effect of cationic surfactant on the kinetics of interaction of $[\mathrm{Ni(II)\text{-}Gly\text{-}Tyr}]^+$ with ninhydrin

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The effect of cationic surfactant of cetyltrimethylammonium bromide (CTAB) on the interaction of nickel dipeptide complex $[\mathrm{Ni(II)\text{-}Gly\text{-}Tyr}]^+$ (dipeptide = glycyl-tyrosine, Gly-Tyr) with ninhydrin have been studied spectrophotometrically at 80°C and pH 5.0. The reaction followed first- and fractional-order kinetics with respect to $[\mathrm{Ni(II)\text{-}Gly\text{-}Tyr}]^+$ and [ninhydrin], respectively. Increase in the total concentration of CTAB from 0 to 35×10^{-3} mol/dm^3 resulted in an increase in the pseudo-first-order rate constant (k_Ψ) by a factor of *ca.* 3. The results obtained in the micellar medium were treated quantitatively in terms of the kinetic pseudo-phase model of micelles (proposed by Menger and Portnoy and developed by Bunton and Romsted). CTAB micelles decrease the activation enthalpy and make the activation entropy less negative. The kinetic data have been used to calculate the micellar binding constants K_S for $[\mathrm{Ni(II)\text{-}Gly\text{-}Tyr}]^+$ and K_N for ninhydrin.

2-O9. Synthesis of 2-(aryl mercurithio)-5-phenyl 1,3,4-thiadiazoles

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Some aryl mercuric chlorides were prepared by the reaction of mercuric acetate with substituted benzene in DMF as solvent, under microwave irradiation for a period of 10–15 minutes followed by treatment with boiling aqueous solution of sodium chloride. The reaction time for the preparation of aryl mercuric chlorides microwave induced is reduced about 200 times with improved yield. Structures of the synthesized compound have been established based on chemical analysis; m.p., molecular weight, IR, and NMR.

2-O10. Synthesis and spectral studies of Ni(II) and Cu(II) complexes with a new azamacrocyclic ligand

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The complexes of Ni(II) and Cu(II) were synthesized with the new azamacrocyclic ligand. The ligand [LC: 1,5,8,12-tetraaza-2,3,4,9,10,11-hexamethyl-6(7),13(14)-di(bromopyridine)] was prepared by the reaction of 3-methyl-2,4-pentadione and 5-bromo-2,6-diamino-pyridine. All the complexes have been found to have general composition $[\mathrm{M(L)X_2}]$, where M = Ni(II) and Cu(II) and X = $\mathrm{Cl^-}$, $\mathrm{NO^-_3}$, $\frac{1}{2}\mathrm{SO_4^{2-}}$. All the complexes were characterized by the conductance measurements, magnetic susceptibility measurements, mass, IR, and electronic spectral studies. An octahedral geometry was assigned for Ni(II) complexes and tetragonal for Cu(ll) complexes. The biological actions of the ligand and complexes have been screened *in vitro* against different pathogenic fungi and several bacteria to study their comparative capacity to inhibit the growth.

2-P1. Vinylallenyl sulfoxides, sulfones, and phosphane oxides as versatile synthones in heterocyclic chemistry

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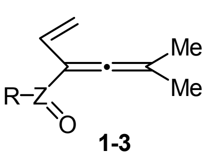
As a part of our long-standing programme on the cyclization reactions of mono- and bi-functionalized allenes we prepared and investigated 1- and 3-vinylallenyl sulfoxides **1** and **4**, sulfones **2** and **5**, and phosphane oxides **3** and **6**, possessing a vinyl group at 1- or 3-place in the allenic system [1]. We studied the reactions with different electrophilic reagents and showed [1–6] that a heterocyclization of vinylallenic system of double bonds proceeds in most cases leading to formation of thiophenes or selenophenes or/and 1,2-oxathiolium or 1,2-oxaphospholium salts depending on the type of electrophile. 2,5-Dihydrothiophene 1,1-dioxides, phthalates, *Z*-*endo*-benzofuran, and *endo*-norbornene were synthesized by regio- and stereoselective reactions of cheletropic addition of sulphur dioxide [7] to vinylallenes, Diels-Alder reaction with dimethyl but-2-ynedioate [8] and with maleic anhydride [9] in absence or presence of a Lewis acid as a catalyst, respectively.



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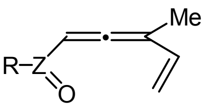

4-6

1, **3**: Z = S, R = Ph
2, **4**: Z = S=O, R = Me
3, **6**: Z = P-Ph, R = Ph

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2-P2. Antitumour activity of novel 1,10-phenanthroline and 5-amino-1,10- phenanthroline complexes

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Synthesis and impact on the tumour growth of palladium(II) complex of 5-amino-1,10-phenanthroline $Pd(5\text{-}NH_2\text{-}phen)_2(NO_3)_2$ and the protonated dimmer $(phen)_2(H^+)(BF_4^-)$ have been studied. In the experiments, a cancerous (100% lethality) myeloid subcutaneous tumour (with Graffi-tumour origin) in hamsters was used. The longest mean survival time (1.65 times longer than the controls) was achieved when the substance $Pd(5\text{-}NH_2\text{-}phen)_2(NO_3)_2$ was injected into the animals. One of the animals even survived until the 71st day, which is 2.2 times longer than controls. The compound $(phen)_2\ (H^+)(BF_4^-)$ prolonged the mean life-time of the animals 1.4 times in comparison to controls. Our experience concerning the effect of other drugs on this tumour has shown a survival time of no longer than 4–5 days after the death of the controls.

2-P3. Synthesis of new bicyclic α-aminophosphonic acids *via* Kabachnik-Fields reaction as potential biologically active compounds

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Aminophosphonic acids constitute an important class of biologically active compounds, and their synthesis has been a focus of considerable attention in synthetic organic chemistry as well as in medicinal chemistry. The interest in the structures of aminophosphonic acids is because of the biological role of their derivatives. These compounds are endowed by a constellation of biological activities including anticancer, antiviral, antibacterial, antifungal, etc. The established antiproliferative effects together with the low mammalian toxicity of these agents have conditioned tremendous interest towards designing novel antineoplastic agents [1]. Conformationally constrained amino acids are of great interest owing to their dominant role in both synthetic and medicinal chemistry. Because of that reason the methods of synthesis and characterization of new enantiopure steric amino acids is also significant [2].

In the present work, we describe the synthesis of new bicyclic aminophosphonic acids through interaction of 1-aminobicyclo[2.2.2]octane-2-carboxylic acid with different aldehydes and dimethyl-H-phosphonate by Kabachnik-Fields reaction. Their structures have been characterized by NMR (^{1}H, ^{13}C, and ^{31}P) spectra.

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2-P4. Synthesis of 2-(aryl mercurithio)-5-phenyl 1,3,4-thiadiazoles

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Some aryl mercuric chlorides were prepared by the reaction of mercuric acetate with substituted benzene in DMF as solvent, under microwave irradiation for a period of 10–15 minutes followed by treatment with boiling aqueous solution of sodium chloride. The reaction time for the preparation of aryl mercuric chlorides microwave induced is reduced about 200 times with improved yield. Structures of the synthesized compound have been established based on chemical analysis, m.p., molecular weight, IR, and NMR.

2-P5. Synthesis of novel octapeptide analogues of somatostatin with potential anticancer activity

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Peptides are a new alternative of drug therapy or drug delivery vector to increase efficacy of anticancer therapy and avoid the resulting damage. Somatostatin receptors (SSTRs) are inhibitory G-protein-coupled receptors that are expressed in normal and cancer cells. Somatostatin (SST), a cyclic tetradecapeptide hormone secreted from the hypothalamus and peripheral tissues, is the natural ligand for Somatostatin receptors (SSTRs) and act as inhibitory regulators of hormone secretion and proliferation. A large number of analogues of SST have been synthesized in order to increase its biological activity and plasma half-life. Some of them have already been used in clinical practice and others are under clinical development. Octreotide (D-Phe-c(Cys-Phe-D-Trp-Lys-Thr-Cys)-Thr-ol) and Vapreotide (D-Phe-c(Cys-Tyr-D-Trp-Lys-Val-Cys)-Trp-NH_2) are two well tolerated SSTR2/SSTR5 selective somatostatin analogues (SSA) that have been used in the treatment of cancers. The aim of the present study was the synthesis and the biological screening of new octapeptide analogues of Octreotide modified at positions 5 and 6. In order to elucidate the influence of the length of the side chain on the antitumour activity Lys at position 5 was substituted by Orn, Dab (diaminobutanoic acid) and Dap (diaminopropanoic acid). To stabilize the desired conformation necessary for biological activity of the new analogues we replaced Thr at position 6 by steric restricted amino acid Tle (t-leucine). To increase plasma half-life and biological activity of our analogues were C-terminal amides. The peptides were prepared by solid-phase peptide synthesis: Fmoc-strategy. Fmoc-Rink-Amide MBHA resin was used as a solid-phase carrier, and TBTU was used as a coupling reagent. The coupling and deprotection reactions were checked by the Kaiser test. For direct disulphide bond formation on the solid phase $Tl(CF_3CO_2)_3$ in DMF has been employed. The peptide purity was checked by electrospray ionization mass spectrometry. The biological trails are in progress.

2-P6. Modified ribavirin: a promising alternative of antiparasitic and antiviral drugs

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Recently, due to rapidly and dramatically changing climatic conditions, our environment is also varying quickly. Simultaneously, we are witnessing the emergence of several new and more resistant viruses such as HIV virus, AH1N1 influenza virus and an ever-increasing resistance of viruses to applied drugs. In this global context, synthesis of completely new or modified antiviral agents and vaccines is of a great interest for medical practice. Ribavirin, an antiviral drug discovered in 1972, is interesting and important for three reasons: (i) it exhibits antiviral and antiparasitic activity against a broad range of viruses and parasites; (ii) it is currently used clinically to treat hepatitis C virus infections, respiratory syncytial virus infections, and Lassa fever virus infections; and (iii) its mechanism of action has remained unclear for many years. Certain nucleosides have been reported to exhibit antiparasitic properties. Herein, we report a total synthesis of modified ribavirin at position 5' of ribose residue in order to be further linked to cell penetrating peptides. In our case, these peptides could play a multiple role: (i) to vectorize ribaverin into liver cells; (ii) to transport ribaverin molecule through cell membrane; (ii) to increase the biological properties of ribaverin; and (iv) to protect ribaverin molecule from proteolysis. A short orthogonal scheme was designed in order to obtain the modified ribavirin at position 5' of ribose residue by COOH or NH_2 group [3].

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2-P7. Cell penetrating peptides: a promising alternative to various molecular cargo

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Cell penetrating peptides (CPPs) are short peptides that facilitate cellular uptake of various molecular 'cargo' (from small chemical molecules to nanosize particles and large fragments of DNA). The 'cargo' is associated with the peptides either through chemical linkage *via* covalent bonds or through non-covalent interactions. The function of the CPPs is to deliver the cargo into cells, a process that commonly occurs through endocytosis with the cargo delivered to the endosomes of living mammalian cells. CPPs hold great potential as *in vitro* and *in vivo* delivery vectors for use in research and medicine. CPPs are of different sizes, amino acid sequences, and charges but all CPPs have one distinct characteristic, which is the ability to translocate the plasma membrane and facilitate the delivery of various different molecular cargoes to the cytoplasm or an organelle. There has been no real consensus as to the mechanism of CPP translocation. CPP transduction is an area of ongoing research. Cell penetrating peptides CPPs found numerous applications in medicine as drug delivery agents in the treatment of different diseases including cancer, virus inhibitors, contrast agents for cell labeling a classical example is green fluorescent protein GFP, as MRI contrast agents, quantum dots. Herein, we report the synthesis of some CPPs in order to be further used as vehicles for antiviral and antiparasitic drugs.

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2-P8. Improving the enantioselectivity of *Candida rugosa* lipase in racemic resolution of fluorine-containing chiral compounds

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The importance of chirality has constantly increased in the last decades and it is today a central issue of organic and pharmaceutical chemistry, especially in the development of new drugs and agrochemicals. Fluorine-containing chiral compounds play an important role in this field, since they often show better performance in comparison to the non-fluorinated analogues. In recent years, the number of fluorinated organic molecules, reaching commercial status as crop protection products and pharmaceutical drugs, is steadily increasing. At the market, the fluorinated compounds have been successfully offered as insecticides, fungicides, herbicides, and pharmaceuticals. Chiral 2-chloro- 3,3,3-trifluoropropionic acid (TFCPA) is an attractive building block, which might be used, similarly to 2-chloropropionic acid, as a precursor for herbicides of the aryloxyphenoxy-propionate family.

In this work, the possibility to get enantiopure TFCPA by means of enzymatic racemic resolution of its esters has been assessed. Around fifty commercial enzymes have been screened for enantioselectivity in the hydrolysis of racemic methyl and ethyl esters of TFCPA. Lipase from *Candida rugosa* and esterase from *Pseudomonas flurescens*, which are known to be highly enantioselective in the hydrolysis of various non-fluorinated as well as fluorinated substrates, have been found to be suitable catalysts for preparative resolution of the target compound. Lipase from *Candida rugosa* appeared to be less active and enantioselective than esterase from *Pseudomonas flurescens*, however, it is a cheap biocatalyst available in bulk quantities, and thus improving its enantioselectivity is of great interest. The influence of various process parameters (type of substrate, organic solvent and buffer; temperature, ionic strength, pH, stirring speed) on activity and enantioselectivity of the enzyme has been evaluated.

2-P9. Some toxicological and bioanalytical tests on the neurotoxin vipoxin

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Vipoxin is the main toxic component found in the venom of the East nose-horned viper (*Vipera ammodytes meridionalis*) populating mainly in the Bulgarian area. The neurotoxin is a heterodimeric postsynaptic ionic complex of two protein subunits: the basic and strongly toxic His48 phospholipase A_2 ($sPLA_2$) enzyme and an acidic enzymatically inactive and nontoxic component. Both the subunits have the same polypeptide length (122 amino acids) and are closely related sharing 62% sequence identity.

In the present study we report the results of acute toxicity of vipoxin on mice (i.p.) LD_{50}, the influence on hemocoagulation and its effect on red blood cells. The LD_{50} was assigned 2.6 mg/kg b.w. The anticoagulant activity was evaluated by measuring PT, TT, aPTT, and RT, which characterize the influence on intrinsic (contact activation pathway) and extrinsic (tissue activation pathway) as well as common coagulation pathway. Additionally, reptilase time was also tested. The results indicate weak anticoagulant activity of vipoxin *in vivo.* Blood cells morphology gives information about the type and shape of blood cells. We observed hypochromic cells and anisocytosis 24 h after vipoxin intoxication (1/2 LD_{50}).

The present study describes for the first time the blood toxicity of vipoxin. The data obtained present important information about the toxicity of the toxin and its evaluation *in vivo.*

2-P10. Heterogeneous protein crystallisation on some novel surface organic templates

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The crystallisation of proteins is the focus of very active research in the last few decades as good quality protein crystals are important for XR structure determination of protein molecules. In addition, the crystal state is a desirable option of delivery for some therapeutic proteins. The process of protein crystallisation is usually difficult, expensive and often prolonged in the time. The nature of the surfaces in contact with protein solutions were found to impact on the processes of heterogeneous crystallisation. The crystallisation of polar compounds is influenced by the presence of surface charges on a solid surface. Influence of surfaces properties on protein crystallisation has been reported. Most protein molecules (excluding membrane proteins) contain ionisable groups, but also more or less hydrophobic patches on their surfaces. It is challenging to establish if polar interactions govern the crystallisation process, or whether hydrophobic have the key role in governing of the process. Here, we present results for newly prepared glass surfaces covered by different hydrocarbon moieties either with or without heteroatoms. These were characterised by contact angle measurements and their surface energy was determined, with special attention to the polar and dispersive components. They were then used for crystallisation experiments with several proteins, which differ in sizes, complexity, and overall charges, using a hanging drop crystallisation method. The influence of surface chemistry on protein crystallisation is evident, but the effect of surfaces is not universal and associated with the specific protein molecule chosen and all the other crystallisation conditions, including pH, temperature, additives, and concentrations.

2-P11. Spectroscopic studies of Cr(Ill) complexes with a new azamacrocyclic ligand

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The complexes of Cr(III) were synthesized with the new azamacrocyclic ligand. The ligand was prepared by the reaction of 3-methyl-2,4-pentadione and 5-bromo-2,6-diamino-pyridine. All the complexes have been found to have general composition $[M(L)X_3]$, where M = Cr(III) and X = Cl^-, NO^-_3. All the complexes were characterized by the conductance measurements, magnetic susceptibility measurements, mass, IR, and electronic spectral studies. An octahedral geometry was assigned for Cr(Ill) complexes. The biological actions of the ligand and complexes have been screened in *vitro* against different pathogenic fungi and several bacteria to study their comparative capacity to inhibit the growth.

2-P12. Synthesis and chacterization of Co(Il) complexes with a new azamacrocyclic ligand with pendent arms

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The complexes of Co(II) were synthesized with the new azamacrocyclic ligand with pendent arms. The ligand was prepared by the reaction of 3-ethyl-2,4-pentadione and 5-bromo-2,6-diamino-pyridine. All the complexes have been found to have general composition $[M(L)X_2]$, where M = Co(II) and X = Cl^-, NO^-_3 and $[M(L)]X_2$, where M = Co(II) and X = $½SO_4^{2-}$. All the complexes were characterized by the conductance measurements, magnetic susceptibility measurements, mass, IR, and electronic spectral studies. An octahedral geometry was assigned for chloride and nitrate complexes of Co(ll) and tetrahedral geometry for sulphate complex. The biological actions of the ligand and complexes have been screened in *vitro* against different pathogenic fungi and several bacteria to study their comparative capacity to inhibit the growth.

3-K1. 'M'A(S) NMR

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Implementation of high speed magic angle has opened some unanticipated prespectives. With a technology for 80 kHz and more available, MAS rotation rate can be used as a quantitative variable as opposed to usual qualitative condition. MAS effect becomes a function MA(S). As an example, we shall demonstrate a shape measurement of large scale molecular assembly [1]. Another MAS, or rather 'M'AS variable, is the actual angle of the spinning. Spin-interactions, restored temporarily in a secular form, can be used for measuring >4Å distances even in a multispin system [2].

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3-O1. Rare earths chemistry: scientific, technological and production activities and thin films deposition at the Department of Inorganic Chemistry of Sofia University

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This report summarizes the main results of investigations on the chemistry and small scale production of rare earths (RE) performed (1985–2010) at the Department of Inorganic Chemistry, Sofia University, in the following fields: (i) chemistry of some methods for RE recovery from waste materials, (ii) RE separation and high purity oxide production, (iii) mechanochemistry of RE, (iv) RE-based materials, and (v) thin film preparation. The main results can be summarized as follows: (i) methods for RE silicates synthesis and purification have been proposed; (ii) methods for RE recovery from waste and by-products have been developed; (iii) mechanochemical effects on RE oxides are shown and mechanochemically assisted methods for synthesis of RE silicates and diketonates are proposed; (iv) the chemical nature of solid RE complexes with ethylhexyl phosphoric acid is elucidated and the possibility to be used for La separation is shown; (v) the chemistry of the processes involved in the polymerized complex method applied for preparation of RE-based compounds is clarified; (vi) spray-pyrolysis deposition of thin films using mixed-metal citrate complexes is proposed; (vii) synthesis and immobilization of RE diketonates in a number of types of matrices is realized; (viii) a highly sensitive optical oxygen sensor is developed; (ix) the influence of RE on the photocatalytic activity of TiO_2 is studied; (x) production routes for some RE compounds are developed and then carried out in practice.

3-O2. *p*-Tert-butylcalix[4]arene tetrakis(N,N-dimethylacetamide) as a second ligand in the complexation of trivalent lanthanoids with thenoyltrifluoroacetone in solution and investigation of a solid Eu(III) complex

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Solvent extraction of 14 lanthanoids by thenoyltrifluoroacetone (HTTA) in the presence of tert-butylcalix[4] arene tetrakis(N,N-dimethylacetamide) (S) from perchlorate medium at constant ionic strength $\mu = 0.1$ was investigated. The complexation properties of the extractants in the organic phase were examined and the parameters of the extraction process were determined. The stoichiometry of the extracted species was determined by a classical log–log plot analysis. The composition of the extracted species was found to be $[Ln(TTA)_3S_2]$. The values of the equilibrium constants were calculated. The presence of calix[4]arene has caused a significant synergistic effect up to 5 orders of magnitude. The values of the synergistic coefficients as well as the values of separation factors of the ions of the entire 4f-series were calculated. The studied synergistic system combines high synergistic enhancement with good selectivity.

The formation of a solid ternary complex of Eu(III), HTTA, and S was studied using elemental analysis, IR, ^{1}H NMR. The stoichiometry of the complex was found to be $Eu(TTA)_3$ S.

3-P1. Injectable bone cement based on tricalcium phosphate-tricalcium silicate-collagen composites

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The development of injectable bone cement has been recognized as a promising strategy to fulfil the complex requirements of biomaterials for micro-invasive surgeries. The purpose of this study was to develop a novel injectable bioactive bone cement based on α-tricalcium phosphate (α-TCP)-tricalcium silicate (TCS)-collagen (Coll) composites. Highly reactive TCP powder was prepared by solution combustion synthesis route using urea as a fuel. The salts $Ca(NO_3)_2.4H_2O$ and $(NH_4)_2HPO_4$ were used as reaction precursors with Ca/P ratio of 1.5. The products were composed of α- and β-tricalcium phosphate. After heating the products at 1350°C for 4 h followed by quenching in a steel plate, pure α-tricalcium phosphate was produced. TCS was prepared *via* normal solid state reaction at 1400°C using SiO_2 (5 μm) and $CaCO_3$ as precursors.

A novel injectable bone cement formulation based on α-tricalcium phosphate-tricalcium silicate-collagen was investigated. Different formulations were prepared by varying the TCS and Coll contents in order to control the injectability, mechanical properties, and bioactivity of the final composites. Added TCS increased the bioactivity of the cement. The produced silicon-hydroxyapatite-collagen nanocomposites *via* a cement type reaction have good handling properties, compressive strength, and biodegradable properties.

3-P2. Synthesis of calcium phosphates prospective as biomaterial

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Calcium phosphate-based ceramics and cements are used for bone reconstruction and remodelling because structurally they are close to the inorganic component of bone hard tissues.

Since the synthesis conditions strongly influence the composition, size, and morphology of calcium phosphates particles, we have studied the effects of reaction medium, methods and techniques of precipitation, and further precursor treatments. Biomimetic precursor precipitation was studied in three electrolyte systems – simulated body fluid – and its modifications with propylene glycol or olive oil. Fast mixing and continuous co-precipitation were applied. The effect of pH, Mg^{2+} and Zn^{2+} additives, and initial solution concentrations were followed. Xanthan gum gelling and lyophilization were used as porosifiers before precursor sintering at 1000°C. Fine powders of calcium phosphates with a Ca/P ratio of 1.4–1.6, mineral composition close to that of the hard bone tissues and separated well-shaped spherical grains in the range of 150–500 nm were prepared. Mg^{2+} and Zn^{2+} ions substitution affected both the particle shape and phase composition. Mono-phase zinc-modified β-TCP powders with $Zn^{2+}/(Zn^{2+}+Ca^{2+}) = 0.01–0.13$, containing idiomorphic crystals and mono-phase magnesium-modified β-TCP with $Mg^{2+}/(Mg^{2+}+Ca^{2+}) \geq 0.02$ and spherical grains and bi-phase mixture of magnesium-modified β-TCP and HAP, when this ratio is lower than 0.02 were obtained.

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3-P3. A study on the spontaneous crystallization of $Na_2SO_4.7H_2O$

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$Na_2SO_4.10H_2O$ tends to form supersaturated solutions possessing remarkable relative stability. Under sterile conditions, these solutions do not crystallize spontaneously at all. However, when supersaturated solutions of $Na_2SO_4.10H_2O$ are kept at low temperatures around or lower than 10°C, $Na_2SO_4.7H_2O$ crystallizes spontaneously. Well-formed transparent crystals with a size of several millimetres are formed.

The spontaneous crystallization of $Na_2SO_4.7H_2O$ has been studied in the temperature interval from 10°C till the eutectic temperature at which the system freezes. It was established that $Na_2SO_4.10H_2O$ crystallizes spontaneously only when an eutectic temperature $Na_2SO_4.7H_2O$-H_2O (–3.6°C) is reached.

The spontaneous crystallization of $Na_2SO_4.7H_2O$ is a probability process – in some cases crystallization does occur, in others – not. At temperatures around or lower than 0°C we found, however, that crystallization always occurs – implying that the supersaturated solutions have transmuted from metastable into labile ones with respect to $Na_2SO_4.7H_2O$. It was also established that on dilution of the solutions this temperature of $Na_2SO_4.7H_2O$ crystallization is lowered.

3-P4. Infrared spectroscopic study of the vibrational behaviour of matrix-isolated SO_4^{2-} guest ions included in selenate matrices ($BeSeO_4{\cdot}4H_2O$ and $K_2Be(SeO_4)_2{\cdot}2H_2O$)

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Using matrix infrared spectroscopy the vibrational behaviour of SO_4^{2-} ions included in selenate isomorphic salts was studied. The influence of different crystal parameters (size of ionic radii, volume of elementary cells, respectively repulsion effect of the matrix, positional symmetry of ion-host lengths of the Me-O bonds) on the number and location of the infrared bands corresponding to normal vibrations of matrix-isolated sulphate tetrahedra is analyzed. The degree of energetic distortion of the SO_4^{2-} guest ions was assessed from the values of $\Delta\nu_{as}$ (site-group splitting) and $\Delta\nu_{max}$ (difference in values of wavenumbers of the asymmetric and symmetric stretching and bending vibrations). The analysis of the infrared spectra shows that matrix-isolated SO_4^{2-} ions exhibit higher effective spectroscopic than crystallographic symmetry to bending vibrations, i.e. tetrahedral ions undergo a strong deformation in terms of the O-S-O bond angles compared with that of the S-O bond lengths.

3-P5. Synthesis and spectral characteristics of $[Bi_6O_6(OH)_2](NH_2C_6H_4SO_3)_4$

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A new Bi(III) complex after the reaction of basic Bi_2O_3 with aqueous solution of sulphanilic acid at pH 2.7 was synthesized. Complex composition was studied by CHNS-mode elemental analysis, FTIR, and XRD techniques. The results from elemental analysis indicate that there is a very good coincidence between calculated and experimental data. Furthermore, FTIR spectra confirmed the presence of sulphanilic acid ligands, as the vibrations of the $-NH_2$ and $-SO_3^-$ groups as well as of the *p*-disubstituted benzene moiety were clearly distinguished. Powder XRD analysis demonstrated only one phase that makes possible to determine the crystal system (tetragonal), unit cell parameters and to perform indexation.

3-P6. Synthesis and thermal decomposition of potassium peroxo-titanate to $K_2Ti_2O_5$

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In recent years, quite intensive work has been done on preparing titanates. Titanates deserve special attention due to their valuable properties. Potassium titanates, having a general formula of $K_2O{\cdot}nTiO_2$ where n=1–8 depending on composition and structure, may find application as semiconductors, photocatalyst and catalyst supports, sensors, ionic conductors. $K_2Ti_2O_5$ is known to be applicable as inorganic ion exchanger and layered host framework for synthesis of inorganic-organic nanocomposite materials. $K_{0.5}Bi_{0.5}TiO_3$ and $K_{0.5}Bi_{0.5}TiO_3{\cdot}PbZrO_3$ possess ferroelectric properties.

Potassium peroxo-titanate was synthesized by the peroxo method *via* thermal decomposition after which $K_2Ti_2O_5$ can be obtained. The isothermal conditions for decomposition of $K_2[Ti_2(O_2)_2(OH)_6]{\cdot}3H_2O$ were determined on the basis of DTA, TG, and DSC results. The DTA and TG curves were recorded in the temperature range 20–900°C at a heating rate of 10°/min. The obtained intermediate compounds were characterized by means of quantitative analysis and IR spectroscopy. The mechanism of thermal decomposition of $K_2[Ti_2(O_2)_2(OH)_6]{\cdot}3H_2O$ to $K_2Ti_2O_5$ was studied. The optimal conditions for synthesizing $K_2Ti_2O_5$ were determined (770°C for 10 h).

3-P7. Experimental determination, calculation, and prognosis of the specific molar capacity of rare earth tellurites

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The development of high technology and the search for new materials for practical purposes boosted the interest towards the tellurites of rare earth elements. Data on the thermodynamic properties are necessary to develop industrial technologies for synthesis of compounds containing rare earth elements and products on their basis with pre-selected properties. The compositions studied in this work were of the type $Ln_2(TeO_3)_3$ where Ln = Y, Er, Yb. They were synthesized in evacuated ampoules and characterized by chemical and X-ray analyses. The specific molar capacities (C_p) of the compounds studied were determined in the temperature range 399–587 K using DSC. The values measured were computer processes by the linear regression method to obtain empirical formulae for the corresponding compound and to determine a, b and c coefficients in the equation $C_p = a + bT + cT^2$. The dependencies of the experimentally measured and calculated values of C_p for the compounds studied, $Y_2(TeO_3)_3$, $Er_2(TeO_3)_3$ and $Yb_2(TeO_3)_3$, had regression coefficients R^2 close to unity which means that the calculation procedure used was precise and correct. This provided a possibility to employ regression analysis to predict C_p for temperature ranges for which there are no experimental data. On the other hand, the specific molar heat capacities calculated allowed determination of the temperature dependences of entropy (ΔS^0_T), change of enthalpy ($\Delta H^0_T - \Delta H^0_{298}$) and Gibbs function ($\Delta G^0_T$) as well as to predict thermodynamic values for non-studied temperature intervals.

3-P8. Investigation of the structure, adsorption capacity, and mechanism of hydrogen storage on modified sorbents for using the process in automobile manufacturing

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This work examines the possibility of application of new materials for hydrogen storage and subsequent use in car building (automotive industry) with a view to efficiency and safe operation.

Retention of hydrogen by samples made at the Institute of Chemical Engineering of the Bulgarian Academy of Sciences has been studied. The following samples were investigated: (i) charcoal (active carbon) AC35, (ii) AC35+Ni, (iii) AC35+Ni+La, and (iv) AC35+Ni and a mixture of approximately 50% cerium, 25% lanthanum, and small amounts of neodymium. Modifying the structure of the activated carbon AC35 is related to the possibility of storing hydrogen by combining physical adsorption on the inner surface of the material and the formation of metal hydrides of these metals to increase the total storage capacity.

Analyses have been conducted to establish the amounts of implanted metal particles in the inner structure of the activated carbon as well as the change of structure with the purpose of determining the dominant mechanism for retaining hydrogen.

3-P9. Mechanochemically induced transformations of 5f-element compounds

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This presentation summarizes results of studies on the mechanochemistry of uranium and thorium compounds and daughter products of theirs. Mechanochemically induced changes in the structure of 5f-element compounds are discussed in respect to the material of triboreactors, duration of treatment, reaction media, and chemical properties of the actinides. Differences in the mechanochemical behaviour of uranium and thorium compounds were established. The influence of mechanochemical treatment on the leaching of uranium and thorium daughter products with mild reagents is reported.

A novel mechanochemically assisted method to produce UO_{2+x}, uranium-thorium, uranium-cerium, and uranium-lanthanum mixed oxides at a relatively low temperature is described. The method is based on external sol-gel synthesis and overcomes its disadvantage (producing a mixture of U(IV) and U(VI) compounds) by utilizing the finding that mechanochemical activation in air in stainless steel vessels causes nearly full reduction of U(VI) to U(IV). The potential applicability of mechanochemical activation for dry processing of spent nuclear fuel by its mechanochemical activation with lanthanides oxides (added as isotopic and isomorphic carriers of fission products to form solid solutions) and aiming to decrease the radioactivity release during long-term storage is considered.

3-P10. Nickel-manganese cationic order, particle size distribution, and lithium intercalation in $Ni_{1/2}Mn_{3/2}O_4$ high voltage electrodes

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The development of inexpensive and safe cathode materials for the next generation of lithium-ion batteries is currently a major focus of research. Nowadays research is turned to the improvement of their electrochemical performance by elaboration of nanostructured composites and by metal substitution. The aim of this contribution is to provide data on relationships involving the Ni/Mn cationic order, particle size distribution, and lithium intercalation in $LiNi_{1/2}Mn_{3/2}O_4$.

Structural and morphological characterizations of the spinels were carried out by powder XRD, SEM, and TEM analysis, and EPR spectroscopy. The electrochemical lithium intercalation was analyzed in model lithium cells using a galvanostatic mode. XRD analysis indicated that from oxalate precursors a pure phase of $LiNi_{1/2}Mn_{3/2}O_4$ with a statistical distribution of Mn and Ni over the 16d spinel sites (s.g. Fd3m) was obtained in the temperature range of 400–600°C , whereas at 800°C Ni and Mn showed 1:3 cationic ordering (s.g. $P4_332$).

The oxalate precursor method was adapted for the preparation of $LiNi_{1/2}Mn_{3/2}O_4$ spinel with a bidisperse particle-size distribution. Acid treatment of $LiNi_{1/2}Mn_{3/2}O_4$ allows tuning of the particle size distribution. The electrochemical performance of the spinels with mono- and bidisperse distribution was compared. Using ^{7}Li NMR spectroscopy the interaction of the $LiNi_{1/2}Mn_{3/2}O_4$ electrode with the electrolyte was examined.

3-P11. Nanostructured pure and Cr-doped $NaAl(WO_4)_2$ and $Al_2(WO_4)_3$ synthesized by co-precipitation method

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Cr^{3+}-doped crystals of $Al_2(WO_4)_3$ and $Sc_2(WO_4)_3$ are suitable laser hosts having a wide emission spectrum and permitting diode pumping. Cr-doped $NaAl(WO_4)_2$ is a potential laser active medium because of high absorption, efficient pumping with the use of visible-range semiconductor diode lasers and broad laser emission. However, the production of single crystals as laser active media from these tungstates is related to a number of problems, first due to significant evaporation of WO_3 in the case of Czochralski growth or low growth velocity and anisotropy. An effective approach to overcoming the crystal growth problems is to produce transparent ceramics that replace single crystals. The technology of optical ceramics includes three main stages: fabrication of nanopowders, preparation of highly dense compacts, and sintering of the compact to non-porous ceramics. As a first step to this task nanostructured $NaAl(WO_4)_2$ and $Al_2(WO_4)_3$, pure and Cr-doped, were synthesized by co-precipitation method. The dimensions, size distribution, morphology, and reactivity of the particles were tested depending on the conditions of powder preparation as well as on Cr concentration. X-ray, DTA, TEM, and SEM analyses for powder characterization were used. Some microstructure features of the nanostructured powder compared with a single crystal of the same chemical composition were established by EPR and NMR methods. It was found that the co-precipitation method gives good possibilities to obtain pure nanosized double tungstates. Particle sizes could vary within 20–50 nm when different conditions for powder preparation were used.

3-P12. Green synthesis, optical properties, and structural characterization of starch-stabilized gold-silver nanoalloys

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Starch-stabilized gold-silver nanoalloys with varying mole fraction were prepared in aqueous solution by ultrasound-assisted co-reduction of $H[AuCl_4]$ and $AgNO_3$ by D-(+) glucose under basic conditions. The optical response (plasmon absorption) was examined by UV-Vis spectroscopy and compared to theoretical calculations using the Mie theory. Structural information was provided by means of TEM, HRTEM, XRD, and DSC. UV-Vis spectra of the aqueous dispersions showed only one absorption band, red-shifted with increasing Au/Ag ratio. The absorption maximum depended linearly on the molar fraction of gold, indicating the formation of a Au-Ag nanoalloy. An agreement between experimental data and calculations using the dipole approximation of the Mie equation was found provided that one uses a novel dielectric function for the alloy particles in the form: $\varepsilon(\chi)=\chi^{\alpha(\chi)}\varepsilon(Au)+(1-\chi)\varepsilon(Ag)$. These simulations were able to reproduce both the experimental linear dependence of the absorption maximum on particle composition and the shape of the plasmon resonance. The nanoparticles (11.8–15.4 nm in diameter) had narrow size distribution and their size gradually decreased with an increase in the Au content. HRTEM revealed that both the mono- and bimetallic alloy nanoparticles contained multiple twins as well as stacking faults. The particles have decreased crystallization ability due to incorporation of Ag atoms in the gold crystal rather than lattice mismatch. These starch-stabilized Au, Ag, and Au-Ag alloy nanoparticles of variable composition, synthesized *via* the developed green procedure, are applicable in catalysis, sensing, and biomedical fields.

3-P13. DTA and TGA study of some tetrazolium salts

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Several commercially available tetrazolium salts (TS) have been investigated by differential thermal analysis and thermogravimetric analysis: 2,3,5-triphenyl-2H-tetrazolium chloride (TTC), 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl-2H-tetrazolium bromide (MTT), 3-(1-naphthyl)-2,5-diphenyl-2H-tetrazolium chloride (TV), 2-(4-iodophenyl)-3-(4-nitrophenyl)-5-phenyl-2H-tetrazolium chloride (INT), and 3,3'-(3,3'-dimethoxy-4,4'-biphenylene)-bis(2,5-diphenyl-2H-tetrazolium) chloride (blue tetrazolium chloride, BTC). Some special features of their thermal behaviour are discussed. All the investigated TS were stable enough to be applied trouble-free in green technologies and green analytical methods, which demand heating.

3-P14. Cytotoxicity of Monensin metal(II) complexes against permanent human tumour/non-tumour cell lines and virus-transformed animal tumour cell lines

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Extensive research on the coordination ability of monovalent polyether ionophore Monensin to complex with biometal(II) ions afforded the isolation and structure characterization of series of compounds with a composition of $[M(Mon)_2(H_2O)_2]$ (M = Mg, Ca, Mn, Co, Ni, Zn). The activity of the new complexes was evaluated against Gram(+) microorganisms to show that most of these metal(II)-containing compounds are highly effective compared to the non-coordinated antibiotic. The enhanced antimicrobial effect of the polyether ionophore complexes raised a question whether the presence of metal(II) ion will influence the antitumour properties of Monensin against cell lines of various origin.

At present, we report data on the evaluation of the cytotoxic activity of divalent metal complexes of Monensin treating human tumour/non-tumour and virus-transformed animal tumour cell lines.

The study showed that generally Monensin complexes exhibit an enhanced cytotoxic activity (lower cytotoxic concentration 50, CC_{50}) than the initial compound. The cytotoxicity values of some metal(II) complexes were comparable ($[Co(Mon)_2(H_2O)_2]$, $[Mn(Mon)_2(H_2O)_2]$) or even higher ($[Mg(Mon)_2(H_2O)_2]$, $[Co(Mon)_2(H_2O)_2]$) with respect to the properties of cisplatin and 5-fluorouracil, respectively.

3-P15. Influence of pyrolysis temperature on the percentage and composition of fluids finely dispersed on carbonized rice husks

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The process of carbonization of rice husks is associated with release of fluids, some of which disperse over the surface of the solid C/SiO_2 residue. In this work, the effect of pyrolysis temperature on the quantity and composition of these fluids was studied. The determination of the amount of fluid was related to the adsorption effectiveness of the carbonized rice husk used for cleaning oil and petroleum products from water.

The rice husks were pyrolyzed at different temperatures in the range of 250 to 700°C. FTIR spectroscopy of carbonized rice husks has shown different functional groups, which are present on the surface of the solid residue. The quantity of these fluids was determined gravimetrically by extraction with acetone. Gas chromatography/mass spectrometry analysis showed that along with oxygen-containing compounds such as acids, phenols, esters, aldehydes, and ketones the extracted fluids contained sulphur and nitrogen compounds as well as alkanes, cycloalkanes, and arenes.

The results obtained show that, under pyrolysis of rice husks in the temperature range 350–480°C, dispersed oleophilic fluids occur on the surface of the resulting composites, which account for the effectiveness of the carbonized husks used as sorbent for removal of oil spills.

3-P16. Influence of pyrolysis temperature on the porosity and fluid content in composite C/SiO$_2$ materials prepared from rice husks

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In this study C/SiO$_2$ composite materials prepared by pyrolysis of rice husks within the temperature range 250–700°C were investigated. Pyrolysis temperatures were selected based on data on complex thermal analysis (TG-DTA). The morphology of the samples was determined by the Brunauer-Emmett-Teller (BET) method and mercury porosimetry. The amount of the finely dispersed fluids on the hard pyrolysis residue was determined gravimetrically by extraction with a suitable solvent.

In addition, by mercury porosimetry the pore size distribution of composite materials, before and after extraction, was determined. It was found that pyrolysis at 250°C leads to intensive emission of fluids and the formation of microporous structure of the composite. On increasing pyrolysis temperature up to 350°C the quantity of the dispersed fluids decreased and the resulting material was characterized by a maximum content of micro pores. At higher temperatures of pyrolysis, 480 and 700°C, the amount of fluids increased again.

After extraction, the content of micro pores in the samples was reduced while the content of the macro pores was increased. The composite material obtained at 480°C possessed optimum porosity and fluid content, which determined it as a suitable adsorbent for removal of oil and oil product spills.

3-P17. Thermodynamic modelling of inorganic chemical species in surface water systems. Some case studies

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The knowledge of chemical species and the processes related to the chemical behaviour of metal and nutrient pollutants in natural waters is of great importance for understanding the environmental geochemical and biochemical mechanisms as well as for planning the environmental management in order to reach the target of sustainable development.

Thermodynamic modelling was used to support monitoring studies in the assessment of the water quality of several case studies. They were fresh, estuary, marine and hyper-saline waters from the following Bulgarian regions: (i) Kamchiya and Ropotamo rivers, (ii) Asarel-Medet open pit copper mine, (iii) Lead-Zinc company area in Kardzhali town, and (iv) Burgas bay.

A combine model based on the ion-association model (PHREEQCI computer program, version 2.11, Debye-Hückel theory) and on the ion interaction model (PHREEQCI computer program, version 2.11, Pitzer theory) using a new *pit2010.dat* database was elaborated for more precise calculation of the chemical species of macro- and micro components in all the natural waters: fresh, marine or hyper-saline.

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3-P18. Determination of the contact angle between chemically modified ceramic surface and water drop

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In the present work, the contact angle between a water drop and a porous alumina support modified by octadecyltrichlorosilane was determined. Octadecyltrichlorosilane ($CH_3(CH_2)_{17}SiCl_3$) is an amphiphilic molecule consisting of a long-chain alkyl group ($C_{18}H_{37}$-) and a polar head group ($SiCl_3$-). A grafting process, leading to an increase of the hydrophobic properties, can be performed by a reaction between the OH surface groups of the alumina and a polar head group ($SiCl_3$-) present in silane compounds. The silanization process can be divided into three steps. Firstly, the alumina samples were boiled in 30% hydrogen peroxide for 30 min followed by boiling the sample in distilled water for 50 min. Secondly, the samples were dried at 90°C for 40 min and placed with 120 ml of toluene into a triple-neck flask. Then 6 ml of the octadecyltrichlorosilane and 12 ml toluene were added. Octadecyltrichlorosilane and toluene mixture were added into the flask and rinsed the neck of the flask with additional 10 ml of toluene. In the third place, modified alumina was placed in 400 ml toluene and soaked for 10 h. The samples were dried at 60°C for about 24 h. The contact angle is a quantitative measure of the wetting of a solid by a liquid. It is defined geometrically as the angle formed between a liquid drop and a solid body. In this work, the measured contact angle between a water drop and modified alumina was over 90°. On a hydrophobic surface water forms distinct droplets. As the hydrophobicity increases, the contact angle also increases. Surfaces with contact angles higher than 90° are designated as hydrophobic. This means that the initial hydrophilic alumina surface transforms into a hydrophobic one due to silanization with octadecyltrichlorosilane.

4-K1. Advances in on-line separation and miniaturization in flow injection analysis

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Two promising directions in the development of flow injection analysis (FIA) and related flow techniques are on-line separation and miniaturization. The present work gives a brief overview on new developments in these areas and reports in more detail on novel applications of polymer inclusion membranes (PIMs) for on-line separation in FIA and the potential of paper-based microfluidic devices for miniaturization of flow analysis.

Polymer inclusion membranes have shown considerable promise for selective separation of metallic and non-metallic chemical species. Their use offers an attractive alternative to conventional solvent extraction by drastically reducing the amount of solvent required and allowing simultaneous performance of the extraction and back-extraction processes. PIMs are homogenous, optically transparent and flexible materials, incorporating a base polymer, such as polyvinyl chloride (PVC) or cellulose triacetate, and a suitable extractant, such as Aliquat 336 or di(2-ethylhexyl)phosphoric acid (D2EHPA). In some cases, a plasticizer/modifier can also be added to improve the homogeneity and/or transport properties of the membrane. This work describes the first application of PIMs for on-line separation in FIA where the membrane contains PVC and D2EHPA and the analyte is Zn(II).

Paper-based microfluidic devices are a new class of analytical microsensors, which meet the increasing needs of rapid, accurate, and low-cost monitoring and analysis in environmental protection and healthcare. They utilize the capabilities of cellulose fibres in paper, which form a hydrophilic porous matrix, to transport liquids by capillary force only. By selectively hydrophobizing paper, it is possible to form liquid penetration channels and detection zones, where an analytical reaction takes place. In most cases, colour reactions are used and the intensity of the detection zone colour can be visually compared to colour charts to assess the approximate analyte concentration. More accurate colour density measurements can be conducted when the paper-based device is scanned and the colour density value determined by suitable software. The possibility of printing the cellulose reactive hydrophobization agents on paper using conventional ink-jet printers allows mass production of these devices at a very low cost. This work describes the development and application to environmental monitoring of a paper-based microfluidic device for the determination of nitrite and nitrate in aqueous samples.

4-O1. Development of methods for trace element determination in accordance with Green chemistry principles

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This lecture presents our efforts to develop environmentally benign analytical methods for trace element analysis by FAAS, ICP-OES, and ICP-MS, reducing sample consumption, utilizing non-hazardous reagents, applying better energy efficiency for sample preparation and system miniaturization.

A microwave-assisted solid phase extraction (MW-SPE) using a microcolumn packed with thioureido propyl functionalized silica gel was developed for Pd and Pt retention followed by elution with 0.5% thiourea under microwave irradiation. In this work, microwave energy was applied for the first time for acceleration of the elution process of trace levels of Pd and Pt in environmental and biological samples.

For the first time the idea of microwave-assisted cloud point extraction (MW-CPE) was studied. MW-CPE based on the use of the non-toxic surfactant Triton X-100 was found to be a green and efficient alternative to classical liquid-liquid extraction. Examples of group preconcentration of Rh, Pd and Pt using 2-mercaptobenzothiazole, N,N'-diphenylthiourea or ammonium O,O'-diethyl dithiophosphate prior to ICP-OES and ICP-MS analysis are presented. Micro sampling (350 µl) by air segmented discrete introduction (ASDI) was performed for determination of Zn in blood serum from children suffering from zinc deficiency.

Another method for separation of Zn, Cu, Cd, and Pb after MW-CPE with ammonium pyrrolidine dithiocarbamate (APDC) was developed. By the combination MW-CPE and ASDI-FAAS the detection limits were lowered by a factor of 10 (Zn, Cu, Pb) or 9 (Cd) compared to the direct FAAS analysis.

A new area of investigation with a high ‘green’ potential is the use of nanoparticles in the sample preparation process. Magnetic nanoparticles-solid phase extraction (MNPs-SPE) of trace metals (V, Co, Ni, Cu, Zn, As, Se, Pb, and Cd) as complexes with APDC was developed. Due to the very high surface-to-mass ratio, quantitative extraction was achieved using only 10 mg of MNPs and 5 min for complex formation and sorption. MNPs with retained metal complexes were easily separated from the bulk solution by a permanent magnet. The combined MNPs-SPE procedure was applied to analyze urine samples by ICP-MS. The method is a ‘greener’ alternative to classical solid phase extraction of metal chelates due to the application of a smaller amount of sorbent phase.

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4-O2. Kinetic-spectrophotometric determination of *p*-toluidine based upon its oxidation by periodate catalysed by MnII

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The Mn(II)-catalysed periodate oxidation of *p*-toluidine in acetone-water medium is first order with respect to catalyst, substrate and oxidant each. The reaction progress was followed by monitoring the increase in the absorbance of reaction intermediate. The main reaction product, characterized on the basis of melting point and spectroscopic studies, is 4-methyl-1,2-benzoquinone. The effects of pH, dielectric constant of medium, ionic strength, and free radical scavengers were studied with a view to establish the conditions for determination of *p*-toluidine in the range 74.84 to 429.04 µg/ml. The characteristics of various calibration curves, Sandell’s sensitivity, molar absorptivity, percentage recovery, effect of interference, and correlation coefficient were evaluated. An attempt was made for proposing a suitable mechanism for the reaction studied. Thermodynamic parameters are also reported.

4-O3. NMR crystallography: the new application of combined theoretical and spectroscopic approach to structural description in the solid state

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Experimental spectroscopic methods are usually used to study the molecular properties either in the solid state or in solution. The conventional way of quantum chemical treatment, however, is usually limited to isolated molecules in vacuum. Nevertheless, the development of more sophisticated quantum chemical models enables a proper description of chemical substances also taking into account the effect of the surrounding media. More recently, quantum mechanical methods using plane waves were applied to describe the structure and properties of compounds in the solid state accounting for the intermolecular interactions present in the crystal.

In this talk, representative examples of a combined experimental and theoretical study on the structure and spectroscopic (NMR) properties of a series of organic compounds is presented. NMR spectra of compounds as obtained in solution and in the solid state are the main subject of the study. Here, we demonstrate for the first time the application and the performance of a new quantum chemical package (QuantumEspresso) for calculating the structure and the nuclear magnetic shielding tensors of dithiohydantoins and 2-substituted 1,3-indandiones. Comparison between the calculated and experimental NMR data permits to estimate the role of intermolecular interactions in the solid state; to verify and even predict the crystal structure and packing for compounds where no reliable X-ray diffraction data could be obtained.

4-P1. Preparation of secondary standards for X-ray fluorescence analysis of molybdenum concentrates

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The accurate determination of element concentration in molybdenum concentrates demands rapid analytical methods for industrial application. X-ray fluorescence (XRF) analysis is an appropriate method for such purposes. For quantification, XRF utilizes different types of calibration. The most used one is the method of the calibration curve. Secondary standards with known analyte concentration are necessary to build the calibration curves. Such standards and reference materials are not available for analysis of molybdenum concentrates. Molybdenum manufacturers use homemade secondary standards and wet-chemistry methods.

In the present study, the preparation and use of secondary standards for quantitative XRF analysis of molybdenum concentrates are described.

4-P2. Selective solid-phase extraction of copper(II) using new Cu(II)-imprinted polymer microbeads

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Molecular- and ion-imprinted polymers (MIPs and IIPs) are synthetic materials with artificially generated recognition sites able to specifically rebind a target molecule/ion in preference to other closely related compounds. Their stability, ease of preparation and low cost for most of the target analytes make them attractive for numerous applications in separation sciences, catalysis, molecular sensing, and drug delivery.

Ion-imprinted polymer particles were prepared by copolymerization of 4-vinyl pyridine as functional monomer, trimethylolpropane trimethacrylate as crosslinking agent and 2,2-azo-bis-isobutyronitrile as initiator in the presence of Cu(II), a Cu(II)–4-(2-pyridylazo)resorcinol (Cu(II)-PAR) complex, and PAR only. The chemical structure and morphology of the Cu(II)-imprinted microbeads were analyzed using elemental analysis, FTIR, SEM, and BET. The separation and preconcentration characteristics of the IIPs for copper were investigated by batch procedure. The optimal pH value for quantitative preconcentration was 7, and full desorption was achieved by 2M HNO_3 for 15 min. The maximum adsorption capacity and the relative selectivity coefficients of imprinted beads for Cu(II)/Cd(II), Cu(II)/Ni(II), and Cu(II)/Pb(II) were also calculated. The imprinted with Cu(II)-PAR complex polymer had a higher capacity and selectivity than the non-imprinted polymers. It showed a metal ion affinity in the competitive conditions of Cu(II)>Cd(II)>Pb(II)>Ni(II). The results suggest that these Cu(II)-PAR IIPs can be used several times without considerable loss of adsorption capacity. The determination of Cu(II) ions in sea water showed that the interfering matrix does not influence the preconcentration and selectivity values of the Cu(II)-PAR IIPs.

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4-P3. Influence of complex-forming reagents on the determination of Hg(II) by CVAAS

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The effect of different complex-forming ligands on the determination of Hg(II) by cold vapour atomic absorption spectrometry (CVAAS) was examined. The chemical species present in the sample matrix, forming stable complexes with Hg(II) or reacting with the reducing agent, could partially or totally inhibit Hg(II) reduction and hence the efficiency of Hg vapour generation. The aim of the present study was to evaluate the influence of selected ligands (thiourea, L-cysteine, citric acid, tartaric acid, EDTA, humic acids, $S_2O_3^{2-}$) on the reduction of Hg(II) by using different concentration levels of $NaBH_4$ and also 5% m/v $SnCl_2$ solutions as reducing agents. The research was conducted by model solutions of different ligand concentrations and pH to evaluate the optimal conditions for quantitative Hg(II) reduction. The reduction of Hg(II) in alkaline medium was also investigated as an alternative method. Further, analytical procedures for direct Hg(II) determination in wine and bee honey by CVAAS minimizing observed matrix interferences will be developed.

4-P4. Synthesis, spectral properties, antibacterial activity of Salinomycin complexes with Cu(II) and Zn(II) transition metal ions

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Sodium salinomycin (SalNa) reacts with divalent metal ions (Cu, Zn) to produce novel compounds, the latter being characterized by various spectroscopic methods. The interaction of metal(II) ions with SalNa resulted in the formation of mononuclear complexes with a general formula of $[M(Sal)_2(H_2O)_2].nH_2O$ (n = 0, 2) where the divalent cation extracts Na^+ ions from the cavity of sodium salinomycin. Spectral studies demonstrated that the metal(II) complexes reported here are isostructural and possess an octahedral molecular geometry. Two salinomycin anions (salinomycinates) are bound to the metal centre in a bidentate coordination mode *via* their carboxylate function and one of the secondary hydroxyl oxygen atoms. Two water molecules occupy the axial positions in the inner coordination sphere of the metal ions to complete their octahedral environment. The antibacterial activity of the new metal(II)-containing compounds was evaluated using the double layer agar hole diffusion method. Data on the minimum inhibitory concentration have shown that the new disalinomycinates of Cu(II) and Zn(II) ions possess an enhanced antibacterial activity against Gram(+)-microorganisms compared to sodium salinomycin and salinomycinic acid (SalH), respectively.

4-P5. Conductometric study of the protolysis of tannic acid (Chinese tannin)

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Two samples of tannic acid ($C_{76}H_{52}O_{46}$, molar mass of 1701.20 g/mol) from different natural sources were studied, containing a small or a high fraction of molecular tannins compared to average amount. Their identical composition with respect to the functional groups was proved based on UV and IR spectra of the acids. The structure of Chinese tannin and the values of the stepwise protolytic constants $k_1 > k_2 \approx k_3 \approx \dots$ were determined using potentiometric and conductometric titration. The absence of gallic acid was established by HPLC. The conformational flexibility of the tannin molecule was used to measure the first stepwise protolytic constant pk_1. Using direct conductometry the concentration range of $5\times10^{-2}\div5\times10^{-4}$ mol/L of the acids was investigated by determining their degree of dissociation (α). Results of the exponential dependences on concentration and thermodynamic protolytic constants pk_1^C and pk_1^T could be unified and described by analysis of variance with corresponding values: $pk_1^C \pm \Delta pk_1^C = 4.19\pm0.02$ and $pk_1^T \pm \Delta pk_1^T = 4.22\pm0.02$, $n = 26$, $\alpha = 0.05$. It is shown that $pk_2^T \approx 6.2$.

4-P6. Application of LA-ICP-MS for characterization of archaeological glasses found in Bulgaria

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Glass has been used on Bulgarian territories since the end of the 6th century BC. During the first millennium, together with intense import from Egypt, Byzantium, and the Near East, glassmaking started in this country. The objective of the present study are fragments of two late-antique Roman window glasses and four medieval glass bracelets excavated in different parts of Bulgaria.

Laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) was used for determination of major, minor, and trace elements in the investigated glass samples. The reference materials NIST 610 and NIST 612 certified for trace elements in glass matrix were used as external calibration standards, while the amount of Si determined by scanning electron microscopy with energy dispersive X-ray spectroscopy was used as internal standard. LA-ICP-MS analytical data provided information concerning the type of glass, the fluxing agents, the typical colouring and decolouring elements and the recipe norm. LA-ICP-MS proved to be a fast and powerful method for characterization of archaeological glasses.

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5-K1. Recent progress in the catalytic petrochemical processes

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This report outlines the future technology needs in the area of petrochemistry. Catalysis science and technologies are fundamental drivers of the economic and environmental progress of the chemical and petrochemical industries. The new developments in catalysis science and catalytic technologies are among the major factors promoting the viability of industry.

Some of the most important results of the following processes will be discussed:

- selective conversion of methane and ethane to higher molecular weight products;
- Fischer-Tropsch synthesis;
- selective oxidation of alkanes and olefins;
- hydrogenation and dehydrogenation.

Possible directions of catalysis research in the field of petrochemistry will be discussed.

5-O1. Comparative texture study of dried and reduced Ni/silica gel catalyst precursors for vegetable oil hydrogenation

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The most commonly used catalyst for vegetable oil hydrogenation is the Ni/SiO_2 system. The aim of this work is to study the texture properties after drying and after reduction-activation of Ni/silica gel catalyst precursors at two different temperatures (430 and 530°C). The precursors, of identical composition (SiO_2/Ni=1.0), were synthesized by precipitation method on three types of silica gel (SIG) with different pore structure.

The texture of all dried precursors was characterized by the presence of aggregates of plate-like particles having non-rigid slit-shaped mesopores as a common feature of the Ni-containing phase formed on SIG supports. This phase may consist of $Ni(OH)_x(CO_3)_y$ and/or Ni^{2+}-O(OH)-Si entities. Isotherm shape and the type of hysteresis loop were preserved after the reduction-activation procedure at both temperatures. However, changes in the texture parameter values were observed. Reduction of the precursors at 430°C caused uniform pore size distribution and pores filling, being mono-dispersed after reduction at 530°C.

It may be concluded that the specific location of the Ni-containing entities in the dried nickel-silica gel catalyst precursors is preserved after the reduction-activation procedure at 430°C as well as at 530°C.

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5-O2. Effect of silver modification on component interaction in Mg-Ni/SiO_2 precursors of vegetable oil hydrogenation catalysts

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Metallic nickel supported on different sources of silica is one of the most widely used catalysts for partial hydrogenation of vegetable oils.

Silver-modified Mg-Ni/SiO_2 precursors of SiO_2/Ni = 1.15 and Mg/Ni = 0.1 ratios, differing in Ag content (Ag/Ni = 0.0025, 0.025 and 0.1), were prepared by precipitation-deposition on SiO_2 support derived from water glass. The effect of silver presence and silver content on the interaction between nickel species and silica support in the as-synthesized and reduced at 430°C precursors was evaluated by X-ray diffraction and infrared spectroscopy techniques. The following was found: (i) presence of Ni-phyllosilicate phase in the Mg-Ni/SiO_2 sample only and occurrence of Ag_2CO_3 and metallic Ag in the unreduced modified samples; (ii) appearance of Ni-phyllosilicates after reduction of the Ag-containing samples; (iii) enhanced reduction of the Ni^{2+} ions accompanied by formation of small metallic nickel particles, the latter being more pronounced in the sample of the highest Ag loading.

It was established that by changing the content of the silver modifier to adjust precursor composition one could control the strength of the Ni-O-Si interaction, the reducibility of the Ni^{2+} ions, and the degree of nickel metal crystallization.

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5-O3. Dry reforming of methane over PrO_x-Al_2O_3 supported Pt catalysts

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The effect of modified support material of γ-Al_2O_3 with praseodymium oxide (1–20 wt.%) on the structure and catalytic performance of Pt-PrO_x/γ-Al_2O_3 catalysts in the reaction of carbon dioxide reforming of methane was examined. Samples were characterized by ICP, XRD, DRS, TPR, and XPS methods. The existence of well dispersed PrO_x particles strongly interacting with the alumina surface via the formation of Pr-O-Al bonds was confirmed by XRD, XPS, and DRS analysis. It was found that modification of the support with praseodymium oxide results in a considerable improvement of the catalytic activity and stability of the supported Pt catalysts. The high values of CH_4 and CO_2 conversions as well as the H_2 and CO yields observed for the PrO_x containing catalysts were related to the existence of intimate contact between the particles resulting in a high dispersion and easy reduction of the metallic Pt and Pr oxide species. It was suggested that the oxygen transfer ability of the Pr oxide species has a significant effect on the resistance to coke formation on the surface of the PrO_x-promoted Pt/γ-Al_2O_3 catalysts.

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5-O4. Study of nanosized ferrite materials prepared by co-precipitation method

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Nanosized magnetic particles are currently used as magnetic fluids, catalytic agents, and ceramics for information storage, light-emitting diodes, pigments in paints and cosmetics. Much attention has been directed to the preparation of such nanocrystalline materials, because of difficult synthesis procedures and special techniques, which are typically used. Co-precipitation has proved to be a successful method, since direct co-precipitation of Fe^{2+} and Fe^{3+} in alkaline medium can be done to obtain directly the ferrite material.

The compounds magnetite (Fe_3O_4) and $Me_{0.5}Fe_{2.5}O_4$ ferrite (Me = Mg^{2+}, Co^{2+}, Cu^{2+}, etc.) are the members of solid solution series, which permits synthesis of samples of various magnetic properties and degree of electron delocalization. The aim of this investigation is to synthesize and characterize nanosized magnetite-type samples. The phase composition and dispersity of synthesized samples were studied by many physicochemical methods: XRD, Mössbauer spectroscopy, IR spectroscopy, and DSC. The obtained results show the formation of one phase of nanosized ferrite: Fe_3O_4 and $Me_{0.5}Fe_{2.5}O_4$, respectively. The catalytic behaviour of these ferrite materials in environmentally important reactions will be studied regarding their different electronic properties.

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5-P1. Oxidative steam reforming of ethanol over Co-promoted Ni/γ-Al_2O_3 catalysts

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The effect of Co addition on the structure and redox behaviour of Ni/γ-Al_2O_3 catalyst used in the reaction of oxidative steam reforming of ethanol (OSRE) was studied as a function of Co content. A series of CoNi/γ-Al_2O_3 catalysts was synthesized by incipient wetness impregnation by varying CoO content (1, 3 and 6 wt.%). The reduction of the oxide samples under hydrogen atmosphere and the redox behaviour of the catalysts under the conditions of OSRE were studied via *in-situ* temperature resolved XANES spectroscopy. The samples were also characterized by means of N_2 adsorption-desorption isotherms, XRD, XPS, and TPR. The results clearly indicated that the addition of Co into the Ni/γ-Al_2O_3 system has a considerable effect on the metal-support interaction by assisting the formation of NiO and Co_3O_4 species weakly interacting with the alumina surface. It was found that the reducibility of the bimetallic CoNi/γ-Al_2O_3 catalysts increases with increasing the Co content. The Co-promoted Ni/γ-Al_2O_3 catalysts exhibited higher resistance to oxidation compared to that of the monometallic systems in the reaction of OSRE. It was suggested that a synergistic promotion effect between the Ni and Co components reflects to a significant extent on the stability of the bimetallic CoNi/γ-Al_2O_3 catalysts in the OSRE reaction with time on stream.

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5-P2. Preparation of cobalt/carbon catalyst from ground coffee waste

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Catalysts, based on active carbon support, are traditionally prepared by depositing the precursor of the active phase on active carbon, the latter being prepared and selected in advance to feature appropriate porous texture parameters and chemical nature of the surface. However, a series of non-traditional methods have also been proposed aimed at preparing carbon-based catalysts, for example, the methods put forward by Feraz, Barnes et al., and others. The aim of this study was to prepare Co/carbon catalyst based on ground coffee waste by introducing the active component into the carbonaceous precursor followed by thermal treatment in inert medium. As a result of investigations carried out by low-temperature adsorption of nitrogen and X-ray photoelectron spectroscopy and after comparison with Co/carbon catalyst, prepared by the impregnation method on active carbon originating from ground coffee waste, the following was established:

– A high dispersion degree of the phase and uniform distribution in the bulk and on the surface of the carbon support;

– The development of a porous texture in the process of thermal treatment of the carbonaceous precursor (ground coffee waste), impregnated with cobalt nitrate, should proceed under deficiency of the oxidizing agent, but not complete absence of the latter;

– Cobalt ions display a catalyzing effect on the process of formation of the porous texture. The presence of the cobalt phase leads to development of wider mesopores in addition to the main micro-mesoporous texture of active carbons prepared from ground coffee waste under analogous conditions.

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5-P3. Cu catalyst for NO_x reduction based on a hybrid support

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The problem of protecting environment from NO_x emissions can be solved in different ways. Today, the catalytic reduction of nitrogen oxides, emitted by various sources, finds widest application. Our preliminary investigations have shown that diatomite (kieselguhr) – a natural material having high silica content – demonstrates good properties as catalyst support for various active phases in the reaction of NO_x reduction. However, one can point out its shortcomings: insufficiently developed porous texture, low specific surface area and dominating presence of Brönsted type acid sites, which, in some specific cases of active phases, do not contribute to the promotion of catalyst activity. For this reason, the purpose of the present investigation was to obtain a diatomite-based catalyst that is a combination between an optimal porous texture of the support with favourable chemical nature of the surface and comparatively low production expenses, having a highly active copper phase deposited in the form of copper-ammonia complex. Such parameters can be achieved simultaneously only by forming a hybrid support based on diatomite through formation of secondary porosity and by modifying the chemical nature of the surface. For this purpose we used active carbon as a structural modifier and introduced Lewis acid sites, involving consecutive hydrolysis of $Al(NO_3)_3.9H_2O$, with the aim to achieve a favourable ratio of Brönsted to Lewis acid sites. In conclusion, we should note that the achieved texture parameters, specific surface area, and favourable ratio of Brönsted to Lewis acid sites ensure a high degree of dispersion of the active phase and a high activity of the catalyst.

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5-P4. Surface and porous texture parameters of depleted fullerene soot in relation to its possible application as a sorbent

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A possible alternative to reduce fullerenes (F) price is to find application of the residual product remaining after fullerene extraction from fullerene soot (FS), i.e. the so-called depleted fullerene soot (DFS). Different options have been proposed to make use of DFS. The aim of this study was to determine the surface and porous texture parameters of various DFS samples, prepared from initial FS with varying fullerene content and treated by identical method of extraction, with a view to evaluate to what extent DFS's of different origin are suitable for adsorbents of organic vapours in the air. Extraction of FS and consecutive vacuum treatment (at 393 K) of all the studied samples caused an increase in BET specific surface area. The increase in the specific surface area is not proportional to the amount of F in the initial FS. Since the residual quantity of F after extraction is very close in value with all the samples, independent of initial content of F in FS, it follows that the value of the specific surface area depends on the composition and on the quantity of the accompanying compounds. Vice versa, the formation of mesoporous texture in DFS is proportional to the initial content of F in FS. The volume of the micro-pores in the initial FS and in DFS (on their basis?) is insignificant and practically it does not change after the process of extraction. The low values of the volume of the micro-pores in the case of DFS imply an insignificant physical adsorption of organic vapours on these materials. Therefore, one can conclude that the use of DFS's as sorbents of these vapours in the air can be realized only after additional modification.

5-P5. ZnO thin films prepared by two different coating methods and annealing temperatures: a comparative study of the photocatalytic degradation of Malachite Green and Reactive Black 5

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Nanocrystalline ZnO thin films were deposited onto aluminium foil substrates by two different chemical methods: (i) polymer-modified spray pyrolysis and (ii) sol-gel dip-coating of zinc acetate complex solutions. The ZnO films were characterized by means of scanning electron microscopy, X-ray photoelectron spectroscopy, and X-ray diffraction. The films prepared by procedure (i) possess a porous structure, while the films obtained by procedure (ii) have ganglia on the surface. The influence of the thermal treatment temperature (350 or 450°C) on both the film microstructure and photocatalytic activity toward Malachite Green (MG) and Reactive Black 5 (RB5) dyes was investigated. It turned out that the films prepared by both methods have a higher photocatalytic activity toward RB5 than MG due to the weaker N=N bond in comparison with the C–C bond between the central carbon atom and the N,N-dimethylaminobenzyl in MG.

5-P6. Transparent films of silver-doped TiO_2 for application as self-cleaning surfaces

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Architectural glass is becoming a popular material in modern building. This leads to higher maintenance costs and more energy required to clean the transparent surfaces. This explains why the interest in the preparation of self-cleaning surfaces has also increased in the past decade. The self-cleaning effect comes from super-hydrophilicity of the surface, photocatalytic action or a combination of both. Titania is one of the most attractive materials for such applications. Along with unique optical properties and chemical stability, it offers a high photocatalytic activity and becomes super-hydrophilic when exposed to UV illumination.

We have used a simple dip-coating technique to deposit uniform and transparent films of TiO_2 on glass slides. The starting materials for the sol were titanium butoxide, citric acid and ethanol (1:1:45 molar ratio). 5 mol.% of $AgNO_3$ in respect of the butoxide were added to achieve Ag doping. The films were coated on standard glass slides at a rate of 0.9 mm/s, dried, and calcined at 500°C. Films with 1, 3, 5, and 7 coatings were prepared. The samples were characterized by UV/Vis spectroscopy, SEM, and XRD. The photocatalytic properties were evaluated by measuring the rate of photooxidation of Methylene Blue dye inside a custom-built batch reactor under UV and visible light illumination. The hydrophilicity was measured by the sessile drop method. The contact angle of a water droplet was measured before and after different periods of UV illumination. The results show that the as-prepared transparent films were highly uniform with a thickness of up to 1 μm and TiO_2 was mainly in the form of anatase with crystallite size of 12 nm (calculated from Scherrer equation). Inspection of the XRD spectra revealed that Ag doping catalyze the transition to rutile yielding 22±1 wt.% (with less than 3 wt.% detected in the undoped samples). Both doped and undoped films showed a high photocatalytic activity (up to 10% conversion in 100 ml of 1 ppm of Methylene Blue dye solution in 30 min) and express superhydrophilicity under illumination (26° water contact angle decreased to full wetting under illumination). Silver doping did not change the activity of titania under UV illumination, but promoted such under visible light. The as-prepared transparent films are good candidates for application as coatings for self-cleaning surfaces.

5-P7. Physicochemical study of materials based on biogenic iron oxides

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Biogenic materials, which are product of the metabolic activity of bacteria from the *Sphaerotilus-Leptothrix* group, were investigated. The bacteria were isolated and cultivated under laboratory conditions and their ability to produce sufficient amount of iron oxide based materials was tested.

The phase composition and the physicochemical properties of the obtained biogenic products were studied by a series of physicochemical methods: X-ray diffraction, Mössbauer spectroscopy, IR spectroscopy, DTA, and SEM. All the characterization methods show the presence of both amorphous and crystal phase. Acquired data reveal that the crystal phase contains ultra-dispersed and highly dispersed particles of nanosized α-FeOOH as a main phase. The possibility to apply the obtained material in catalytic reactions important for environmental protection was considered.

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6-K1. Theoretical problems in chemical engineering

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Chemical engineering uses various methodologies to solve practical problems of chemical applications in industry. A comprehensive theoretical analysis of various aspects and applications of chemical engineering are considered in this presentation.

The simple and more complicated models of transport phenomena, taking into account some non-linear heat and mass transfer processes, are discussed. Different theories appearing in the development of chemical engineering in time are compared and analysed. The effects of hydrodynamic stability related to the transfer processes performance are also taken into account.

Mathematical methods and their applications are also considered. Two different aspects are considered: the quantitative study of transport phenomena and unit operations and complex modelling and optimization of integrated plants and technological flow sheets.

6-K2. New technology for purification of flue gas from sulphur dioxide

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This work presents a new type of installation for removal of SO_2 that is further used for producing gypsum. It ensures conditions under which a flue gas with high concentration of SO_2 is absorbed by slurry of low pH avoiding in this way formation of low soluble $CaSO_3$ on the particles of $CaCO_3$, which leads to elimination of the diffusion resistance in the solid phase. Under these conditions, the increase of pH does not reduce significantly the driving force of absorption. On the contrary, at low concentrations of SO_2 in the gas phase the pH of the slurry is high which leads practically to zero value of the equilibrium concentration in the gas phase increasing very strongly the driving force of the process and its rate in comparison with existing installations. Because of low concentrations of SO_2 under these conditions, the building of $CaSO_3$ on the particles of $CaCO_3$ is strongly limited. Under the described conditions, the absorption process is practically gas-side controlled by elimination of resistance in the liquid phase boundary layers between gas and liquid and between liquid and solid $CaCO_3$ used as adsorbent. This gives a possibility to calculate the absorption degree using literature data, which makes unnecessary performing experiments for the given system and absorber construction. The absorbers are constructed as packed bed columns filled with Holpack: a packing of horizontal expanded metal sheets with high mass transfer coefficient and low-pressure drop. Of all existing packings, it is characterized by the greatest ratio of effective to specific surface area at low liquid superficial velocity, which in the selected variant of packing reaches three. Another advantage of the new installation is associated with optimal conditions for oxidation of the $CaSO_3$ to gypsum by air, which is preliminary humidified and saturated in SO_2 to provide stable high temperature of oxidation and stable low pH.

The new technology is compatible with extremely high absorption capacity, over 99%, for small dimensions of the absorbers, low-pressure drop, and high quality of the obtained gypsum.

6-O1. Numerical analysis of local field distribution in multi-phase composites

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Transport processes in small-scale heterogeneous systems offer opportunities for wide range of sophisticated applications and usually differ significantly from those at the macro-scale. Thus, numerical modelling and simulations can be useful for understanding the relationship between microstructures and complex phenomena that composites exhibit.

The objective of this contribution is to predict the influence of interface boundary in the field of processing of tri-phase dielectrics. 2D numerical simulations, based on a parallel plate capacitance model, were performed. The system under study consisted of periodic arrays of non-overlapping circular inclusions (2D spheres) distributed in a matrix. Small size isolated inclusions or thin coating layers with a third material were introduced in the reference two-phase composite. The exact results for the steady electric field distribution were obtained by solving the mixed boundary-value problem for the Laplace's equations. Finite element simulations were performed using FEMM (finite element method magnetics) software package in the quasi-static approximation. A parametric study was performed at different interface area-to-volume ratios and dielectric permittivity of each phase. The behaviour demonstrated by three-phase systems was completely different from that based on two-phase systems, even for low additive content (less than 10%). Electric intensity was shown to be enhanced from each nonlinear region because the field can be concentrated in both the interior and the exterior neighbourhoods of the inclusions depending on the dielectric permittivity ratio. The enhancing effect of coating layer was well above those obtained by single inclusions. Therefore, the process of local dispersion of the additives seems to have a significant influence on the resulting material performance.

For mathematical analogies reasons, the methodology and the local field distribution laid out in this work for dielectric composites can be extended to other field phenomena including velocity field for flow through porous media, and temperature and concentration fields for conduction and diffusion in heterogeneous media.

6-O2. Potentials of CFD characterization in 'green' production of exopolysaccharides

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The restricted volume of plant polysaccharides poses a problem in many industrial areas of modern society that suggests a successful replacement of plant by microbial polysaccharides. Research on new bioproduction systems, methods and operations has been extended and simulation techniques have been also included. This work presents an overview of the simulation of stirred bioreactors aimed at bioprocessing of exopolysaccharides. The study is focused on exopolysaccharides (EPS) produced by extremophilic microorganisms. Single phase and two-phase (gas-liquid) flow conditions and characteristics relevant for the specific bioproduction were obtained and illustrated. Stirred vessels with single and double impellers of semi-tech scale were included. The variation of bioreactor parameters accompanying the rheological changes in the time-course of bioreaction is considered. Different impeller designs were examined and the results were evaluated in terms of power efficiency and availability of substrates. The potentials of two-phase bioreactor modelling are revealed and discussed in the context of advanced laboratory green technologies now considered for practical evaluation.

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6-O3. Heavy metal adsorption in fluidized bed: experimental and modelling

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The purpose of the present study is to investigate the behaviour of activated carbon from apricot stones (ACAS) in a closed circuit fluidized bed (CCFB) for removal of Pb, Cu, Cd, and Zn ions from aqueous solution. Adsorption equilibrium was calculated by the Langmuir model for single and multicomponent systems. An intraparticle diffusion coefficient, calculated by the model of Morris and Weber, was used to evaluate the total adsorption of Pb, Cd, Cu, and Zn in the CCFB. The expansion characteristics of the bed were studied. The behaviour of single and binary solid phase in liquid fluidization was also studied. Layer inversion velocity was obtained by visual observation and was photographically verified. The homogeneous solid phase diffusion model, using kinetic and equilibrium parameters obtained from laboratory batch adsorption runs, satisfactorily described mass transfer in the solid phase. The piston-dispersion model for the liquid phase was compared to the calculations assuming perfect mixing conditions in the whole CCFB adsorber due to the influence of the recirculating flow. A close correspondence between batch and fluidized bed operation modes for experimentally determined time evolution of the adsorbed amounts supports the observation that the CCFB can be described by a stirred batch adsorption model.

6-P1. Sensory properties of Bulgarian yoghurts with *Lactobacillus* strains as probiotic adjunct cultures

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Yoghurt market is highly sophisticated, complex, and, diverse and its evolution has been dictated by market forces and consumer preferences. Recently, many kinds of yoghurt and yoghurt-type products have been introduced into the market and the sensory properties of yoghurt and fermented milk products have become one of the principal factors that affect the consumers' choice.

The objective of this work was to study the effects of four different probiotic *Lactobacillus* strains on sensory properties of yoghurts enriched with these cultures. The products were appreciated by panelists (especially taste, appearance, texture, and aftertaste) using descriptive sensory analysis. The experiments were conducted to establish differences between probiotic and standard yoghurt – a control fermented only by symbiotic starters of *Lactobacillus bulgaricus* and *Streptococcus thermophilus*. Evaluation of the physicochemical properties of the same products was also carried out. From the inoculation until the 28th day the product acidity, firmness and rheological parameters were determined. A comparison was made between the properties of the yoghurts and their sensory perception.

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6-P2. Comparative study of antioxidant contents in different medicinal plants

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Bulgaria is rich in medicinal plants containing polyphenols that are widely used in traditional healing practices. Recently the scientific interest in better understanding of the process has risen enormously especially for pharmaceutical, nutritional, and cosmetic products. Phenolic compounds represent a majority of the natural antioxidants presently identified. The most important classes of natural antioxidants include tocopherols, flavonoids, and phenolic acids, which are common to all plant sources.

Conventional extraction techniques based on water/ethanol solutions have been applied to extract natural antioxidants from some traditional Bulgarian botanical species and compared to exotic plants. Their total polyphenol content and antioxidant activity was used as a basis for comparison. A routine extraction protocol was used to establish the complex composition of the antioxidant compounds of the natural source.

The extraction efficiency was found to be affected by variable operational parameters, as temperature, ethanol concentration, and solid-to-liquid ratio. In this study, the optimal conditions for antioxidant extraction were investigated. The optimal conditions for a maximum antioxidant extraction were obtained and data on different plants were compared.

6-P3. Aeration non-uniformity of stirred fermentors in presence of exopolysaccharides

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Aeration non-uniformity has been analyzed experimentally by measuring local gas hold-up in semi-industrial bioreactor (50 L) in presence of various exopolysaccharide (EPS) concentrations. As an EPS, xantan gum was used. The gas hold up axial profiles obtained in various radial position selected close and far from the wall in the bulk area reveal high aeration non-uniformity. The effects of the design of two impeller types equipped with flat and curved blades have been studied. The novel blade shape could account for up to a 50% balance of non-uniformity in this specific biotechnological case.

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6-P4. Modelling of bioreactor for autothermal thermophilic aerobic digestion by using artificial neural network

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Mathematical modelling is one of the research methods that is capable to predict the behaviour of ATAD processes in batch bioreactors under different scenarios. Bearing in mind the lack of complete knowledge on the biological sludge degradation carried out in bioreactors and the uncertainties in incoming fresh sludge temperatures as well as their amounts and composition because of fluctuations over the different seasons and days we proposed an artificial neural network (ANN) to be applied for modelling of ATAD bioreactors.

Using real set of data; two ANN bioreactor models were built and trained. Both models differed in their structure and number of neurons in hidden layers. Model verification showed acceptable coincidence with rested for verification group of real data.

Both proposed models could be used for ATAD bioreactor modelling.

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6-P5. Hybrid process for production of lemon balm extracts with high content of antioxidants

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The beneficial action of an antioxidant substance is expressed by neutralization of free radicals in the human body, which prevents DNA damage, as well as improper cell reproduction leading to many diseases (premature aging, cancer, heart disease, etc.). For this reason, antioxidants are used as ingredients of medical pharmaceutical preparations. These compounds play also an important role in food technology because of their usefulness as preservatives against lipid oxidation that develops unpleasant odour and flavour. The conserving action of antioxidants is an important feature increasing storage life of food products, also determining their use in cosmetic and flavouring industry. Unlike synthetic chemical substances, those obtained from natural raw materials are preferred as ingredients of consuming products.

Extracts from lemon balm (*Melissa officinalis L.*) have antioxidant activity, mainly due to the presence of rosmarinic acid (RA). This activity is proportional to RA concentration. Conventional extraction methods produce extracts with many ballast components and low concentration of active substances. The aim of this work was to develop a process for production of extracts from lemon balm with higher concentration of rosmarinic acid, i.e. with stronger antioxidant activity. This complex process is based on integration of different separation methods: treatment of the plant material by carbon dioxide at supercritical conditions (high pressure) coupled with a process of solid-liquid extraction by ethanol-water mixture. Both processes were optimized and the result of the integrated scheme was a product of higher content of rosmarinic acid and higher antioxidant activity.

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6-P6. Extraction of antioxidants from coffee residues

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Coffee is a most common everyday drink with proven effect on human physiology. The annual consumption in the European community and USA is about 5 kg of roasted coffee *per capita.*

There are essentially three ingredients responsible for the physiological effects: caffeine, diterpene alcohols: cafestol and kahweol, and polyphenols with chlorogenic acid (CGA) as a major representative. CGA and the majority of other polyphenols in the coffee are well soluble in methanol, ethanol, and their mixtures with water. For this reason, they are used for extraction of these antioxidants. Although ten times less, the solubility of CGA in water is not negligible (2.5 g/l).

During coffee preparation (hot water extraction) the polyphenols are only partially extracted, while 20–60% of their initial content remains in the solid residue. Consequently, they may be recovered by additional treatment turning the coffee wastes into a source of antioxidants for nutritional industry. After this second extraction, the coffee residue can be used as an animal feed or as a natural fertilizer.

The aim of this work is to study the extraction of polyphenols from solid residues after coffee drink preparation using water and ethanol-water mixtures as solvents and applying a subsequent adsorption of CGA by Amberlite resin.

The results showed that the coffee residues obtained after standard espresso preparation are sources still rich in antioxidants, which might be recovered by additional water or ethanol-water extraction. Water extraction yield was slightly lower than that of ethanol-water treatment, but the composition of extracts was similar. The extracts obtained contained 25–30% polyphenols that can be used in the nutritional industry on condition that their dark colour is not an obstacle. Further enrichment of the final product could be obtained by additional treatment using an appropriate ion exchange resin.

6-P7. Spent coffee grounds for production of biodiesel

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Solutions to our fuel issues can be found in unlikely places that we only have to see. Coffee dregs, of one of the most used beverages in the world, have values as an oil source for production of biodiesel. Research shows that spent coffee grounds contain from 11 to 20% oil, which is slightly less than other biodiesel feedstock.

Spent coffee grounds might be a source of green energy. It is estimated that more than 7.3 billion kilograms of coffee are produced globally per year, so there is a cheap and constant supply of coffee waste, which could be used to make 1287 million litres of biodiesel. Since coffee is rich in natural antioxidants, the resulting biodiesel is predicted to be more stable than those from other sources are.

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6-P8. Separation of dimer and polymer carbohydrates by biphasic systems based on ionic liquids

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In the present study, biphasic systems based on imidazolium ionic liquids, a hydrophilic [C_8mim]Cl and a hydrophobic [C_6mim][BF_4], were investigated as an alternative to the volatile organic solvents commonly used in recovery and crude separation of dimer and polymer carbohydrates, which are both present in the aqueous bioreaction media of extracellular polysaccharide (EPS) producing strains. Model aqueous solutions of various concentrations of maltose and xanthan were employed in extractions by the ionic liquids. [C_8mim]Cl could only form aqueous biphasic systems upon addition of a structure-making (kosmotropic) salt, K_2HPO_4. A binodal curve of the system [C_8mim]Cl/K_2HPO_4 was determined and an extracting composition of phase-forming components was selected. Individual extractions of single maltose or xanthan were performed. It was established that the disaccharide preferably resides (by a fraction of 97%) in the lower aqueous K_2HPO_4-rich phase, while the polysaccharide entirely migrates (extraction efficiency of min. 99%) into the upper ionic liquid-rich phase. The same trend was kept in simultaneous extractions of both maltose and xanthan: 80% of the maltose was separated in the aqueous phase and the xanthan was completely transferred to the ionic liquid phase.

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6-P9. Some possibilities for separation of copper, zinc, and iron by means of bifunctional extractant Kelex 100

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The aim of this study was to find out possibilities for separation of copper, zinc, and iron from combined hydrochloric acid initial solutions by means of solvent extraction using a bifunctional extractant Kelex 100 (7-(4-etyl-1-metyloktyl)-8-hydroxyquinoline). The solvent composition was 20 vol.% Kelex 100, 65 vol.% kerosene, and 15 vol.% *n*-octanol.

The separation process involved the following steps: (i) extraction of metal anion chloride complexes from the hydrochloric acid medium; (ii) scrubbing of loaded organic phase using water or ammonia; (iii) stripping of metals ions from the organic phase by means of sulphuric acid; and (iv) conditioning of the organic phase by a sodium chloride solution. After that, the extractant was ready for a new extraction step. The conditions of carrying out the individual steps of the method were studied.

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6-P10. Pressure drop of vertical plates with inclined capillary grooves for a redistribution packing layer of packed columns

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The uniform distribution of the liquid phase over the cross-section of a packed column is a major prerequisite for its effective operation. Regarding various distributor designs, the best uniformity is achieved with devices where the liquid divides into jets with equal flow-rates. The final liquid redistribution, to obtain uniformity over cross-section areas of the size of a packing element, takes place in the packing itself or in a specially designed redistribution layer. For this purpose, a new packing, especially proper for low liquid superficial velocity, was developed and investigated. It consists of parallel vertical plates with inclined crossing capillary grooves stamped on them.

A computer procedure is for calculating the height of the redistribution layer under a distributor with a given distance between the feed points. The calculated height ensures, with a selected precision, equality of the flow-rates of the liquid phase leaving the capillary grooves.

Experimental data on the pressure drop of the new packing at different gas and liquid superficial velocity have been obtained and compared with data on other packings for redistribution layer.

The hydrodynamic investigation and comparison with other devices shows that for a given degree of uniformity the new packing is characterized by significantly smaller height and lower pressure drop.

6-P11. Liquid distributor for soiled and viscous fluids in packed column apparatuses

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Of interest are the possibilities of liquid distributors regarding flow rate and hence the density of irrigation and the uniformity of the different liquid jets. For this purpose, a distributor for a column with diameter of 426 mm with 12 bevel pipes with bevelling angle of 45° was studied. The pipes were Ø53×1.5 and the feeding pipe – Ø70×2. Experiments were carried out by water at a plant, in which liquid flow was measured by a flow meter and the uniformity of the liquid jets was determined by volumetric method. The free section in the area of the distributor was 58%.

The experiment has shown stable operation in the loading range within 1.0–8.5 m^3/h. These values depended on the height of the hydrostatic layer in the plate above the lower end of the slots. The relationship of the two variables was directly proportional in the most part. The experiments showed that, because of technical irregularities in pipe welding in height by about 0.8–1 mm, at low flow rates there was a considerable non-uniformity (standard deviation is 0.03–0.07). In this liquid feed and location of the overflowing pipes, no significant influence of liquid gradient on jets uniformity was observed. It was also found that a greater difference between the bottom of the distributing pipes and the packing layer might cause greater non-uniformity due to a variation of jets trajectory.

In conclusion, it can be stated that the studied liquid distributor ensured good uniformity with standard deviation less than 0.03. The operation range of the distributor with such uniformity is within 2.0–8 m^3/h. The distance between the distributor and the packing layer must be 30 to 50 mm.

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6-P12. Equilibrium partial pressure of SO_2 over absorption slurry in case of purification of the flue gas from sulphur dioxide using gypsum technology

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The most widely used process for purification of flue gases from SO_2 is their absorption by slurry containing $CaCO_3$. Until now, there exist installations only for high capacity boilers with low degree of absorption. The present work is a part of a project funded by the National Science Fund of Bulgaria in partnership with a Bulgarian trade and technology joint-stock company for creation of an installation for small and middle capacity boilers. The knowledge of the equilibrium between the gas and liquid phase is the first condition for developing a proper technological scheme and dimensioning the necessary absorption equipment. Because of the low solubility of the main solid components of the slurry circulating in the absorbers, SO_2 concentration and SO_2 partial pressure in the gas phase at a given temperature is practically a function only of pH. Data on the necessary equilibrium for the temperature in the absorbers are not available in the literature.

Equilibrium data were obtained by passing a pure inert gas through a succession of thermostated absorption flasks. SO_2 partial pressure was calculated from the pressure in the last flask and SO_2 concentration in the out gas measured by a precise gas analyzer. The fact that the measured concentration is actually the equilibrium one was proved by changing the number of the absorption flasks. By increasing this number, a constant SO_2 concentration was attained, which was assumed the equilibrium one. The studies were performed at different temperatures and pH values.

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6-P13. Investigation of conditions for decreasing the inlet gas flow maldistribution in four configurations of gas distribution device

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In an experimental installation with column diameter of 0.47 m, four different configurations of gas distribution device (GDD), representing a bent toward the bottom of the column tube, were tested. Configuration 1 was a GDD with added water mirror, while configuration 2 was a GDD without water mirror. Configuration 3 was a GDD without water mirror and an empty section with a height of 0.5 m added, and configuration 4 was a GDD without water mirror and with 2, 4, and 6 redistributive grids of horizontal sheet packing. The local velocities of the gas flow were measured by thermal anemometer in 123 points along the cross section of the column, after each of configurations output, for three different inlet gas flow velocities (1.3, 1.6, and 2 m/s). Results are presented as velocity iso-lines contour maps. Maldistribution coefficients for gas flows in relation to these maps were also calculated. It was found that the initial maldistribution of incoming gas stream for configuration 1 (~60%) decreased to about 38% by removing the water mirror (configuration 2), and after adding an empty section (configuration 3) it was further reduced depending on the initial velocity (16, 31, and 28%). The most significant decrease of the maldistribution coefficients was observed with configuration 4, around 20–23%, depending on the number of grids (6 grids for 2 m/s and 2 grids for 1.3 and 1.6 m/s). These results well agree with literature data and can be used to improve column performance.

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6-P14. Study of hydrodynamic and mass exchange characteristics of the sieve plate in distillation

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Rectification is one of the methods of separating liquid mixtures based on different distribution between the liquid and vapour phases of the components in the mixture. Vapour and liquid flows are passed counter current, repeatedly interacting with one another through special apparatuses – rectification columns, in which part of the vapour (or liquid) leaving the column is recovered after condensation (in the case of vapour) or evaporation (in the case of liquid). A contact between the two phases takes place on contact devices (trays) horizontally located along the height of the column.

The purpose of this work was to study the influence of load of the steam phase on hydraulic resistances, the height of the gas-liquid platelayer, and the efficiency of separation of the rectification model (methanol-water mixture). Experiments were conducted in a glass laboratory column with three tray exporters with the following geometrical characteristics: diameter 0.1 m, number of holes with a diameter of 3 mm 50, and 4.7% free section. The cube of the column holding, 0.015 m, was equipped with adjustable electric heating with power of 11 KW, which allowed loading the steam phase to the entire section of column, 1 m /s.

Based on experimental results it was found that the change in velocity in the column ranged from 0.12 to 0.38 m/s, the hydraulic resistance of the plate was changed in the range of 3 to 15 mm WS, the height of the gas-liquid layer being 5–50 mm, and the Murphree efficiency 40–72%.

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6-P15. Gas-liquid mass transfer coefficient in sieve-tray laboratory column

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The influence of plate geometry on the characteristics of fluid flow and mass transfer in a laboratory column was experimentally examined using different binary blends. The volumetric gas-liquid mass transfer coefficient depends on fluid properties, hydrodynamic regime, and configuration of the gas-liquid contacting device. Prediction of mass transfer coefficients is an important part of gas-liquid contactor design. The individual terms in volumetric mass transfer coefficients are difficult to measure directly.

The aim of this work was to perform an experimental study of the kinetic coefficients in distillation of binary blends in a laboratory column under conditions close to a model of ideal mixture for a liquid phase and ideal displacement for a vapour phase.

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6-P16. Surface tension effects in sieve-plate distillation columns

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The main feature of the rectification process is its efficiency. It has long been known that the gas-liquid bubbling layer formed on the trays and the ongoing mass-exchange process upon rectification is influenced by the change of the surface tension gradient during the mass-exchange process. Binary mixtures with respect to the change of the surface tension effect can be divided into positive ($d\sigma/dx<0$), when the high-boiling component of the mixture has a greater surface tension effect, negative ($d\sigma/dx>0$), when the high-boiling component of the mixture has a lower surface tension effect, and neutral ($d\sigma/dx=0$), when both components of the mixture have similar values of surface tension effect. To assess the effect of surface tension on mass transfer the stabilization index quantity (M-index) is used, representing the product of the liquid phase process momentum and the surface tension gradient in the composition of the liquid phase.

The purpose of this work was to study the effect of surface tension on the rectification efficiency of methanol-water mixture under the conditions of complete mixing of the liquid phase and the ideal displacement regime in the vapour phase as well as to compare the results with those of chloroform-benzene mixture according to experimental data.

Based on the obtained experimental results it was found that on increasing the M-index the values of the local coefficient of performance COP (E_{OG}) for methanol-water mixture increased. For the chloroform-benzene mixture, the change of M-index did not influence E_{OG}.

6-P17. Wet flue-gas desulphurization process with waste alkaline suspension

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Desulphurization may be divided into dry, semidry, and wet methods. In the wet processes, the removal of sulphur dioxide is achieved by chemical absorption using limestone or slaked lime slurry as a sorbent in spray towers.

The present work deals with wet flue-gas desulphurization process with alkaline suspension. The interaction between gas mixtures of air/SO_2 and N_2/SO_2 with various contents of sulphur dioxide and alkaline suspensions was experimentally studied. The absorbents used were waste suspensions from the manufacture of sodium carbonate, filtrate of the suspension as well as model solutions of different mass concentration of the solid phase.

Experiments were carried out in a glass reactor, the absorber being of bubble type. The liquid phase was placed in the reactor and a magnetic stirrer was started. Different contents of sulphur dioxide ($1.41\div17.32\times10^{-2}$ mol/Nm^3) in the gas mixtures with waste suspension from sodium carbonate manufacture and with model solutions of different mass concentration of the solid phase ($5\div60$ kg/m^3) were used. A gas analyser, MSI Compact dragger, was applied to measure the concentration of sulphur dioxide in the gas phase before and during experiments.

The obtained experimental data give possibilities to plot kinetic curves of sulphur dioxide and alkaline suspension. A comparison between the experimental data on waste suspension and model solutions was made. The results provide possibilities to calculate the mass transfer coefficients of both the gas and liquid phases. These coefficients allowed the assessment of the kinetic features of the wet desulphurization process.

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6-P18. Oxidation of $CaSO_3$ by air in a technology for purification of flue gases from SO_2

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Gypsum technology is the most widely used process for purification of flue gases from SO_2. According to this process the $CaSO_3$, obtained by absorption of SO_2 in $CaCO_3$ slurry, is oxidized by oxygen (air) to $CaSO_4{\cdot}2H_2O$. The latter is transformed by drying to gypsum ($CaSO_4{\cdot}0.5H_2O$) for building purposes. The existing technology is created for big boilers, which reflects on the type of SO_2 absorbers and apparatuses for oxidation of the obtained $CaSO_3$ that are not proper economically for small and middle capacity boilers. The severe limitations to the maximal concentration of SO_2 in the purified flue gases connected with Bulgaria's membership to EU and their regular tightening call for better solution of the problem.

The distribution of the oxidizing air over the cross section of the apparatus in the existing installations takes place by means of a system of agitators. In comparison with evenly distributed small orifices, this system has one advantage and two disadvantages. The advantage, which determines the usage of agitators in all existing installations, is that they have no problems with fouling. One disadvantage is the great energy consumption for the agitators. Another drawback, which is important for some SO_2 absorber constructions, is the equal value of pH of the slurry distributed over their cross section independent of SO_2 concentration in the flue gas entering the apparatus. This leads to reduction of the driving force in the absorber and in this way to reduction of its efficiency.

A new technology using small orifices gas distributor by preventing the effect of their fouling has been created. Data on dimensioning of the oxidation reactor at different pH, temperatures, and catalysts are presented. They are used for construction of an industrial oxidizer, which soon will be implemented in industry.

6-P19. Determination of the main characteristics of carbonate nanoparticles obtained by the method of reverse micelles

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Recently, microemulsions have shown their potential as an interesting alternative reaction medium for the production of relatively monodisperse small colloidal nanoparticles. Nanosized particles of alkaline carbonates have specific characteristics and they are important materials for industry. The aim of this work is determination of the main characteristics of carbonate nanoparticles prepared by the method of reverse micelles. The proposed reverse micelle method allows for a purposeful regulation of the particle size during synthesis. The shape and size of the particles were determined by electron microscopy. The obtained carbonate nanoparticles were spherical with a size of 20 to 30 nm. The main characteristics of the resulting carbonate nanostructures, such as specific area of the nanoparticles, average diameter, and number of particles per unit mass were calculated.

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6-P20. Non-linear mass transfer from a solid spherical particle dissolving in a viscous fluid

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Theoretical study of non-linear mass transfer from a solid particle suspended in a viscous fluid is presented. In the case of intensive mass transfer, the process is completed by the secondary flow as a result of the big concentration gradients and the decrease of the particle radius as a result of particle dissolution. Under these conditions, the liquid-solid interphase mass transfer rate is obtained and analyzed. Comparison analysis shows that the effect of non-linear mass transfer on mass transfer rate is bigger than the effect related to changes of the radius.

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6-P21. Parameter identification of multiequation models

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A very important stage of model development is parameter identification through inverse problem solutions.

The kinetics of many chemical, biochemical, photochemical, and catalytic reactions is very complex, the kinetic model consisting of many equations and parameters. Model parameter identification in these cases is very difficult because of the multiextremal least square function or because of the fact that some minima are of ravine type. The solution of this problem needs very good initial value approximations for the parameters (in the attraction area of the global minimum) for the minimum searching procedure. A polynomial approximation of the experimental data permits to propose a hierarchical approach to obtaining initial parameters values in the global minimum area, using a consecutive approximations method.

The hierarchical approach to parameter identification of multiequation models was tested for two bioprocesses: modelling of fermentation systems and microalgae growth kinetics. Model parameter values were obtained on the basis of actual experimental data.

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6-P22. Bio-electrodenitrification of nitrates

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Nitrates pose a serious risk to environment, human and animal health. Nitrate ions cause many diseases all over the world. For example, they oxidize Fe atoms in hemoglobin from Fe^{2+} to Fe^{3+} and in this way they are unable to bind oxygen which is transferred from lungs to every cell in human body.

One of the most effective and economically worth method for wastewater treatment is the biological denitrification in the presence of microorganisms whose enzyme systems reduce nitrates to nitrites. When combined with weak electric field this method increases its rate. Electric field affects the active site of nitrate reductase, where Mo is contained. Probably this is the main reason for faster nitrate reduction.

The effect of temperature was also considered. The optimal temperature for nitrate reductase activity is 30°C. We established that denitrification without applying electric field is accompanied by tunnel effect. The impact of electric field is due to decreased activation energy for the reduction of nitrates to nitrites and partial elimination of the tunnel effect. In this case, the maximum reaction rate follows the Arrhenius equation. Isolated and purified nitrate reductase also showed a certain activity in both types of experiments with and without applying constant electric field.

In the cases of high nitrate concentration, the temperature effect is slightly observed. This may be due to substrate inhibition.

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6-P23. Fed batch processes for biodegradation of monochloroacetic and dichloroacetic acids

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Monochloroacetic acid (MCA) and dichloroacetic acid (DCA) are strong organic pollutants and met as big amounts in the environment. Their biodegradation was able with *Xanthobacter autotrophicus GJ 10* strain.

These carboxylic acids were used as carbon substrates of inoculate in fed batch processes under the same conditions. It has been established that the highest consumption of substrate in a laboratory bioreactor was achieved at an agitation rate of 500 rpm and airflow 1.0 l/min.

Unlike MCA, the biggest daily consumption of DCA was 15 mM. We have fed the reactor with DCA two or three times a day. Instantaneous concentration of dissolved oxygen and its influence on the processes has been studied.

The total quantity of degraded acid was 300 mM MCA for 10 days and 80 mM DCA for 8 days.

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6-P24. Biotransformation of glycerol by *Pseudomonas denitrificans* 1625 with production of 1,3-propanediol

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Glycerol is a waste product from biodiesel production. There are many efforts to find reasonable applications for it and one of them is to produce some diols, e.g., 1,3-propanediol (PD).

In the present study, the ability of the strain *Pseudomonas denitrificans* 1625 for this purpose was checked. Both batch and fed-batch modes of this biotransformation carried out under rotary shaker conditions were tested.

It was observed that a homo-fermentation process prevails and PD was produced with no traces of other products, when the glycerol initial concentration was sufficiently low (10 and 20 g/dm^3). At initial substrate concentration of 30 g/dm^3, the process was substrate-inhibited with a longer lag phase.

In the case of fed-batch process higher yields of PD were observed but at a lower rate. Some small amounts of 2,3-butanediol have been observed.

These preliminary results give confidence that crude glycerol may find practical application for producing chemicals that are manufactured from petroleum.

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6-P25. Sulphuric acid autoclave dissolution of Ni-Co sulphide deposit

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During processing deep ocean manganese nodules from the Clairon-Clipperton fraction zone of the Pacific Ocean by combined pyro-hydrometallurgical route, the non-ferrous metals were concentrated in two sulphide deposits: copper and mixed nickel-cobalt. In the present work, experimental results on sulphuric acid autoclave dissolution of Ni-Co sulphide deposit containing as mass %: 30.37 Ni, 3.13 Co, 8.36 Fe, 0.08 Cu, 0.16 Mn, and 36.8 S are presented. The effect of the main technological parameters on nickel and cobalt extraction and iron hydrolytic precipitation from the solution were studied. The degree of nickel and cobalt extraction at 90°C, Po_2 = 0.35 MPa, $\Delta H_2SO_4/\Delta Ni{+}Co = 0.19$, s:l ratio = 1:10, and dissolution time = 240 min was 97.71 and 96.25%, respectively, while the degree of iron hydrolytic precipitation was 99.68%.

7-K1. Enzymes for green chemistry and environmental quality

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Enzymes are versatile catalysts with a growing number of applications in biotechnology and, progressively, in mainstream chemical operations. The properties of enzymes render them also attractive for waste/pollutant treatment processes and their use is often advantageous over conventional treatments. In addition to the ease and reliability of enzyme usage, the biocatalytic properties of enzymes can be manipulated thanks to protein engineering, enzyme immobilization/insolubilization and bioreactor design.

The ligninolytic enzymes of white-rot fungi (WRF) such as peroxidases and laccases are particularly suited to the degradation of emerging micropollutants of concern, such as endocrine disruptor compounds (EDC), pharmaceuticals and personal care products. Thanks to their relatively low substrate specificity, these oxidoreductases can oxidize various micropollutants of phenol-like structure plus several non-phenolic substrates indirectly *via* the oxidized form of mediator molecules.

The re-usability of enzymes and their separability from reactants and products is ensured by carrier-based immobilization or by formation of cross-linked enzyme aggregates (CLEA). The initial CLEA concept developed by Sheldon's group at Delft has gained considerable attention during the last decade. CLEAs are produced by precipitating the protein(s) of interest with a suitable agent and subsequently linking the protein molecules covalently to each other with a bifunctional molecule. This methodology is simple, does not need highly purified enzymes and results in biocatalysts of high specific activity, solely consisting of protein.

In our group, laccase-CLEAs have been successfully produced and applied for the treatment of EDC in adapted reactor systems. Furthermore, we have identified key factors for the production of CLEAs of laccases alone or of combined oxidoreductases, and we have improved these novel biocatalysts by applying rational experimental design and optimization methodologies. An illustration of the powerful possibilities afforded by multi-enzyme aggregates involves our co-aggregation of laccases from *Coriolopsis polyzona*, with an acidic pH-optimum, and from *Coprinopsis cinerea*, with a neutral pH-optimum, in a single biocatalyst. The combi-CLEAs obtained showed activity over a broad pH-range implying their suitability for the treatment of real wastewaters with varying pHs. The creative fusion of biocatalysis, chemical engineering fundamentals, and nanotechnology opens up particularly attractive horizons towards a new chemistry and engineering for sustainability.

7-K2. Dust reduction by fuel additives

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Particulate matter (PM) is a general term describing small particles in the ambient air, such as dust, marine-derived particles, liquid droplets, smog components, and soot. PM in exhaust gases from combustion facilities is called as dust. Soot consists of small PM particles, amorphous carbon and polycyclic aromatic hydrocarbons (PAH). Soot becomes a part of black carbon/ smoke when present in sufficient particle size and quantity in exhaust gases resulting from incomplete combustion of hydrocarbon fuels. $PM_{2.5}$ is a term used for PM having particle size less than 2.5 μm that constitute a significant portion of soot and are able to affect the deeper parts of lungs leading to asthma, chronic bronchitis and heart diseases. Black carbon originating from combustion processes, scatters and absorbs the incoming solar radiations, contributes to poor air quality and induces respiratory and cardiovascular problems. In outdoor air, diesel particulates contribute to the total concentration of total suspended particulates. All diesel particulates can be classified as PM_{10}.

Because small particles like those under PM_{10} are capable of penetrating the filtering mechanism of the respiratory tract and can be deposited in the bronchi or lung tissue, aerosols stemming from combustion processes are unwanted particularly in the areas where they can be inhaled by humans. Medical studies have shown that non-volatile ultrafine particles with diameter <100 nm, can cause inflammation and respiratory diseases and the effect depends upon the surface area of inhaled particles and not on the particle mass. These particles can adsorb the hazardous substances and transport them into human organism. PAH are such typical adsorbates from combustion sources and many of these are carcinogenic. The ultrafine particles reduce visibility and may influence the climate-related effects like cloud formation. The probable carcinogenic PAH are chrysene ($C_{18}H_{22}$), benzo[a]anthracene ($C_{18}H_{12}$), benzo[b]fluoranthene ($C_{20}H_{12}$), benzo[a]pyrene ($C_{20}H_{12}$), dibenz[a,h] anthracene ($C_{22}H_{14}$) indeno[1,2,3-c,d]pyrene ($C_{22}H_{12}$), etc.

Environmental legislations are becoming increasingly restrictive over emission limits. Moreover, the need for fuel savings is also an objective of power producers for both economic and environmental reasons. The meeting of both of these targets is often difficult and it becomes more difficult in case of low quality of fuel especially in terms of stability. The typical combustion PM emissions (in g/kg of fuel) are 0, 1, 0.05–2, 0.05–0.5, 1–20, 1–10, 0.1–0.4, and 0.05–0.3 for power generation by natural gas, heavy residual oil, coal, municipal waste combustion, wood or coal open fires/stoves, diesel engines, Otto engines, and Otto engines using 3-way catalyst (although the data depend on the process and fuel specification), respectively.

Therefore, recent developments in the field of application of various types of fuel additives for reduction of particulate matter/dust in exhaust gases resulting from incomplete combustion of hydrocarbon fuels have become important. Different aspects of these emissions like the concern about polycyclic aromatic hydrocarbons adsorbed on soot particles, the trade-off between PM and NOx emission, etc., are being addressed worldwide today.

The metallic, organometallic and non metallic additives including oxygenates, nitrogenates, and nitro-oxygenates are being employed these days for PM/dust reduction during combustion of various types of fuels like heavy fuel oil, diesel, mixed fuels, biodiesels, and gaseous fuels. New additives like metal-based nanofluids/catalysts are being explored and investigated. Much progress has been made in deciding the probable mode of action of these additives.

7-K3. Green chemistry and sugars: a fruitful mixing for new amphiphilic molecules (or surfactants)

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Amphiphilic molecules (or surfactants) are key components of organized systems as emulsions and micro-emulsions. Depending on the applications of these systems, it is important to use an appropriate amphiphile for the process under consideration.

In this context, surfactants based on sugars are very important, the sugar part bearing together hydrophilicity, biocompatibility, and/or bioactivity.

Moreover, considering the crucial importance of developing green chemistry, the use of renewable sugars is also an important goal. Generally, these derivatives from sugars are not readily synthesized, as the starting sugars require protection. We present here routes, avoiding protection of the starting carbohydrates, to new series of surfactants derived from lactose and rhamnose, two natural sugars.

All these compounds form aggregates in aqueous solutions with corresponding biological properties and vectorization ability (of drugs) depending of the nature of the aggregates. Moreover, some of these compounds are now commercialized leading to new formulations of drugs for different cutaneous applications.

7-K4. Development of agro-derived green epoxy resin

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This study an approach of green chemistry, also known as sustainable chemistry. Green epoxy materials have been developed from epoxidized soybean oil (ESO) and anhydride-curing agent. Varying the anhydride/epoxy ratio (R) showed significant effect on the resulting properties of the materials. The materials have been characterized and compared by mechanical testing such as tensile tests, flexural tests, izod impact, scanning electron microscopy (SEM), and thermo gravimetric analysis (TGA). The glass transition temperature reaches the maximum at stoichiometric ratio. Thermogravimetric studies reveal that the materials are thermally stable but thermal stability exhibit a rapid decreases as the anhydride/epoxy ratio increases. Thus, the developed materials would be green alternative for achieving strong and environment friendly qualities.

7-K5. Organized molecular systems as reaction media for green chemistry

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Media are one of the most important factors to realize organic synthesis in soft and non-polluting conditions, answering the conditions of sustainable development. Organized molecular systems (OMS) are very efficient for the application of the twelve green chemistry principles, more precisely to replace organic solvents (VOC), to realize reactions in water, in catalysis and biocatalysis, for the molecular economy (and, of course, of atoms), or to work with low energetic conditions. These OMS possess a number of advantages: solubilization of substances that are not normally soluble in the continuous phase of OMS (organic or aqueous), localization of reactants and products, relative orientations and stabilization of the various entities in the various stages of the reaction. Rapid and selective reactions of preparative amounts of substrate can be carried out in such media, which are also well suited for mechanistic studies. For example:

– reaction in water: Wacker process, latex and functionalized latex preparations;
– selectivity: macrocycles synthesis *vs*. polymers formation;
– molecular economy: amidation of olefins;
– environment: decontamination of chemical weapons;
– clean products: surfactants with sugar heads;
– catalysis and biocatalysis: use of soy lipoxygenase, enzyme model.

By using model of rigid micelles, it is also possible to realize chiral synthesis with high stereoselectivity.

7-K6. A comparative study of R12, R134a, and mixture of R290 and R600a in a domestic refrigerator

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In the recent years, a non-azeotropic refrigerant mixture (NARM) of propane (HC290) and isobutane (HC600a) is considered to be a prominent substitute of CFC12 because it gives zero ozone depletion potential (ODP) due to no chlorine atom and also have very low global warming potential (GWP). In this paper, vapour compression cycle analysis has been carried out and a computer programme developed for pure CFC12, new eco-friendly alternative HFC134a, and NARM of HC290/HC600a having compositions 45/55, 50/50, 55/45, 60/40, 65/35, 70/30 by mass and parameters, viz., pressure ratio, discharge temperature, volumetric efficiency, mass flow rate, refrigerating capacity, power, heat rejected and COP have been evaluated and compared with available data.

7-O1. Studies on fungal biodegradation of lactic acid based rubber sheets

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The degradation of polymer based in general and natural rubber latex based product in particular have become a very challenging task. The consumption of natural rubber latex for making surgical gloves, ball bladders, etc., has increased many fold and accordingly disposal/handling challenges have increased tremendously. Due to environmental consideration and health threat, the problem of degradation of natural rubber latex products have reached to alarming level and the scientific world is searching desperately to find some eco-friendly technique for disposal of natural rubber latex product. In the present work, we made a successful attempt to develop biodegradable rubber. Sheets were prepared by using latex and lactic acid based resin. These sheets were subjected to fungal biodegradation. *Penicillium* sp., *Rhizopus* sp., *Mucor* sp., *Alternaria aternata*, *Aspergillus clavatus*, *Aspergillus Versicolor*, and *Aspergillus fumigatus* were taken for the biodegradation. The fastest biodegradation was found through *Aspergillus niger.* The biodegradation was analyzed by loss in tensile strength and SEM.

7-O2. Characterization of oil palm empty fruit bunch (OPEFB) as a source of biomaterial

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There is a massive generation of oil palm agro-wastes in Malaysia especially in the form of OPEFB. This calls for co-ordinated effort to manage the wastes and to develop value-added products from them. OPEFB can be exploited as an economical and greener source of value-added materials. It consists of compact lignocellulosic material, which is a natural biopolymer that has characteristics of renewable and biodegradable biocomposites and derivatizable material. Extractive treatment was applied on the lignocellulose of OPEFB with different solvents. The morphological and chemical characteristics were analysed using field emission scanning electron microscopy (FESEM), X-ray diffraction (XRD), transmission electron microscopy (TEM) and Fourier transmission infrared spectroscopy (FTIR). Morphology of lignocellulose as observed under FESEM showed rough network of fibres with cavities. Silicon network of OPEFB ash was found as a better substrate site for fillers to make silicon composites. XRD patterns depicted the lignocellulose as comprising of amorphous and crystalline regions. 2θ values of 22.331, 22.442, and 22.796° within the range of 19–23° reported the presence of cellulose. FTIR spectra showed different peaks at 900 and 1051 cm^{-1} of glycosidic and C-O-C linkage. Ash FTIR spectra described the Si-O-Si, Si-Si, and Si-OH bands at 1009, 1114, and 1454cm^{-1}. Characterization of OPEFB opened up avenues for material developments in the field of biomaterials.

7-O3. Enhancement of solubilization of polycyclic aromatic hydrocarbons by gemini conventional mixed surfactant systems

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Surfactant enhanced remediation (SER) is a promising technology for the removal of sorbed hydrophobic organic compounds (HOCs). The hydrophobic core of surfactant micelles may be used as a cargo space for encapsulation of a variety of sparingly soluble HOCs. Such encapsulation substantially increases their availability for microbial remediation. The superiority of gemini surfactants is found almost in all fields of surfactant applications compared to the conventional surfactants; this being due to their special physicochemical properties especially their low cmc and efficient ability to lower surface tension. Since using less compound to achieve the same effect and also having clear economic advantages and can thus be regarded as a green surfactant, recent years have witnessed rapid interest in a variety of areas of applications using gemini surfactants. Mixing of gemini surfactants with conventional surfactants are important from industrial as well research point of view. The work is a step forward as the results are better than systems involving conventional or conventional-conventional mixtures and thus add sense of topicality to the SER related research. As in practical fields, the properties of mixtures of surfactants are important; gemini surfactants used in combination with conventional surfactants will have properties more interesting than pure surfactants and thus be cost effective. In the lecture, studies of aqueous solubility of slightly soluble polycyclic aromatic hydrocarbons (PAHs – naphthalene, anthracene, pyrene), investigated in presence of pure and mixed gemini-conventional surfactants, will be described. The reasons to synergistically solubilize PAHs in gemini-conventional mixed surfactant systems will be discussed with the viewpoint of results to be exploited for the use of surfactant mixtures for environmental remediation. Furthermore, using a novel cationic dimeric (gemini) surfactant containing ester linkage in its spacer (that makes it biodegradable) for the SER will also be highlighted.

7-O4. Bio-energy crop sugarcane developed through tissue culture technique for sustainable environment

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India is the largest producer of cane and sugar in the world; however, the cane and sugar production per unit area is lower than several other cane-producing countries. Thus, sugarcane production offers continuing challenge to the development of high yielding high sugared and disease resistant clones. Sugarcane, belonging to the *Saccharum* (Poaceae) genus, is an important industrial crop and accounts for about 70% of sugar production all over the world. Attempts to evolve productive varieties of sugarcane are being made by conventional breeding method for last several decades. Tissue culture technique is now becoming an important tool of crop improvement as well as rapid micropropagation of selected clones. Achievements of this variety are highly significant and commendable; the deeper understanding of the genome of sugarcane along with cell and whole plant physiology will surely accelerate the biotechnological outcomes of sugarcane commercially. There are strong basis to anticipate that the rapid developments being brought about by the scientists globally would lead to boost the sugarcane production. The present paper deals with the effect of light intensity, photoperiod and growth room temperature on *in-vitro* morphogenetic responses of leaf sheath explants of sugarcane varieties CoS 96258 and CoS 99259. High frequency callus initiation was recorded in leaf sheath explants incubated in dark for 10–15 days and then transferred in light. Maximum shoot regeneration and number of shoots per culture could be recorded less than 16 h photoperiod of 4000-lux light intensity at a growth room temperature of 25±2°C in both varieties of sugarcane.

7-O5. Biogas recovery from waste organic materials: a comparative experimental study

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Biogas production from organic waste is already traditional method for treatment of agricultural waste with simultaneous energy recovery in the form of biogas. However, biogas can also be produced efficiently treating organic waste from beverage industries and biodiesel production. In the latter case, huge amounts of crude glycerol are released posing severe problems with their treatment. The main obstacle to the efficient waste treatment by anaerobic digestion is the sensitivity of the methanogenic bacteria toward pH variations. When the digester is overloaded, high concentrations of organic acids are produced damping the activity of methanogenes. This problem can be overcome by separating the digester into different compartments, enabling the development of the consecutive processes of hydrolysis, acidogenesis and methanogenesis in different spaces.

In the present study results of biogas production from poultry litter, stillage from ethanol production, and crude glycerol from biodiesel manufacturing are presented. The experiments were carried out in a continuous baffled anaerobic reactor. It was established that the process with glycerol utilization was too sensitive toward the loading because of intensive acid formation as intermediates. The process with stillage as substrate was stable and well steered for months with very high biogas yield (350 l/kg COD) at high production rate, i.e. up to 4 vvd^{-1}. The microbial profiles, the pH values and the intermediate concentrations along the reactor were determined and correlated with the biogas yield. Different microbial strains and profiles for the different substrates were observed. In the case of glycerol digestion, almost one bacterial genus, i.e. *Klebsiella* sp., was detected besides the methanogenes, which enables to make speculations about the pathway of competitive intermediate, biogas, and final products formation.

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7-O6. Removal of chromium from water with the help of aromatic amide prepared by pet waste

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Now-a-days, contaminated water is the major problem all over the world. Heavy metals like Hg(II), Cd(II), As(II), Pb(II), and Cr(II) are classified as toxic to the water. Adsorption, ion exchange, precipitation, reverse osmosis, phytoextraction, ultra filtration, and electrodialysis are the methods used for the removal of heavy metals. In adsorption method, use of PET waste and adsorbent such as charcoal or activated carbon, N-N'-dimethyl terephthalamide, terephthalic dihydrazide shows the maximum adsorption. Different columns are made with the adsorbent. Samples containing different concentration of Cr(II), heavy metals is made in ppm. They can be determined by atomic absorption spectrophotometer. The degradation of PET waste flakes was studied with methylamine and the products of PET waste with methylamine and hydrazine hydrate are soluble in different solvents. White precipitates were obtained, which were separated by simple filtration and dried under vacuum at 80°C for 5 h. The white precipitates obtained from the degradation reaction of PET waste were characterized by spectroscopic techniques (IR, NMR) and DSC. It is concluded that the amides prepared by PET waste act as good adsorbent and take less time for removal. A new adsorbent was prepared by this study and on the other hand, PET waste was also utilized.

7-O7. Investigations of radon exhalation rates, natural environmental radioactivity, and radiation exposure from Indian commercial granites

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In the present study, measurements of radon exhalation rates for granite samples used as construction material mainly as flooring material and as ornamental stones were carried out through sealed can technique using LR-115 type II detectors. Natural radioactivity in granite samples has been measured by low-level gamma ray spectrometer using HPGe detector. Higher and wide variation in radon exhalation rates were found in the samples. Radon activity was found to vary from 380.00 to 4258.57 Bq/m^3, whereas radon exhalation rate varied from 227.44 to 2548.81m Bq/m^{2}h. The variation could be correlated with the colour of the granites. Effective dose equivalent, estimated from exhalation rate varied from 26.82 to 300.56 μSv/y. From the activity concentrations of ^{238}U, ^{232}Th, and ^{40}K in the granite samples, radium equivalent activity (Ra$_{eq}$) due to the presence of radionuclides varied from 34.64 to 1144.84 Bq/kg. The total absorbed gamma dose rates varied from 6 to 535.61 nGy/h. Indoor and outdoor annual effective dose rate from these granite samples varied from 0.08 to 2.63 mSv/y and 0.02 to 0.66 mSv/y, respectively. The use of these granites as construction material can be done without posing significant radiological threat. However, care should be taken in the use of any granite slab.

7-O8. *Jatropha curcas*: sources of bioenergy for environmental protection

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Bio-fuels are renewable sources of energy derived from biological raw material. Two sources of biofuels, ethanol and bio-diesel, are gaining worldwide acceptance as one of the solutions for the problems of environmental degradation, energy security, restricting imports, rural employment, agricultural economy, owing to reduce dependence on oil import; savings in foreign exchange and reduced vehicular pollution. Two major biofuels for the transport sector, bio-ethanol and bio-diesel, are becoming popular in many countries across the world. *Jatropha curcas* L. commonly known as physic nut, Ratanjot, purgative nut or nut. *Jatropha curcas* L. has unique pride among the various plants because of its multiple uses like ethnomedical value, nutritional value, ornamental value, carbon sequestration potential, comparatively better fuel properties, etc., are worthy to mention. *Jatropha curcas,* an oil bearing, drought hardy shrub with ecological advantages has already being successfully grown and harvested as a bio fuel in countries. By the use of tissue culture technique *Jatropha* can be grow at higher level. By the development of tissue culture, technology for rapid multiplication of disease-free planting material has greatly facilitated mass production of quality seed with high content of bio-diesel in *Jatropha*. In recent years this plant has received extensive attention of many scientists in view of its great economic importance, medicinal significant and for its seed oil as commercial source of fuel. The superior quality oil can be extracted from the seeds. The oil can be used as a mixed fuel for diesel/gasoline engines. National networks namely ‘national network on jatropha and karanja’ constituted by involving state agricultural universities and institutions, such as CSIR, ICFRE, ICAR, CFTRI, TERI, and IIT Delhi.

7-O9. The psychochemistry of pollutants: effects of chemicals on human behaviour

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Pollutants may have many deleterious effects on bodily health, but the most insidious effects are those in which the entry of pollutant species affects the central nervous system (CNS) and results in changes in normal behaviour. Human beings are still ignorant about the long-range effects of number of pollutants, but effects of a few in the environment have now given extensive consideration. More attention is needed to be given to this problem, so that the effects of the pollutant species that our developing system introduces into the environment on our capability to adjust to our ecosystem can become known, understood, and controllable.

The study, that how the brain or CNS is working under the influence of chemicals (external or internal), is psychochemistry. According to this view, two major interactions are involved: first, change in biochemical processes introduced by the entry of chemicals into the body, and second, a consequent alteration of normal relations between biochemical processes and the behaviour, which appears as a change in the later.

Basic to effects on behaviour are the neurochemical events, which take place particularly in CNS. Activity between the neurocells results from the flow of neurotransmitter substances across the gaps and the activity can be recorded as a change. The following reaction summarizes the step reactions involved in the synthesis and inactivation of neurotransmitter.

$$\text{Acetate + Coenzyme–A} \rightarrow \text{Acetyl coenzyme–A + Choline} \xrightarrow{\text{Ch-acetylase}} \text{Acetylcholine} \xrightarrow{\text{Ch-esterase}} \text{Acetate + Choline}$$

Acetylcholine: $(CH_3)_3\text{–}N(OH)\text{–}CH_2CH_2\text{–}O\text{–}COCH_3$

7-O10. Development of integrated bioenergy devices for improvement of quality of life of poor people

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Sudan is enjoyed with abundant solar, wind, hydro, and biomass resources. Like many tropical countries, Sudan has ample biomass resources that can be efficiently exploited in a manner that is both profitable and sustainable. Fuel-wood farming offers cost-effective and environmentally friendly energy solutions for Sudan, with the added benefit of providing sustainable livelihoods in rural areas. Biogas from biomass appears to have potential as an alternative energy in Sudan, which is potentially rich in biomass resources. This is an overview of some salient points and perspectives of biomass technology in Sudan. Current literature is reviewed regarding the ecological, social, cultural, and economic impacts of biomass technology. This presentation provides an overview of biomass energy activities and highlights plans concerning optimum technical and economical utilisation of biomass energy available in Sudan.

7-P1. Improved sustainability of bioenergy crops through underground communication between roots and the soil microbiome

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The underground world is a lively place with plant roots and soil microbes waging a continual battle for resources. Plant roots take an active role in this conflict through the exudation of various chemicals, yet key areas of this process remain mysterious: what genes and gene networks control exudation? How do plant root exudates influence the microbial community of the soil? Finally, if plant roots do play a large role in soil microbial composition, what effect does this have in making plants more sustainable and self-reliable?

Our studies in this area have proceeded on three fronts. On the first front, we have looked at how a specific set of genes, the ATP-binding cassette (ABC) transporter genes, influences root exudation. On another front, we have examined how plant root exudates influence the soil microbial community. Current studies involve the analysis of how specific Arabidopsis ABC transporter mutants differently influence native soil microbes depending on their root exudate profile. Finally, a model will be presented that will synthesize knowledge about the active communication between roots and soil microbes and how this exchange of information affects soil microbial diversity, plant fitness and biomass production.

7-P2. Exergetic life cycle assessment of the sulphuric acid production

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The present investigation is an attempt at assessing the life cycle of one of the most important products in inorganic synthesis, namely sulphuric acid. Technological schemes for the manufacture of sulphuric acid from liquid sulphur, copper sulphide concentrates and zinc sulphide concentrates using double conversion have been analysed. The technological flowcharts include the principal processes to give sulphuric acid, namely:

– making SO_2-containing gas from sulphur or metal sulphide concentrates;
– gas purification and heat exchange;
– conversion of the SO_2-containing gas;
– absorption of SO_3 obtained in water to give H_2SO_4.

The assessment has been made using the exergy method of thermodynamic analysis. The exergy concept can be used as a measure of depletion and use of material and energy resources and as an indicator for total environmental impact.

The degree of utilisation of renewable natural resources used in the processes, the energy technological efficiency of the principal chemical technological stages and of the overall systems as well as the anthropogenic emissions in the environment characterisation have been carried out. The environmental impact was given in the form of impact categories (acidification, global warming potential, ozone layer depletion, human toxicity, etc.) which helps evaluating and proposing further improvements to the systems.

The studied installations of sulphuric acid production have good exergy and ecological indices, defining them as effective processes both in thermo-technical and in ecological aspects.

7-P3. Influence of climate changes on the migration ability of technogenic radionuclides

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Global warming and climatic changes in the last decade focus the attention of scientists worldwide. Changes in climate variables (winds, precipitation, currents, temperature, etc.) affect the transport, transfer, and deposition of contaminants in the environment. Numerous investigations show the strong impact of climatic parameters like temperature and precipitations on soil characteristics, and especially on soil organic matter, which plays a significant role in the migration behaviour of the contaminants in the environment. This defines the need of special attention on elucidation of the impact of temperature and precipitations on the chemical behaviour of the radionuclides. This work presents initial results of a research project aiming to elucidate the influence of climate changes on the migration and bioaccumulation of natural and technogenic radionuclides in terrestrial ecosystems. Different types of soils were contaminated by technogenic radionuclides (^{241}Am, ^{137}Cs, and ^{60}Co) and conditioned under different temperatures and soil humidity, simulating sharp climatic variations. Chemical fractionation of the radionuclides was studied by using two different procedures for sequential extractions, followed by radiation detection by gamma-spectrometry. Evaluation of the chemical behaviour of the investigated radionuclides with respect to soil characteristics, temperature and humidity variations and duration of conditioning was performed. Initial conclusions on the influence of the climate changes on the migration ability of radionuclides of different oxidation states were made.

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7-P4. Prediction of the biodegradation and toxicity of naphthenic acids

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Naphthenic acids are most significant environmental contaminants. They are comprised of a large collection of saturated aliphatic and alicyclic carboxylic acids found in hydrocarbon deposits. They are toxic components in refinery wastewaters and in oil sands extraction waters. There are many industrial uses for naphthenic acids, so there is a potential for their release to the environment from a variety of activities. Studies have shown that naphthenic acids are susceptible to biodegradation, which decreases their concentration and reduces toxicity.

The presence of naphthenic acids in the environment is seldom studied and little is known about their fate. Studies that used actual naphthenic acids focused on the biodegradation of these compounds as a group, because current analytical methods do not allow the study of individual compounds in the mixed state. The aim of this study was to predict the biodegradation of individual naphthenic acids and the possible toxicity of the parent structure and their metabolites. The software used in this study for prediction of the microbial metabolism of the naphthenic acids was the OECD (Q)SAR Application Toolbox. Toolbox is a software application intended to be used by governments, chemical industry, and other stakeholders in filling gaps in (eco) toxicity data needed for assessing the hazards of chemicals. Degradation pathways used by microorganisms to obtain carbon and energy from 200 chemicals are stored in a special file format that allows easy computer access to catabolic information. Most of pathways are related to aerobic conditions. Single pathway catabolism was simulated using the abiotic and enzyme-mediated reactions *via* hierarchically ordered principal molecular transformations extracted from documented metabolic pathway database. The hierarchy of the transformations was used to control the propagation of the catabolic maps of the chemicals. The simulation started with the search for match between the parent molecule and the source fragment associated with the transformation having the highest hierarchy.

7-P5. Recovery of platinum from spent SiC-DPFs

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A diesel particulate filter is a device designed to remove diesel particulate matter or soot from the exhaust gas of a diesel engine. The aim of this work was to determinate platinum content in Mercedes-Benz ML 350 DPF and to develop the technology for recycling such type of spent DPFs. According to X-ray diffraction analysis, the honeycomb ceramic matrix of this DPF is made of silicon carbide. The silicon carbide body is coated with a mixture of alumina and ceroxide. This mixture serves as a carrier layer for the catalytic converter. The carrier layer is coated with platinum, which acts as the catalyst. The dissolution of the ceramic matrix in carbonate melts at different molar ratios at a temperature of 1000°C was investigated. Separation of the ceroxide was achieved by dissolving the products obtained from silicon carbide corrosion in water. The content of silicon carbide in DPF was determinate by fusion with lead oxide. The obtained results were used to develop the fire assay methodology for determination the platinum content in spent DPF. Flux mixtures consist of potassium carbonate and lead oxide. In order to prevent platinum loss a silver chloride was added to the charge. Lead oxide is reduced from silicon carbide to metallic lead, which collects platinum. The resulted alloy after cupellation contains of 5.44% Pt and 94.56% Ag. This means that platinum content in analyzed DPF is 0.115 mass %. This methodology is a basis for technology development for recovering platinum from spent SiC-DPFs.

7-P6. Synthesis of hybrid materials based on sol-gel films for optical sensor construction

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The sol-gel technology is being increasingly used for the development of optical sensors and biosensors, due to its simplicity and versatility. By using this process, porous thin films incorporating different chemical and biochemical sensing agent are easily obtained at room temperature giving final structures of mechanical and thermal stability as well as good optical characteristics.

Optical sensors, or optodes, represent a group of chemical sensors in which electromagnetic radiation is used to generate the analytical signal in transduction element. These sensors can be based on various optical principles (absorbance, reflectance, luminescence, and fluorescence), covering different regions of spectra (UV, visible, IR, NIR) and allowing the measurement not only of the intensity of the light, but also of related properties, such as refractive index, scattering, diffraction, and polarization.

Enzymes, in combination with optical fibre biosensors, have almost exclusively been utilised in their immobilised form. The immobilization of the enzymes confers a number of advantages for their application in optical biosensors. In many cases, the immobilised biomaterial achieves greater pH, thermal, and storage stability. Immobilization also allows the reuse of the enzymes over an extended period, hence leading to greater reagent economy. Furthermore, it allows easier sensor manipulation and operation.

The aim of this study was to develop a sol-gel method of synthesis of new hybrid membranes, with immobilized biocatalysts (enzymes) for optical biosensor construction and xenobiotics detection. This study showed that hybrid organic-inorganic membranes were successfully synthesized.

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7-P7. Biocapacity of thermophilic bacteria from Bulgarian hot springs for generation of 'green' polysaccharides

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The restricted volume of plant polysaccharides poses a problem in many industrial areas of modern society that suggests a successful replacement of plant by microbial polysaccharides. This study is focused on exopolysaccharides (EPS) produced by thermophilic bacterial strains originating from Bulgarian hot springs. Multiple samples taken from Bulgarian hot springs were analyzed extensively in laboratory and thermophilic bacterial strain EPS producers were found. Two bacterial strains isolated from these samples were identified as *Geobacillus tepidamans* and *Geobacillus pallidus* and were characterized by bacterial growth and EPS production capacity. The biopolymer produced by *G. tepidamans* was identified as glucan. In view of evaluating the applicability of these strains for large-scale production, a feasibility study has been carried out both in laboratory flasks and in semi-tech scale stirred bioreactors. A maltose-containing medium was found to be preferable by the microorganisms with pH being maintained close to neutral, 6.5–7, and temperature close to moderate at 55–60°C. EPS production has been found to be strain-dependent with the majority of the batch runs producing between 20 and 100 mg of polymer dry mass per litre of fermented maltose medium. No significant increase of apparent viscosity with EPS production could be registered what is an important property for implementation of the bacterial strains in large-scale EPS production. The typical bioprocess dynamics has been registered and will be illustrated, including the most recent results and conclusions of the study. Although thermophilic Geobacillus strains generally display low EPS yields, a large biodiversity with respect to yields, monomer compositions and molecular masses as well as functionalities is expected. Further classification based on monomer composition of the EPS produced by the strains and EPS databases can be added/built. These may be used for further research on structure-function relationships and to predict the effect of the properties on value-added materials, such as cosmetics and food.

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7-P8. Biodecomposition of Jordan phosphorite by phosphate solubilizing fungi

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The soil naturally has microorganisms capable of biomeliorating soil phosphorus by converting the insoluble forms into soluble orthophosphates that can be taken up by the plant. Microorganisms substantially influence the soil productivity by solubilizing this insoluble phosphorus through their metabolic processes in the soil.

The bio-solubilization of Jordan phosphorite by the phosphate-solubilizing fungi (*Aspergillus niger*) was investigated. The effect of the phosphate concentration in the liquid medium, the duration of biodecomposition, the concentration of citric acid generated from the fungus and the effect of the preliminary mechanical activation of the phosphate on the biodissolution has been studied. It was established that the lower the phosphate concentration in the medium the greater the degree of P_2O_5 extraction was. The results obtained showed a correlation between soluble phosphate and citric acid produced by *Aspergillus niger*. A maximum degree of 99.1% of P_2O_5 extraction has been achieved on the 15th day when 0.5% w/v non-activated Jordan phosphorite were added to the medium. Mechanical activation of the phosphate had insignificant effect on the bioconversion process. Investigations with mechanically activated Jordan phosphorite showed that a maximum of 92.4% of the phosphate solubilization has been observed on the 10th day at phosphorite concentration of 0.5 w/v%.

7-P9. Effect of mechanochemical activation on bioleaching of Jordan phosphorite

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In the soil, two reactions, fixation and immobilization, convert applied phosphorus into forms unavailable for the plant. The soil naturally has bacteria capable of biomeliorating the soil phosphorus by converting the insoluble forms into soluble orthophosphates that can be taken up by the plant. The mechanisms of mineral phosphate solubilization by bacteria have been postulated to be due to release of organic acid and/or due to proton extraction. On the other hand, direct application of phosphate rock seems to offer a better alternative in terms of low cost, least energy-intensive and sophistication of processing of the phosphate ore to produce soluble fertilizers.

The role of mechanochemical activation as a pre-treatment method to improve the process of phosphorus biorecovery from Jordan phosphorite by soil bacteria is presented in this study. The effect of the phosphate concentration in the liquid medium and the duration of the incubation period on phosphate solubilization were established. The results indicated the positive affect of preliminary mechanical activation on the bioconversion process. A correlation has been observed between soluble phosphate and titratable acidity. A maximum of 54.3% of P_2O_5 extraction has been reached immediately on the first day of incubation if 0.5 w/v% of mechanical activated Jordan phosphorite were added to the medium. Investigations with non-activated Jordan phosphorite showed that the extraction of P_2O_5 was two times lower than with activated phosphate (26.4%) under the same conditions.

7-P10. Green roof: innovative technologies for sustainable development and improvement of the environment in cities

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The share of green roofs on residential and public buildings is increasing rapidly in recent years. Only in 2008 in the U.S., over 300000 square meters were installed. Development and enforcement of this new type of technology in building fully comply with the principles of sustainable development and help achieve greater energy efficiency with reduced greenhouse emissions. Green roof means not only an impressive exterior, but also a longer life of the waterproofing, and better and sound insulation that has greater energy efficiency and quality of construction – money that is subsequently returned. Besides, the purely economic advantages of green roofs are proving very useful to re-establish ecological balance in the cities. Thanks to the plants, the air was enriched in oxygen, reducing dust and the concentration of greenhouse gases.

This work has analyzed the experience and results of applying this new type of innovative technologies and has analyzed the effect of applying them to different local systems. It is emphasized that due to the inability to provide significant green spaces in cities and heavily polluted environment, green roofs are one of the best alternatives for the use of all available sites for development of plant areas and improve the quality of urban environment.

7-P11. Passive house: future or presence

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The idea of harmony between nature, society and the economy is best achieved through full implementation of the principles of sustainable development, i.e. improved quality of life while minimizing the consumption of natural resources so that next generations have enough opportunities for better life. One of the areas in which business, public needs, traditions, and cultural beliefs with environmental protection is necessary to integrate these principles in deciding to build housing for the population. From the selection of construction, decision today determines the quality of life of residents for a relatively long period. The international Energy Agency shows that buildings consume nearly 30% of final energy and is responsible for more than 40% of greenhouse gas emissions worldwide. The application of the principles of sustainable development is of an extraordinary importance to the construction sector.

This work considered some of the concepts for the development of a new type of construction by building the so-called passive buildings where energy saving and minimizing greenhouse gas emissions is the most significant. The concept of passive houses is based on a strict energy-saving heating, cooling, and ventilation, and can be reduced to such an extent that solar sources are sufficient to ensure a comfortable climate in buildings. Thus, passive houses become the basis for the development of sustainable architecture and construction by helping to reduce the use of non-renewable energy resources, reducing climate change, maintaining natural ecosystems, use 12% less potable water, generate 39% less carbon and 69% less waste and consume 71% less electricity. This work presents data on the development of this type of construction in many countries where the share of passive houses of the total housing stock is already significant.

7-P12. Characterization of Estonian and Bulgarian poultry excrements

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Sustainable agriculture is based on maintaining an optimal balance in content and ratio of nutrients in the soil, care for the ratio of major structural components, moisture, and protects plant and animal species from disease and pests of aggression. This requires the application of different fertilizers, soil, pesticides, and growth regulators. Other factors including selection of the most suitable plant species, mechanical treatment and use of modern irrigation systems are also important. Production of environmentally sound and sufficient in quantity crops requires use of appropriate improvers and fertilizers to nourish and stabilize soil compositions. In this respect, particular interest is manifested to processing of waste from poultry farms in appropriate fertilizers or soil improvers.

Subject of research in this work are four samples of bird excrement (two Bulgarian and two Estonian) from different poultry farms. These samples were characterized by means of X-ray analysis and differential thermal analysis to enable determination of P_2O_5 absorbed species, phase composition, and thermal stability. Based on the results of the experiments, it was found that the two Bulgarian samples had significantly higher content of organic component, which defines them as a good soil improver. Estonian samples contained lower amounts of phosphorus and organic components, which defines them as less effective for use in practice.

7-P13. Study on the possibilities for shared use of excrements from poultry farm with fluorapatite

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Poultry industry in Bulgaria involves between 15 and 22 million birds in recent years for poultry and eggs breeding, these birds producing daily about 4000–6000 tonnes of excrement. In annual terms this defines an amount of 500000 tonnes. Today, about 70 large poultry farms run in Bulgaria, where production does not reply to the requirements of EU law and has not complex license by the Ministry of Environment and Water for development of industries as these farms do not dispose of facilities for environmentally sound treatment of those wastes.

Poultry manure is an excellent source of nutrients and can be incorporated into many programs as fertilizer. Great interest is manifested to the processing of organic waste products of poultry and production of organic fertilizers.

Based on previous experiments, low phosphorus content of faeces was found. This work has investigated the possibility of joint use of bird excrement with fluorapatite to improve the quality of product to be used in agriculture as an innovative green technology for sustainable agriculture.

7-P14. Possibilities for recovery of technogenic contaminated soils by using the new products from solid wastes

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The utilization of solid waste is a major task that ecology has undertaken. The problem is not only its volume but also its chemical composition and great diversity. Declining stocks of primary energy sources and environmental problems arising from their use are just some of the causes behind the demand for alternative energy sources and developing new technologies for their utilization. Significant forest resources available in this country and relatively well-developed agriculture identify high potential for development of green technologies for sustainable agriculture. Along with this aim, problems with solid waste through their use in agriculture should be resolved, namely by restoring polluted technogenic soil. Belonging to this group, solid waste is biomass and ash from it followed by waste from livestock.

Natural resources, being rapidly depleted, and polluting the environment in a geometric progression should speed up the development of methods and technologies to utilize solid waste by environmentally sound way, aimed at closing the cycle of materials used in manufacture.

7-P15. Grape by-products as alternative source for obtaining natural antioxidants

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Grape is one of the most important fruit commodities as an economic plant with good agricultural characteristics. It is a significant source of nutritional antioxidants, health-promoting phenolic compounds. These compounds have been of great interest to the food industry due to their benefits as anti-aging, anticarcinogenic, antimutagenic, antimicrobial, and as the inhibition of human low density lipoprotein oxidation. During winemaking, large quantities of waste such as grape marc (residue after pressing for white wines or vinification for red wines) are produced. This by-product is characterized by high-phenol contents because of poor extraction during winemaking, so that its use supports sustainable agricultural production. By processing 100 kilograms of grape-vine approximately 20–25 kilograms of grape marc is produced. In Serbia, the grape industry produced 431000 tonnes of grapes and 190000 tonnes by-products in 2009. Recently, extraction of polyphenols from grape marc has emerged as an opportunity and vital business for the wine and food industry. The addition of antioxidants is a method of increasing shelf life, especially of lipids and lipid-containing foods. The importance of natural antioxidants for medicinal and food application has been underlined by numerous works. The aim of this work was to evaluate grape marc as a source of natural antioxidant for possible use as dietary supplement or food antioxidants. For this purpose, the antioxidant capacity and contents of total phenolic hydroxycinnamoyl tartaric acid and flavonol compounds of some red grape varieties grown in Serbia were investigated. The results of spectrophotometric analysis of the investigated grape by-products (grape seed, skin, and stalks) show high contents of polyphenolic compounds reflecting their high antioxidant capacity (99.92±0.21%). The grape by-product constitutes a very cheap source for the extraction of antioxidants, which can be an alternative source for obtaining natural antioxidants (dietary supplements), thus providing an important economic advantage.

7-P16. Secondary use of some types of wastes like soil-improvers in cultivation of pepper

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The necessity of achieving sustainable development in all areas of our life and the world shortage of raw materials bring to intensification of investigations aimed at utilizing different types of wastes. In this connection, the creation of complexes with technological cycle without generation of wastes is one of the most efficient directions for achieving control on manufactures.

This work presents possibilities for realization of new ‘green technologies’ for production of new types of soil improvers based on wastes, which are generated from pretreatment of biomass and cleaning of industrial waste gases. The application of these types of soil improvers with the aim of achieving higher yields, prevention of acidification and contamination of the agricultural lands and their recovery is demonstrated by different tests. In this work, analysis and assessment were made of available elaborations for obtaining soil improvers from appropriate wastes and their influence on plant growth and soil structure and properties. Also, experimental data from vegetation tests on two sorts of pepper (capsicum) grown by using different rates of soil improvers are given. Based on these data, optimal compositions for practical application of the prepared soil improvers are recommended.

8-K1. A novel route of synthesis and characterization of bisaminoethyl terephthalamide from polyethylene terephthalate (PET) waste

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Polyethylene terephthalate (PET) is a widely accepted most important commercial polyester polymer. The very large amounts of PET products used each year have poised a potential problem, which involves its disposal. Many research papers have been contributed by several authors for making PET waste recycling economically and ecologically more viable. Some success has been obtained in development of chemical recycling methods, which provides value added products from PET waste. The degradation of polyethylene terephthalate (PET) waste through aminolysis by making use of ethylenediamine was investigated at ambient temperature and pressure. After five days, complete degradation of PET waste was achieved. The aminolysed products so obtained were characterized as bisaminoethyl terephthalamide with the help of various conventional techniques such as chemical tests and spectroscopic techniques namely IR and NMR. The thermal stability of bis-aminoethyl terephthalamide was also studied with the help of thermogravimetric analysis. It shows change in the colour from white to yellow either in sunlight/UV radiation or on heating at 50°C.

8-O1. Study on physical modification of isotactic polypropylene using LLDPE

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Polymer blends have gained significant commercial interest, which increased in the last two decades, outpacing growth in the synthesis of existing polymers by 2–5%. The aim of the present work is to study the possibility of isotactic-polypropylene homopolymer modification by forming a polymer blend with linear low-density polyethylene.

The successful experiment will produce a polymer mixture to replace ethylene compositions obtained by block copolymerization

The possibility of physical modification of isotactic polypropylene homopolymer with a linear low-density polyethylene was studied. The properties of polymer blends with different contents of polyethylene in the range from 5–50 to 100 wt.% polypropylene were also studied.

Incompatible components in the polymer mixture were proved by using the results of thermal and X-ray analysis. The mechanical properties of the resulting polymer blends, PP/LLDPE, were studied by analysis of the observed phenomena and changes of component properties in the composition of the polymer mixture.

Using known theoretical dependencies, values of the glass transition temperature (Tg) of the studied polymer blends were calculated and the lowering of the glass transition temperature of the polypropylene compositions was confirmed, which is one of the objectives of its modification.

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8-O2. Electrospun poly(ε-caprolactone)/ascorbyl palmitate nanofibrous materials

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In the present study the possibility of one-step incorporation of ascorbyl palmitate (AP), an amphiphilic derivative of vitamin C, into nanofibrous mats from poly(ε-caprolactone) (PCL) by electrospinning is shown. AP content in the spinning solutions was selected in a way to be within 9–30 wt.%. It was found that the presence of AP in the spinning solutions led to preparation of thinner fibres, and the fibre mean diameter decreased with increasing the vitamin content. This was attributed to the behaviour of AP as an ionogenic surfactant capable of decreasing the surface tension and increasing the conductivity of the spinning solutions. The successful incorporation of AP into the fibrous materials was evidenced by IR spectroscopy, and the vitamin content was determined quantitatively by means of thermogravimetric analysis. Using the ability of the vitamin C to reduce silver ions, the possibility of depositing elemental silver nanoparticles onto PCL/AP mats is shown as well. AP incorporated into the nanofibrous materials preserved its stability, antioxidant and antibacterial activity as evidenced by UV-Vis spectrophotometric analysis, quenching of the free 2,2-diphenyl-1-picrylhydrazyl (DPPH) radicals studies and microbiological tests against *Staphylococcus aureus*, respectively.

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8-O3. Recent advances in the synthesis and properties of functionalized fluoropolymers as engineering materials

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We have investigated new thermoplastic fluoroacrylated copolymers, synthesized by radical copolymerization of fluoroalkene(s) with 5-membered cyclic carbonate and a third monomer or transfer agent, both containing an OH group susceptible to be used for grafting of photocrosslinkable groups. In the presence of photoinitiator(s), they were crosslinked under UV irradiation in order to obtain optical waveguides. The other family of polymer optical materials were obtained by copolymerization of perfluorodioxolanes with different fluorovinyl monomers. The fibres of the copolymers were flexible and transparent with a low refractive index (1.3350–1.3770 at 532 nm) and high Tg (100–145°C).

Various strategies have been focused on: (i) the radical telomerization of 3,3,3-trifluoropropene (TFP) with isoperfluoropropyliodide or diethyl hydrogenophosphonate to prepare $(CF_3)_2CF(TFP)_x$-R_H or CF_3-CH_2-CH_2-$(TFP)_y$-$P(O)(OH)_2$, and (ii) the radical cotelomerization of vinylidene fluoride (VDF) and TFP, or their controlled radical copolymerization in the presence of $(CF_3)_2CFI$ or a fluorinated xanthate. These strategies led to various highly fluorinated telomers whose chemical changes enabled to obtain original ionic and non-ionic surfactants as novel alternatives to perfluorooctanoic derivatives.

Novel fluorinated copolymers based on VDF were synthesized by iodine transfer copolymerization with hexafluoropropene and α-trifluoromethacrylic acid, either in solution or in emulsion. α,ω-Diiodoperfluoro alkanes were used as the chain transfer agents. According to their concentration in the feed, molecular weights ranged from 20000 to 220000 g/mol. Chemical modification of these fluorinated terpolymers led to original functionalized copolymers containing either sulphonic acid or benzimidazole functions which were processed into membranes for fuel cells, the properties of which were investigated.

8-O4. Photozyme-stimulated pesticide photodegradation

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Photozymes are amphiphilic copolymers forming macromolecular micelles with a core from hydrophobic and chromophoric monomer units and a shell from hydrophilic entities. Their preparation and photocatalytic activity are inspired by natural photosynthetic systems and antenna effect for light harvesting.

In the present work the following photozymes were prepared and tested: (i) xanthenes (fluoresceine and rose Bengal) bound to chitosan, (ii) phthalocyanine dyes and pigments bound to poly(styrene sulphonate-co-vinyl benzene chloride), (iii) heterogeneous photozymes composed by poly(styrene sulphonate-co-vinyl benzene chloride-co-vinyl carbazole) adsorbed on goethite. Their photooxidation efficiencies toward three different pesticide classes (atrazine, chlorpyrifos, and benomyl) were estimated and compared. It was shown that a 60% degradation of these pesticides was achieved by irradiation of their aqueous solution by solar light at usual temperature for less than 10 h in the presence of aforementioned photozymes. The most promising result for practice was obtained with chlorpyrifos for which a full photodegradation took place after 20 h irradiation only, if the photozyme, combining photocatalytic effects of phthalocyanine and xanthene chromophores bound to poly(styrene sulphonate-co-vinyl benzene chloride-co vinyl carbazole), was used.

The results obtained demonstrate a new possibility, based on photozymes, of solar light-stimulated purification of water contaminated by pesticides.

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8-O5. In vitro bioactivity of collagen/calcium phosphate silicate hybrids in the presence of glutaric aldehyde and chondroitin sulphate

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In the present study, novel hybrids of collagen (Coll) and calcium phosphate silicate (CPS) were synthesized. The CPS ceramic was prepared *via* polystep sol-gel method. The dissolution test of CPS ceramic was filled with 1.5SBF solution. FTIR spectroscopy showed that hydroxycarbonate apatite ($OHCO_3HA$) was observed after a 3-day immersion in 1.5SBF solution. Hybrids of C-CPS were produced from diluted in CH_3COOH collagen type I and ceramic powder of different ratios of C to CPS, 25:75 and 75:25 wt.%, in the presence of glutaric aldehyde and chondroitin sulphate. The synthesized hybrids were characterized by FTIR, XRD, SEM, and ICP-OES. FTIR spectroscopy indicated that the red shift of amide I could be associated with the finding that the collagen prefers to chelate Ca^{2+} from partial dissolution of the CPS ceramic. A growth of B-type of carbonate containing hydroxyapatite (CO_3HA) on the C-CPS hybrids soaked in 1.5SBF was observed. The negatively charged carboxylate groups from the collagen could be responsible for CO_3HA deposition. This fact was confirmed by the red shift of the carboxylate groups of collagen in the FTIR spectra. Formation of CO_3HA was observed by FTIR, XRD, and SEM.

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8-O6. Polymers from renewable resources: eco-friendly building materials

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The need to reduce the use of fossil fuel derived monomers in the manufacture of polymers is apparent because of the spiralling cost and high rate of depletion of the petrochemical derived stocks. This necessitates the investigation and use of natural and renewable sources, which can serve as alternative feedstock of monomers for the polymer industry. The synthesis of polymers from renewable resources has attracted the attention of many research workers in recent past because it substitutes for petrochemical derivatives. A renewable resource means agricultural products and one such agricultural product is cashew nut shell liquid (CNSL). The major components of CNSL are cardanol, cardol, anacardic acid, and 6-methyl cardol. The desired phenolic constituent of CNSL is cardanol. CNSL holds considerable promise as a source of unsaturated phenol, an excellent monomer for the polymer industry. In fact, cardanol and its derivatives can be converted to polymers with better processability, hydrocarbon solubility, and resistance to acids and alkalis than conventional phenol-based systems. This, to a certain limited extent, has led CNSL products to be used as building materials in the form of tiles, sheets, and even foams suitable for partitions and doors, resins and adhesives, varnishes and surface coatings, insecticidal products, anticorrosion paints, friction materials, and composite materials.

8-O7. The influence of high-density polyethylene added to ionic thermoplastic elastomer compounds based on maleinized ethylene-propylene terpolymer rubber

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This work studies the influence of high-density polyethylene on the characteristics of ionic thermoplastic elastomers based on maleinized ethylene-propylene terpolymer rubber (EPDM-g-AM). Ionic thermoplastic elastomers were obtained by processing elastomers containing ionisable groups, namely EPDM-g-AM, by introducing metal salts or polyvalent metal oxides, which can react with functional groups of ionisable molecules forming ionic fields as well as introducing fillers, ionic plasticizers, polyolefins, antioxidants, etc. From the results obtained it was noticed that upon increasing the amount of high-density polyethylene (HDPE) introduced in EPDM-g-AM blends, hardness, modulus, and tear strength increase while elasticity and residual elongation decrease. These effects prove that the properties of polymer blends depend on the characteristics of component polymers and on their molar ratios. The blend containing 80 phr polyethylene was selected, as it had the optimum values of hardness, modulus, tear strength and good values for tensile strength, elongation at break, and elasticity. This blend was used to make ionic thermoplastic elastomer granules in a laboratory extruder-granulator. The new types of granules were characterized and their functionality and the reproducibility of the technology by means of which they were obtained were demonstrated. They can be used to obtain new types of soles and top lifts for footwear, to make protection equipment, to obtain gaskets, hoses, conveyor belts which are resistant to concentrated acids and bases, etc.

8-O8. Predictive modelling and experimental measurement of biodegradable packaging films derived from renewable resources

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The properties of renewable resources are such that makes the material ideal for the purpose of daily routine activities, except a few problems, which can be overcome. Biodegradable plastics have aroused significant interest in the community today to use them as flexible packaging material. Studies have indicated that incorporation of starch into polyethylene renders it bio-disintegrable. Challenge as on date is to get the polyethylene film converted into biodegradable one by suitable filler.

Various compositions of starch with LDPE and LDPE-grafted maleic anhydride (1:1) having 0.5% grafting of maleic anhydride group were prepared and extruded in twin screw industrial extruder. The mixing of potato starch in different percentages was done.

Maintaining 110–140°C temperature extrusion was done and extruded samples were blown through blowing machine under temperature profile of 120 to 160°C and packaging film were prepared and tested.

The effect of particular filler starch on modulus and tensile strength was studied and practical results were compared with theoretical prediction of Nikolis and Narkis geometrical model and results are discussed.

8-O9. Quaternized chitosan-based electrospun nanofibrous materials with antitumour activity

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The use of electrospun micro- and nanofibrous materials as antitumour drug carriers is a promising approach to targeting delivery of the antitumour drugs, because they have numerous advantages, such as improved therapeutic effect, reduced toxicity, and convenience. The appropriate conditions for successful preparation of novel hybrid nanostructured materials by one-step electrospinning of mixed solutions of quaternized chitosan (QCh), poly(L-lactide-*co*-D,L-lactide) (coPLA) and antitumour drug doxorubicin hydrochloride (DOX) were found. *In vitro* cell viability studies revealed that the incorporation of DOX and QCh in the nanofibrous mats led to a significant reduction in the HeLa cell viability similar to that of free DOX. *In vivo* experiments against Graffi myeloid tumour showed that the local application of the nanofibrous mats containing both QCh and DOX in the tumour tissue showed suppression of the tumour volume and extension of the average survival time. Therefore, the prepared novel nanofibrous materials have excellent potential as antitumour drug delivery systems for local application in the treatment of solid tumours.

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8-O10. Monomer participation in the equilibrium between active and dormant propagation radical states of ATRP

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Atom transfer radical polymerization (ATRP) is an effective approach to macromolecular engineering. According to the mechanism of this controlled/living polymerization, proposed by Matyjaszewski, two states of the propagation radical, active (A) and dormant (D), were defined. The equilibrium between them, shifted to D, is conjugated with redox reactions of metal halide complex. It is noteworthy that the monomer does not take part in this equilibrium. However, detailed analysis of this peculiarity shows that two experimentally proved ATRP advantages are disputable: (i) the block-copolymer synthesis by ATRP is not possible after the full conversion of the initial monomer because of the transformation of the propagation radicals into dead chains through the termination reactions of A, (ii) the decrease of polymer polydispersity with conversion is not clear. In addition, it was established that the monomer reactivity ratios in the ATRP copolymerization and conventional one are different, though they should be the same for both copolymerizations if the aforementioned mechanism is true. It is shown that all three poor agreements with experimental data can be overcome by introduction of the monomer into the equilibrium reactions of A with D. It means chain propagation in each equilibrium reaction, in addition to that of the monomer interaction with A. By this way an original modification of the generally accepted ATRP mechanism is proposed, which describes the ATRP experimental data more adequately and fully.

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8-O11. Functionalization of polycaprolactone using glycidyl methacrylate in supercritical carbon dioxide for polycaprolactone-starch blend

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Plastic resistance to biodegradation causes serious environmental problems. Only limited amount of accumulated plastic waste can be reduced. The application of biodegradable plastics is an attractive solution for the problems related to the use of conventional plastics. Blends of starch and synthetic biodegradable polyesters, especially polycaprolactone (PCL), have been widely studied for the synthesis of fully biodegradable products. However, phase separation occurs upon blending of hydrophilic starch and hydrophobic PCL, which leads to undesired poor mechanical properties (e.g. tensile strength). A compatibilizer can be introduced in the blends to improve the interfacial association between these two polymer phases. In this work, we describe ternary blends of starch, PCL and a compatibilizer precursor obtained by grafting glycidyl methacrylate onto the PCL backbone (PCL-g-GMA). Two different approaches were used for the grafting process, normal melt processing and under supercritical CO_2. The latter is a green solvent widely studied in combination with polymer processing. Different functionalization degrees and compatibilizer intakes were used to investigate changes in mechanical properties of the blends. In addition, the ratio of PCL and starch is also systematically changed. GPC analysis of PCL-g-GMA shows that there was no degradation/cross linking during the reactions in supercritical CO_2. In contrast, changes were observed from the compatibilizer prepared in the melt. The use of compatibilizers improves the mechanical properties of the blends. The amount and functionalization degree of the compatibilizer did not significantly affect the mechanical properties. However, blends with compatibilizers prepared in supercritical CO_2 have better mechanical properties with respect to those with compatibilizers prepared in the melt.

8-O12. Impact of zinc oxide on the UV absorbance and mechanical properties of UV cured films

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UV curable adhesives are widely used in various industrial sectors, due to their distinct advantages mainly low energy consumption, high quality end products, room temperature operations, and solvent free formulations. Zinc compounds can provide a variety of properties in the plastic field. Zinc oxide is outstanding among white pigments for its property for absorbing UV radiations. In the present work, zinc oxide was added to epoxy acrylate based formulations, which were photopolymerized to form films. These films were analyzed for UV absorbance and mechanical properties such as tensile strength, hardness, percentage elongation, and tensile modulus. It was found that presence of zinc oxide has enhanced UV absorbance of these UV cured films and a remarkable improvement was observed in their mechanical properties.

8-O13. Synthesis of *n*-(dichlorophenyl)maleimides and thermostable copolymers on the their basis

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N-substituted maleimides (RMI) are multifunctional monomers for new polymer synthesis and polymer modification reactions. There has been great interest in development of copolymerization of halogen containing RMI. This work describes the synthesis and characterization of copolymers of N-(dichlorophenyl) maleimide (DCMI) with donor comonomers: N-(2,3-dichlorophenyl)maleimide (2,3DCMI), N-(2,4-dichlorophenyl) maleimide (2,4DCMI) and N-(2,6-dichlorophenyl)maleimide (2,6DCMI). They were synthesized by a two step reaction of maleic anhydride with 2,3-, 2,4-, and 2,6-dichloroaniline.

The radical copolymerization of DCMI with styrene, vinylacetate, and methylmethacrylate was investigated in 1,4-dioxane at 60°C using AIBN as an initiator. Monomer reactivity ratios r1 and r2 were determined by Kelen-Tüdös method.

The experimental data showed that the copolymerization of DCMI is alternating for DCMI-styrene, with alternating tendency for DCMI-vinylacetate, and random for DCMI-methylmethacrylate. The thermal properties of the obtained DCMI-copolymers were investigated by thermogravimetric analysis (TGA, 10°/min). It was found that they possess a higher thermal stability than the homopolymers of styrene, vinylacetate, and methylmethacrylate.

8-O14. Adaptive chemistry. 3. Bayesian approach to dynamer adaptive ability

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Dynamer (D) is a dynamic associate whose components (constituents, C) are molecules (macromolecules), linked through weak reversible connections and has therefore a capacity to modify its constitution by exchange and modification of its constituents. The number of the interconstituent bonds (IB) with which a given C takes part in the formation of D is a measure of its adaptive ability (A). In the present work the quantitative measures for A of C (Ai), dynamer biconstituent fragments (Aij), and of D as a whole (A_D) are defined. For this purpose the formation of IB between free active centres (AC) and those taking part in the formation of intraconstituent junctions are considered. In the latter case the destruction of such junctions passes ahead the IB formation. The Bayesian approach opens a possibility to divide the contributions of these two AC types, which extends our knowledge on the formation and stability of D. The conditional probabilities of IB formation for each C were determined if the junctions are only between non-intraconnected AC. In addition, the relationships for probabilities of IB formation between AC from different types were also deduced. Dependencies of these probabilities on A_D, Aij, and Ai are proposed, too. All these features were determined for two different regimes: spontaneous and progressive D formation. For the latter the algorithm for estimation of the different formation pathways is proposed.

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8-O15. Electrospinning of poly(L-lactide) and poly(L-lactide)/PEG in the presence of some bioactive substances

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New nanofibrous materials from poly(L-lactide) and poly(L-lactide)/poly(ethylene glycol) (PEG) with an incorporated drug: diclofenac sodium (DS), lidocaine hydrochloride (LHC), benzalkonium chloride (BC) or combinations thereof (DS/LHC or DS/LHC/BC), were prepared by one-pot electrospinning. The drugs utilized are organic salts capable to increase poly(L-lactide) and poly(L-lactide)/PEG spinning solutions conductivity. FTIR spectra evidenced that the corresponding drug(s) was/were incorporated successfully into the fibrous materials. The effect of the low molecular organic salts on polymer crystallinity was evaluated by DSC and XRD, and the surface elemental composition of the fibrous materials was determined by XPS. The hydrophilic/hydrophobic behaviour of the new materials was studied by measuring the water contact angle. SEM analysis showed that the fibrous materials consisted of fibres aligned preferably in direction of drum collector rotation. It was demonstrated that the use of a purposely designed multi-needle electrode enabled the self-bundling of the fibres. Release profiles of the incorporated drug were evaluated by UV-Vis spectrophotometry. The new fibrous materials exhibited antibacterial activity against the pathogenic microorganism *Staphylococcus aureus*, as evidenced by microbiological tests.

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8-O16. Studies on development of biodegradable formulation of natural rubber latex

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Natural rubber is a strategic raw material used in the manufacture of more than 40000 products, including over 400 medical devices. Although more than 2500 plant species are known to produce natural rubber, all commercially available natural rubber currently is harvested from a single species, *Hevea brasiliensis* (the Brazilian rubber tree). Primarily due to its molecular structure (cis-1,4-polyisoprene) and high molecular weight (>1 MDa) natural rubber has high performance properties, such as elasticity, resilience, heat dispersion, and abrasion resistance that cannot easily be mimicked by artificially produced polymers. Demand for natural rubber has increased throughout the twentieth century despite competition from synthetic rubber. In the present work, we attempted to make biodegradable inflatable ball bladders.

Natural rubber latex formulation was prepared. Dispersion of chemical additives was prepared and a mixer was prepared with natural rubber latex. Resin additive so prepared was added to natural rubber latex formulation. Samples were evaluated for physiochemical and biochemical changes.

8-P1. Preparation of cellulose ferrite micro- and nanocomposite materials

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Micro- and nanocomposite materials have been of fundamental importance in view of their unique properties and possibilities for applications. Wood polymer metal, metal oxide and ferrous magnetite containing micro- and nanocomposites of high electrical conductivity and microwave absorption properties for electromagnetic wave protection are especially perspective.

A synthesis methodology of new cellulose ferrite micro- and nanocomposites was developed and the properties of these materials were studied.

A new method of modification by a two-component system, Fe^{2+} and Fe^{3+} of microcrystalline cellulose, was developed. After defining the optimal synthesis conditions, the modified microcrystalline cellulose is used as a filler in a composite matrix. The composite materials based on modified microcrystalline cellulose and Fe_2O_3 (micrometer scale hematite), and binding component (polyurethane prepolymer) were prepared *via* pressing method. A number of characterization analyses as DSC, IR spectroscopy, water absorption, physicomechanical properties, and electro conductivity were performed.

8-P2. White top paper improvement by addition of modified fibrous materials

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Corrugated cardboard is the largest group of paper products over the world. Increasingly anonymous brown box is offset by good-looking multicoloured printed text, barcodes, and illustration package. This, of course, requires a white surface and coatings and, in the group of raw materials for corrugated cardboard, this is the area, which is developing quickly. The Duropack mill in Bulgaria produces multi-layers white top paper for liners and uses white wastepaper pulp grades for that.

The purpose of this study is to investigate properties improvement of white top liner by addition of modified fibrous materials from the production of disposable diapers.

Experiments were carried out by different types of waste paper pulp delivered from Duropack Trakia SA (Bulgaria). Modified fibrous materials consist of polymer and super absorbent polymer, which have a clear retention effect. These polymers are now commonly made from the polymerization of acrylic acid blended with sodium hydroxide in the presence of an initiator to form a polyacrylic acid sodium salt (sometimes referred to as sodium polyacrylate).

The modified fibrous materials charge up to 5% lead to best results of the paper prepared by secondary fibrous materials and cationic starch. The pulp strength properties tear index, breaking length, and the brightness of the top layer are visibly improved.

The obtained effects are probably due to the retention action and morphology of the modified fibrous materials. By adding modified fibrous materials, it is possible to reduce the cost of the bleaching agents, retention additive, and starch, which affect positively the production costs.

8-P3. Research on accelerated thermal ageing of printing papers

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Written works, created nowadays, should be saved for the coming ages and in the mean time writings, archives and works of art from the past should be preserved for longer time.

A research on kinetic relations during accelerated ageing of printing and writing papers was conducted. Four kinds of papers were studied: offset paper 60gsm, 70gsm, 80gsm, and two side coated matt 80gsm. The samples were subjected to accelerated thermal ageing at 105 and 120°C. Then variations of optical properties (brightness, colour parameters, reflection curve with different light sources), physicomechanical properties (mostly double folding resistance), and acidity (pH) were studied. The following important conclusions were made.

The optical properties of printing paper are getting worse after accelerated thermal ageing.

Graphical curves of studied optical parameters (brightness and yellowness) are changing equally at both 105 and 120°C, which is evidence that processes with different kind of papers are accomplished according to the same mechanism. Test data show that the brightness is most significantly decreased during the first six hours of experiment.

The physicomechanical parameters are getting worse during the process of accelerated ageing. Most expressive for these changes in the papers is the ‘double folding’ parameter. Because of ageing, the fibres lose their elasticity and become more fragile.

The acidity of papers is getting higher with time, which causes a decrease in pH, thus accelerating the process of ageing.

8-P4. Synthesis and characterization of hybrid materials based on polyvinyl alcohol (PVA)/tetraethyl orthosilicate (TEOS) with embedded silver nanoparticles (AgNps) and their application for purification of wastewater

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Novel hybrid material thin films based on polyvinyl alcohol (PVA)/tetraethyl orthosilicate (TEOS) with embedded silver nanoparticles (AgNps) were synthesized using a sol-gel method. Silver nanoparticles in PVA/TEOS matrix were prepared by reduction of the silver ions using thermal annealing of the films. TEM images clearly demonstrated the formation of spherical silver nanoparticles of size ranging form 5 to 7 nm, which were homogeneously distributed in the PVA/TEOS matrix The successful incorporation of the silver nanoparticles was confirmed using EDX analysis, by exhibiting a peak at approximately 3 keV, which is typical of the absorption of metallic silver nanocrystallites. The formation of silver nanoparticles was also evidenced by means of UV-Vis spectroscopy through the appearance of strong absorption bands at 420 nm. The obtained PVA/AgNps/TEOS hybrid films showed improved thermal stability as demonstrated by TGA analysis in comparison to the pure polyvinyl alcohol. Further, PVA/AgNps/TEOS films were used for immobilization of cells of *Trichosporon cutaneum R57*, which are capable of removing metal ions from aqueous solution. The influence of silver nanoparticles on metal ions removal was also examined.

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8-P5. Solubility parameter of materials: a QSAR study

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The solubility parameter, δ (sigma), plays an important role for determination of the fundamental properties of material like polymers. To predict this parameter a quantitative structure activity relationship (QSAR) model is generated for a set of 51 polymers. A repeating unit of these polymers was used to calculate the quantum-chemical parameters. In this reference, quantum-chemical descriptors were used to model the parameter encode information about the electronic structure of the molecule and thus implicitly account for the cooperative effects between functional groups, charge distribution, and possible hydrogen bonding in the polymers. As it is impossible to measure the solubility of polymers directly due to reason like value obtained from different approaches span a wide range, polymers have wide distribution of molecular weight and possess high molecular weight. Therefore, this field requires new approaches to predict solubility of polymers. In this regard, the QSAR approach can play a significant role. Various parameters like topological, physiochemical, connectivity indices, and other quantum chemical parameters were tried and best one derived to model the parameter. A model generated by this approach provides a good QSAR to predict the solubility parameter. A four-parametric QSAR model was used to predict δ with a good quality factor and less standard error than earlier reported model for the parameter. The model provides a variance of 90.37% (or regression coefficient $R^2 = 0.9037$) which is much better than reported one by other authors. The model is easier to apply with good predictive capability.

8-P6. Ultrasonic synthesis and photophysical properties of perylene derivatives for application as active layers for organic solar cells

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Being soluble in organic solvents perylene derivatives are effectively used as reducers in the active layers of solar cells. Three alkyl substituted perylene derivatives of high yields and purity have been synthesized regarding such an application. They were obtained by ultrasonic synthesis, which, if compared to conventional methods of perylenes preparation, took less time, proceeded at a lower temperature, and resulted in higher yields and purity of the products. The newly synthesized perylene derivatives were proven and characterized by NMR and IR spectroscopy.

The basic photophysical characteristics of the c perylene compounds were studied in organic solvents of various polarities as well as in the solid state as a thin nanosized layer. It was found that in organic solvents the perylene derivatives absorb in the 450–480 nm range and emit intensive fluorescence with a maximum at 560–580 nm. Their colour characteristics were preserved in the solid state. The new materials were proven to be photostable and reliable for application as an active layer in solar cells.

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8-P7. Magnetic treatment of paper furnish for sack paper production

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Annually worldwide paper and board production exceeds 370 mil t. 40% are paper and board for packaging. Sack papers are in these types of papers. It should have good paper structure, high strength, and elasticity with certain hydrophobic properties and excellent printing properties without dusting. For achieving these purposes, several wet-end chemical additives are used. Magnetic treatment of fluids in paper production is technically comfortable and environmentally friendly but it cannot replace the suitable wet-end chemical additives. Their combined usage is an interesting field for examination.

The aim of the present study was to investigate the influence of magnetic treatment on the sack paper furnish behaviour in dependence of anionic high-molecular weight polyacrylamide (Percol$^{®}$156) quantity at constant consumption of other system components. For straightening out the interaction, flocculation volume and sedimentation index of paper furnishes were determined as well as their dewatering ability. The conductivity and turbidity of the white waters were also studied. Beside indirect results for retention, the real parameters of retention were determined by the Britt method. Experimental results showed a positive influence of the magnetic treatment on the behaviour and the properties of paper furnish for production of sack papers. On increasing the retention additive Percol$^{®}$156 consumption the furnish properties were improved: dewatering was quickened, white waters were clarified, and retention was enhanced.

8-P8. Synthesis and characterization of SiO_2/cellulose derivatives nanomaterials for *Trichosporon cutaneum R 57* immobilization

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The purpose of the present work was to clarify the preparation of nanoscale hybrid materials by sol-gel method and to examine their characterization and application. The synthesized materials were based on different silica precursors (TEOS, TMOS, ETMS, and MTES) and cellulose derivatives like methyl cellulose (MC), hydroxypropyl cellulose (HPS), and hydroxypropyl methyl cellulose (HPMC). The phase state and structure of the new nanomaterials was determined by X-ray diffraction (XRD) and infrared (IR) analysis. XRD patterns showed that all nanomaterials had an amorphous nature. IR spectra of the obtained materials showed typical bands of silica at ~1080, 950, 790, 560, and 460 cm^{-1} and of organic components at ~1640 and 1460 cm^{-1}. The pore size and specific surface area were determined by BET analysis and the results suggested that on increasing cellulose derivatives content the specific surface area was decreased while the pore size was increased. The surface topography and morphology was investigated by AFM and SEM analysis.

A silicate synthesized by sol-gel process is a porous material having pores large enough to allow diffusion. The pore size can be easily controlled during the sol-gel process by changing several conditions such as pH, aging time, and mixing procedure. These properties are useful for immobilizing biomolecules while retaining their biological activities and allowing bioreactions to proceed inside the matrix.

The synthesized sol-gel nanomaterials were used for immobilization of cells of filamentous yeast *Trichosporon cutaneum R57* with ability of metal ions removal. Two different techniques of immobilization were used: by attachment and by entrapment. The encapsulation of whole yeast cell within sol-gel silica matrices enhanced their stability in various organic solvents.

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8-P9. Design of amphiphilic star copolymers with a calixarene core

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Recent advances in controlled radical polymerization open new prospects for the design of complex nanostructures. Association of copolymers in solution is one of the routs to achieve desired supramolecular architectures.

The present communication reports on the synthesis of calixarene-based amphiphilic star copolymers and on the results of studies on their self-organization. A full characterization of the copolymers and the nanoparticles is reported, there preparation being performed by means of solutions of selected solvents.

It was established that the calixarene-based star copolymers self-aggregate into various architectures predetermined by different functionalization of the calixarene core. Functionalization allows tailoring particular properties of the copolymers regarding their versatile applications.

8-P10. New synthesis of functional copolymers containing stable tempo radicals

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First method. Alternating multifunctional copolymers of maleic anhydride (MA) with electron donating comonomers: styrene, acrylic acid, vinyl acetate, vinyl butyl ether, vinyl-2-pyrrolidone (VP) (1–5) were prepared by radical-initiated copolymerization in solution at 60 or 70°C. By polymer analogous reactions in DMF at 60°C (N-acylation) of the obtained MA-copolymers (1–5) with 4-amino-2,2,6,6-tetramethyl piperidine-1-oxyl (A-TEMPO) new functional copolymers, containing stable nitroxide radicals, were prepared.

Second method. TEMPO-functionalized copolymers of VP were prepared through reactions between 4-amino-2,2,6,6-tetramethyl piperidine (A-TEMP) and A-TEMPO and carbonyl chloride groups. The reactive copolymers (6) were prepared by free radical copolymerization of VP with methacryloil chloride (MAC) in THF solution at 60°C. Reactivity ratios (KT-method) were as follows: r_1=0.07 and r_2=0.22. By polymer analogous reactions of poly(VP-co-MAC) with A-TEMPO in DMF copolymer (7) was prepared containing stable TEMPO radicals.

A new monomer piperidine methacrylamide (8) was prepared through direct reaction between MAC and A-TEMPO. A polymerized product (9) with pending TEMPO groups was prepared and through oxidation in H_2O_2 solution gave a copolymer of VP (7) containing stable TEMPO radicals.

The structure of the new polynitroxides (1-5) and (7) was investigated by ESR and FTIR spectroscopy.

8-P11. Ultra filtration polymer membranes with modified surface

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A study of the efficiency of plasma-chemical surface modification by phase-inverse method of ultra filtration membranes, made by triple PAN co-polymer, aimed at increasing membrane productivity at a given selectivity is presented. The effect of both barrier discharge intensity and treatment duration on membrane characteristics was studied. A parallel investigation of two-type plasma-chemical modification was carried out, namely: (i) in barrier discharge at atmospheric pressure in air in a diode system and (ii) in magnet-stimulated barrier discharge under the same conditions.

It was found experimentally that these two types of barrier discharge significantly increase water productivity at certain selectivity of the membranes. The magnet-stimulated barrier discharge treatment was accompanied by an insignificant selectivity decrease (about 5–6%) but without change of the general positive effect.

Two-border treatment regimes were clearly distinguished at the studied ultra filtration membranes: at low intensity of the barrier discharge combined with short treatment duration and at high intensity of the barrier discharge combined with long treatment duration. The membrane surface ion activity change was accompanied by additional plasma-chemical activation with the former regime and by surface etching with the latter regime. Another regime passing at the barrier discharge treatment was demonstrated giving a possibility of effective control of the membrane surface properties.

8-P12. Complexes of rice husks ash with heavy metals as catalysts for oxidation

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The method of thermal treatment of raw rice husks helps to solve disposal and pollution problems of the rice milling industry and gives excellent starting materials for preparation of advanced high-quality ceramic powders, such as silicon carbide, silicon nitride, and magnesium silicide, which can be successfully applied to high temperature material engineering, especially in turbine engines. In addition, small amounts of pure silica powder can be widely used for production of high purity elemental silicon for electronics and as adsorbent, catalyst support, thixotropic agent, thermal insulator, rubber and plastics filler, etc.

The aim of the present investigation was to prepare new metal-immobilized complexes based on rice husks and to study their catalytic activity in the oxidation of cyclohexene by tert-butylhydroperoxide.

The corresponding metal complexes were prepared by interaction of raw (RRH) or thermally treated black (BRHA) and white (WRHA) rice husks in nitrogen or air with aqueous solutions of various salts. A commercial product, Aerosil A200, was also used. The rice husks supported metal complexes were identified by FTIR and EPR analysis. The structure of the iron-containing polymeric materials was evaluated by Mössbauer spectroscopy. A possible structure of the complexes is suggested.

The catalytic activity of the molybdenum-containing complex catalyst in the principal epoxidation reaction was higher than that of the vanadium-containing one, whereas an opposite order of activities was found for the side reaction of allylic hydroxylation of cyclohexene. Under selected reaction conditions, the yields of the main reaction products, cyclohexene oxide (1,2-epoxycyclohexane) and 2-cyclohexene-1-ol, were 56.4 and 12.0%, respectively.

8-P13. Hybrid nanofibrous yarns based on N-carboxyethylchitosan and silver nanoparticles with antibacterial activity

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Hybrid nanofibrous materials consisting of yarns from N-carboxyethylchitosan (CECh) and poly(ethylene oxide) (PEO) that contain silver nanoparticles (AgNPs) were prepared by electrospinning [1]. $AgNO_3$ concentration was selected to be 0.02 mol/L or 0.04 mol/L in order the content of the AgNPs in the electrospun nanofibres to be 5 or 10 wt.%, respectively. The self-bundling of the fibres into yarns with a mean diameter of ca. 35 μm was enabled by using a grounded needle electrode. The reduction of the Ag^+ ions to Ag^0 was evidenced by UV-Vis spectroscopy, XRD, and XPS. TEM analysis revealed that AgNPs formed at a $AgNO_3$ concentration of 0.02 mol/L were uniformly distributed within the fibre with a mean diameter of 4±0.5 nm. The increase of $AgNO_3$ concentration to 0.04 mol/L led to preparation of AgNPs with a higher mean diameter as well as to aggregate formation. Studies of the antibacterial activity of CECh/PEO/AgNPs fibrous materials against *Staphylococcus aureus* showed that the mats exhibited bacteriostatic or bactericidal activity at a AgNPs content of 5 or 10 wt.%, respectively.

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1. H. Penchev, D. Paneva, N. Manolova, I. Rashkov, Carbohydr. Res. 345 (2010) 2374.

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8-P14. Preparation, physicochemical characterization and *in vitro* cytotoxicity of poly(butylcyanoacrylate) nanoparticles simultaneously loaded with daunorubicin and 5-fluorouracil

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The present investigation deals with the preparation, characterization, and preliminary *in vitro* evaluation of poly(butylcyanoacrylate) nanoparticles, co-loaded with daunorubicin and 5-fluorouracil during *in situ* anionic polymerization. Drug-loaded nanoparticles were characterized by PCS (size and size distribution) and electrophoresis (zeta potential). The inclusion of Dau and 5-FU in the polymer matrix of nanoparticles was verified by ^{1}H NMR and ^{19}F NMR analyses. The biological experiments were performed on cultured human tumour cell lines 8MGBA (glioblastoma multiforme) and HeLa (cervical carcinoma). For evaluation of the cytotoxic effect of co-encapsulated in nanoparticles drugs on treated cell cultures MTT test was used.

The results obtained demonstrate time and concentration dependent activity of the tested compounds. The cytotoxic assay used for evaluation of cytotoxic effects shows different sensitivity of the human tumour cell lines used toward tested drug combinations. The human tumour cell line HeLa is more sensitive to low concentrations while the human tumour cells 8MGBA are more sensitive to higher concentrations applied.

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8-P15. Nonlinear elasto-viscosity of rubbers at large deformations

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In this work, two compositions were examined: butadiene-nitrile rubber and polyisoprene rubber. Instantaneous stress-strain and vice-versa relations at large deformations were derived in analytical form. These relations were obtained by resolving algebraic equations of third and fourth degree, respectively. The Neo-Hookean and the Mooney-Rivlin models were used concerning thermodynamic potentials. Aforementioned analytical solutions were incorporated in the hereditary integral equations of Volterra to predict the creep and relaxation of such materials at large deformations. One takes into account the physical non-linearity of the viscous behaviour in the presence of similarity in the isochrone stress-strain curves. As kernel in the hereditary integral equations, the singular kernel of Koltunov was used, this describing well the high strain rate at the beginning. Only one restriction in the theoretical developments was involved concerning rubber incompressibility. Our theoretical results were compared with experimental data on two kinds of rubbers and demonstrated very good coincidence.

8-P16. Textile material combining chemisorption with optical sensor properties for metal ions in water solution

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The aim of this work was to develop a textile material possessing the ability to adsorb metal ions from water and having properties of optical sensor for these ions.

A new water soluble 1,8-naphthalimide dye was synthesized and characterized. Its fluorescent properties are pH dependent and its fluorescent emission is quenched at alkaline pH. The dye comprises a receptor fragment for binding metal ions dissolved in water. This process followed up the changes in the fluorescent emission induced by photoinduced electron transfer effect.

The textile material was initially treated with chloroacetyl chloride. The presence of new reactive groups in cellulose fibres after this treatment was confirmed by FTIR spectroscopy. Two coloured textile cotton materials with different fluorescent properties were obtained by applying the new 1,8-naphthalimide dye on the modified cotton: (i) material, dyed at pH = 5, showing a decrease of its fluorescent emission in the presence of cuprum cations, and (ii) material, dyed at pH = 8, showing an increase of its fluorescent emission in the presence of cuprum cations. The possible interaction between 1,8-naphtalimide dye and functionalized cotton cellulose is through a covalent bond.

It can be supposed that the textile-bonded fluorescent 1,8-naphthalimide dye has different properties depending on the interactions between dye and fibre. Probably in the former case, dyeing at pH = 5, the dye sensor fragment reacts with the functional groups of the modified cellulose thus changing metal ion coordination. In the latter case (dyeing at pH = 8) the sensor fragment is free and the dye retains its sensor properties in the dissolved state.

8-P17. Synthesis, properties, and application of peptide-based hybrid copolymers

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Combining biopolymer elements and synthetic polymers into a single macromolecular conjugate is an interesting strategy for synergistically merging the properties of the individual components and overcoming some of their limitations.

Hybrid copolymers in this study were synthesized *via* controlled ring-opening polymerization of N-carboxyanhydride of Z-L-lysine (Z-L-Lys-NCA) initiated by temperature-sensitive amino-functional macroinitiators. Ammonium-mediated ring-opening polymerization described by Dimitrov and Schlaad was applied to obtain copolymers of controlled molar-mass characteristics and functionality. The copolymers obtained were characterized by several methods such as gel permeation chromatography (GPC), NMR, and UV-Vis spectroscopy. The formation of block copolymers with monomodal molar mass distribution was proved by GPC analysis. ^{1}H NMR was used to determine the degree of polymerization of the polypeptide block.

Thermodynamic properties such as enthalpies of melting and crystallization of the synthesized copolymers were studied. A two-stage mechanism of thermo-oxidative destruction was observed.

The potential application of peptide-based hybrid copolymers as carriers for biomacromolecules was demonstrated through a complexation with DNA. Appropriate conditions for the formation of stable polyelectrolyte complexes (polyplexes) with average diameters in the 100 nm range were found. Furthermore, the cytotoxicity of the hybrid copolymers and the polyplexes was assessed.

8-P18. Control of the permeability of polymer membranes through modification by thermoresponsive polymer

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Thermoresponsive copolymers based on polyvinyl alcohol have been used in modification of ultrafiltration polyacrylonitrile (PAN) membranes. Two methods of modification were applied: (i) modification of preformed ultrafiltration PAN membrane, and (ii) modification during membrane formation. In the former method, the basic ultrafiltration membrane has been obtained based on the PAN and butadiene-nitrile rubber followed by introduction of the thermoresponsive copolymer into the membrane pores and its crosslinking with glutaraldehyde. In the latter method, the thermoresponsive copolymer has been added to the polymer solution used for membrane casting. Series of composite ultrafiltration membranes have been obtained and characterized by using FTIR spectroscopy, scanning electron microscopy, and differential thermal analysis.

The former approach aims at obtaining a membrane of well developed macroporous structure suitable for incorporation of high molar mass thermoresponsive modifier.

The latter modification approach involves introduction of the thermoresponsive copolymer directly into the membrane forming PAN solution. In this case, lower molar mass poly(vinylalcohol-co-vinylacelal) of phase transition temperature of 29°C was used. The values of the permeability and selectivity measured showed that at temperatures over the phase transition temperature the higher the amount of the thermoresponsive copolymer introduced, the higher the permeability. At the same time, the selectivity of the modified membranes was preserved.

8-P19. Development of surface properties on leathers and fur skins by using nanosilver-based materials

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Nanosilver-based materials are already used for medical devices and textile treatment with the aim of transferring bactericidal properties as alternative to chemicals used in macro concentrations and exhibiting adverse effects. The use of nanomaterials for leather and fur treatment is almost unknown and opens an interesting area of research in leather and fur skin processing industry. Our experiments were focused on designing different nanomaterials with affinity to collagen and keratin and selection of suitable processing treatment with the final purpose to develop surface properties regarding advanced resistance to fungus attack. The novelty of the research refers to the selected materials based on nanosilver, such as nanosilver deposited on titanium dioxide or doped polyurethane, treatments of collagen and keratin supports and strong resistance of some variants to bacteria and fungus. Assessment of the main surface properties of leathers treated with nanomaterials was carried out by using AFM, XPS, fungus, and bacteria tests and has allowed understanding the relationship between nanomaterials characteristics upon interaction with leather and the surface properties.

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9-K1. Application of nanotechnologies and nanomaterials

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In the present report, we give a brief description of the present state, development, and application of nanotechnologies (NT) and nanomaterials (NM) in some key industries, such as chemical industry and power industry (nanocatalysts, and nanocatalysis, hydrogen storage and fuel cells, artificial photosynthesis and Gratzel's cell, energy efficiency, energy storage); fabrication of consolidated nanostructures (ceramic nanomaterials, nanostructured coatings, production of low-combustibility plastics, nanostructured hard materials, nanostructures with colossal magnetoresistance); fabrication of ultra-high strength carbon fibres; nanotechnologies for environmental protection (adsorption of heavy metals by self-ordered self-organized nanostructure ensembles, photocatalytic purification of liquids, fabrication of mesoporous materials, application of nanoporous polymers for water purification, nanoparticles and environment); medical applications; military applications and fight against terrorism; household applications; energetic and some other [1–7].

In 2010, the European Union and the governments of the USA and Japan each invested over $ 2 billion in nanoscience, which is ample evidence to substantiate the claim that the 21st century will be the century of nanotechnologies. Some of the optimistic forecasts predict that in 2014 the total revenues from NT will exceed those brought by the information technologies and telecommunications combined. At present, more than 800 companies are involved in R&TD in this field (including giants such as Intel, IBM, Samsung, and Mitsubishi) while more than ten Nobel prizes were awarded for research in nanoscience.

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9-O1. Plasma chemical synthesis of multicomponent nanopowders, their characteristics, and processing

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The improvement of parameters of functional and construction materials and the development of new materials is closely related to wide application of nanosized powders and their particulate multicomponent composites as well as with detailed studies of their characteristics and processing. Owing to an increasing importance of nanoparticles many preparation methods have been developed, including mechanochemical and several liquid phase and gas phase techniques. Among these methods, a plasma technique based on the formation of products from a vapour phase provides an attractive alternative for producing multicomponent compounds or particulate composites due to mixing of components at a molecular level and relatively high production rate of a simple one-stage process.

Plasmachemical synthesis has been applied successfully to produce nitride-metals, nitride-carbide, nitride-oxide, oxide-oxide, oxide-metals by introducing and evaporation of coarse-grained commercially available powders of chemical elements, oxides, and salts in nitrogen or air plasma.

Specific surface area and average particle size of powders in the range of 20–90 m^2/g and 10–100 nm, respectively, were determined depending on synthesis parameters, cooling rate of the products, and their chemical and phase composition.

The high activity, regular particle shape, and homogeneity of the produced powders allow the manufacture of dense materials with fine-grained microstructure by using pressureless sintering, hot pressing, or spark plasma sintering techniques.

9-O2. Electronic polarizability, optical properties and chemical bonding of oxide glasses

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The current status of the polarizability approach to glass science has been considered. Four groups of oxide glasses have been established: glasses formed by two glass-forming acidic oxides; glasses formed by glass-forming acidic oxide and modifier's basic oxide; glasses formed by glass-forming acidic and conditional glass-forming basic oxide; glasses formed by two basic oxides. The role of the electronic ion polarizability, $\alpha_{O2-}(n_o)$, as well as of the average single bond strength, $B_{M–O}$, as basic parameters of linear and nonlinear optical properties of oxide glasses has been emphasized. More acidic glasses possess large $B_{M–O}$ (450–350 kJ/mol) which means participation of an average oxide ion in more covalent M–BO (bridging oxygen) bonds such as P–O, Si–O, and Ge–O. The decrease of $B_{M–O}$ could be attributed to formation of M–NBO (non-bridging oxygen) or other bonds with increased ionicity such as La–O, Pb–O, etc. The smallest values of $B_{M–O}$ at about 250 kJ/mol have been obtained for basic tellurite and bismuthate glasses. It has been assumed that these values could be associated with the presence of Te–NBO, Te–BO, and Bi–BO chemical bonds with large ionic contribution. The results obtained probably provide a good basis for prediction of the type of bonding in oxide glasses based on refractive index as well as for prediction of new nonlinear optical materials.

9-O3. Contemporary possibility for utilization of waste vulcanisates

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The generation of used tyres in developed countries is estimated at 6 kg per person per year and, taking into account that the number of cars in developing countries is increasing, the valorisation of this waste material will solve an important environmental problem. The routes for valorisation of used tyres and their economic viability have been the subject of analysis and, furthermore, this has been encouraged by public administrations due to the ever-increasing need for recycling components of automotive waste.

The aim of this study is to present a contemporary possibility for utilization of waste protected vulcanisates.

The reuse of scrap tyre as a very finely ground crumb (granulated rubber) combined with virgin elastomer compounds has limitations due to loss in physical properties and performance. Furthermore, the use of tyres as fuel in cement mills must be strictly controlled due to the atmospheric pollution caused by zinc oxide, dioxins, and polynuclear aromatic hydrocarbons. Considering the lower environmental impact, the use of tyres (particularly as crumb) and asphalt as an additive to cement-based materials for road construction seems to be a promising application. By comparing different options of available disposal, thermal destruction has a promising future because it allows recovering of valuable materials. In general, such products are: char (33 wt.%), gas (20 wt.%), oil (35 wt.%), and metallic residue (12 wt.%). Future exploitation of a tyre thermal process at large scale requires marketing of the products obtained, which has encouraged numerous studies aimed at finding possible applications. Thus, char may be converted to activated carbon, reused as carbon black in the manufacture of new tyres, or used for blends with bitumen to improve the rheological properties of the latter. The oil can be used as a fuel in conventional furnaces and the residual heavy fraction can be utilized as a plastifying material in a different formulation of rubber and for modifying the rheological properties of asphalts. The non-condensable gas, having a heating value of the order of 42 MJ/m^3, is mainly composed of light hydrocarbons (olefins and C_1-C_4 paraffins) together with H_2, CO, CO_2, H_2S, etc., and hence it can be used to heat the reactor of the thermal process.

9-P1. Radio-frequency inductively coupled plasma-chemical installation for preparation of nanodispersed powders

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The wide application of radio-frequency inductively coupled plasma (rf-ICP) is due to the following. Rf-ICPs are clean because these types of plasma do not use any electrode and, hence, are contamination free. Rf-ICPs are stable and can be used over a wide range of operating conditions. They have relatively large volumes and low plasma velocities, which result in complete melting of the solid materials in materials processing because of the longer residence time. The preciseness of the rf-ICPs is important in determining contamination effects (which inevitably occur because of electrode evaporation and nozzle ablation) on gas circuit breaker arcs as well as to predict plasma properties for all materials processing, and any gas or mixture of gases can be excited by the rf fields, so there is wide flexibility when choosing plasma gas(es) depending on the type of application [1].

The experimental plasma set-up used for the production of nanosized powders (carbides, carbon nanostructures (nanotubes, fullerenes), oxides, nitrides, catalysts, pigments, etc.) consists of a radio-frequency generator (maximum power 60 kW, frequency 1÷30 MHz), a water-cooled quartz plasma-chemical reactor with inductor, raw powder and gas supply systems, a gas quenching device, heat exchangers and cloth filter for powder collection. Ar, N_2, Ar+N_2, air, air+O_2, and Ar+H_2 can be used as plasma-forming gases. The quenching gases are air, Ar, N_2, and CO_2. The raw powder is injected into the upper part of the plasma-chemical reactor. A chemical reaction is carried out in the reactor and after complete evaporation of the micron size powder, it enters the quenching device. After that, the nanosized product is captured by the heat exchangers and cloth filter.

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9-P2. Element distribution coefficient in the pyrometallurgical manufacture of agglomerate from manganese concentrate and waste vanadium catalyst

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Laboratory and semi-industrial experiments for pyrometallurgical manufacture of agglomerate from manganese concentrate from Obrochiste deposit (Bulgaria) and deactivated vanadium catalyst in a Tamman furnace and electric arc furnace were implemented. Carbon, aluminium and also silicon plus aluminium were used as a reducing agent. Element distribution coefficients of elements between the metal and the slag phase for vanadium, manganese, iron, silicon, calcium, potassium, aluminium, and magnesium were calculated.

10-K1. Feed properties impact on a fluid catalytic cracking unit: key issues in a diesel market

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Nine heavy vacuum gas oils having different hydrocarbon compositions and different distillation characteristics have been cracked in a fluid catalytic cracking microactivity unit with the aim to determine which feedstock characteristics have impact on diesel (light cycle oil) yield maximization. While it was shown that maximum gasoline yield and the conversion at which gasoline is at maximum depend on fluid catalytic cracking feed hydrocarbon composition the maximum light cycle oil yield and conversion at which light cycle oil is at maximum was found to be independent of feed hydrocarbon composition. The fluid catalytic cracking feedstock parameter that showed to have impact on the maximum light cycle oil yield and the conversion at which light cycle oil is at maximum was the diesel fraction content in the fluid catalytic cracking feed. The lower the diesel fraction content in the feed the higher net diesel yield and the higher conversion at which light cycle oil yield is at maximum was observed. Hydrotreatment of the fluid catalytic cracking feed was found to lower the light cycle oil yield. Increasing the fluid catalytic cracking feed conversion showed to decrease the light cycle oil cetane index. The increase of conversion leads to lowering the low value slurry yield but also deteriorates the light cycle oil quality. This implies that hydrotreatment is always necessary before blending this fraction into the final diesel pool.

10-O1. Synthesis and photophysical properties of fluorescence sensing diester-terminated 1,8-naphthalimide

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The immediate detection and determination of environmental pollutants have been gaining particular importance. In recent years, extensive research has been carried out on fluorescent organic compounds whose photophysical properties are sensitive to environmental changes. Such interest is due to the possibility of tailoring the design of molecular devices for environmental pollution caused by heavy and transition metal ions. Photoinduced electron transfer (PET) using the 'fluorophore-spacer-receptor' format, developed by de Silva, is one of the most popular approaches to the design of fluorescent sensors.

This work reports the synthesis and sensor activity of a 1,8-naphthalimide sensor based on the 'fluorophore-spacer-receptor' format. The diester-terminated 1,8-naphthalimide was found to display sensitive fluorescence signal amplification over a wide pH scale, which has been ascribed to a photoinduced electron transfer from the tertiary amine receptor to the fluorophore. From the changes in the fluorescence intensity, a pKa value of 4.42 was determined, making the synthesized compound of potential use as pH chemosensing material.

In addition, the ability to detect ions has been evaluated in DMF by monitoring the quenching of the fluorescence intensity. Different ions have been tested: Zn^{2+}, Ni^{2+}, Pb^{2+}, Co^{2+}, Cu^{2+}, and Fe^{3+} for this purpose. The results have clearly shown that only Fe^{3+} could be efficiently detected.

10-O2. Dependence of FCC catalyst selectivity on feed hydrotreatment

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Heavy vacuum gas oil and its hydrotreated counterpart have been cracked in a laboratory microactivity test (MAT) unit and in a commercial fluid catalytic cracking (FCC) unit. The increase of conversion in both the MAT and the commercial FCC units during cracking of the hydrotreated VGO was only 2%. The data generated in laboratory showed that the catalyst activity and gasoline selectivities were higher when hydrotreated feed was cracked at the expense of lower selectivities of dry gas, heavy cycle oil, and coke. No change in LPG selectivity was observed. Commercial data indicated that the FCC feed hydrotreatment increased the LPG yield and iso-butane/butylenes ratio. Gasoline selectivity was not changed when both feeds were cracked in the commercial FCC unit. The diesel yield obtained during the hydrotreated VGO cracking in the commercial FCC unit was by 4% higher. Commercial and laboratory data demonstrated the same delta coke, which was 20% lower when the hydrotreated feed was cracked. Because of their technological differences, the two units, laboratory MAT and commercial riser FCC, showed different trends in catalyst selectivity when hydrotreated and unhydrotreated feeds were cracked. The laboratory MAT unit is equipped with a fixed bed reactor, whereas the commercial FCC unit has a riser upward reactor.

10-O3. A novel PET-based fluorescent sensor for protons and transition metal ions

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Fluorescent chemosensors are of great importance in chemistry, biology, and medicine in the last years. By their intensive naked-eye detectable fluorescent signal and high selectivity, they allow immediate detection of different compounds *in vivo* and in the environment. Fluorescent sensors based on photoinduced electron transfer (PET) consist of a receptor fragment attached to a fluorophore (signal fragment) via spacer. 1,8-naphthalimide derivatives are fluorophores of excellent photophysical characteristics and could successfully serve as signal fragment in fluorescent chemosensors.

In this work we report on the design, synthesis and sensor properties of a novel PET sensor molecule based on 1,8-naphthalimide fluorophores. The novel compound was designed according to the 'fluorophore-spacer-receptor' model, where 4-phenoxy-1,8-naphthalimide moiety is the fluorophore and a tertiary amine is the receptor fragment. As expected, the compound showed high fluorescence enhancement in acidic media. In addition, the influence of metal cations (Zn^{2+}, Ni^{2+}, Pb^{2+}, Co^{2+}, Cu^{2+}, Fe^{3+}) on the fluorescence intensity was recorded. The results clearly show that the novel molecule is an appropriate candidate for detection of transition metal ions.

10-P1. Mathematical modelling and optimization of extractive desulphurization of light cycle oil

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World environmental regulations become more stringent. Since 2010, the allowed sulphur content of diesel in Bulgaria has been 10 ppm. Diesel fuel and gasoline with less than 10 ppm of sulphur content were available commercially by the end of 2005 in Japan. The situation is similar in Europe and North America. Zero-emission and zero-levels of sulphur content are being called for worldwide in the coming 5–10 years.

Desulphurization of diesel blending components remains an important research area. There are continuing efforts to develop new technologies such as extractive desulphurization for deep fuel cleaning.

The present work describes mathematical modelling and optimization of extractive desulphurization of light cycle oil (LCO, component of diesel fuel obtained from fluid catalytic cracking) with dimethylformamide. This approach was used to determine optimum values of the following factors: extraction time, content of selective solvent used and amount of water added to the solvent to decrease sulphur content in LCO.

By optimization techniques, we found a suitable combination of these factors as applied to the gasoil from catalytic cracking.

10-P2. Biodiesel production by direct esterification of fatty acids

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Among the alternative sources of energy, biodiesel – mono-alkyl (methyl, ethyl, propyl, etc.) esters of fatty acids, has attracted much attention as a renewable additive to diesel fuel. It is commonly produced by transesterification of natural triglycerides (vegetable oils and/or animal fat).

The most widely used biodiesel production technology uses strong acids as catalysts for esterification of free fatty acids (if present) and then – strong bases for transesterification of the glycerides. However, this technology is known to have numerous problems, related to low yields due to formation of soaps and emulsion, low quality and contaminants in the glycerol phase, incomplete transformation of the glycerides, etc. Alternative transesterification technologies developed at present include solid catalysts, supercritical processes, microbiological catalysis, ultrasonic methods, and even microwave methods, each of which has its own advantages and drawbacks.

An important alternative for biodiesel production, being developed only recently, is the direct catalytic esterification of the free fatty acids, obtained after *a priori* hydrolysis of the glycerides by subcritical water. This hydrolysis is the typical approach used for many years for production of fatty acids (e.g. stearin and olein) by the fats and oil industry. This work presents our laboratory set-up and technology. It also reports experimental results for the esterification of oleic acid with methanol under different conditions.

10-P3. 'Chemical structure – lubricity property' relationships for esters of fatty acids (biodiesel) and other compounds used in diesel fuels

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The requirement for less than 10-ppm sulphur in today's automotive diesel fuels revives lubricating problems, previously controlled by petroleum sulphur compounds, which are now removed. The wear scar diameter, determined by the ISO 12156 standard method on a High-Frequency Reciprocating Rig is used to specify lubricity of diesel fuels. In the USA, a similar method (ASTM D 6709) is applied.

Alkyl (e.g. methyl, ethyl) esters of fatty acids, commonly known as 'biodiesel', are among the most widely used and promising renewable additives for petroleum diesel. Some of the compounds that might be present in biodiesel (esters, fatty acids, glycerol, etc.), depending on their chemical structure, can boost the lubricity of diesel fuels.

The present work describes correlations for prediction of the standard wear diameters and four other lubrication parameters of esters of fatty acids and other compounds used in diesel fuels, from their chemical structure. In addition to the presently known experimental data for around 40 compounds, our correlations suggest estimated values for more than 50 new compounds, important for optimization of biodiesel and diesel composition.

10-P4. Extraction of oil from spent ground coffee

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Bioenergy is the only alternative and cheap source of energy, which can be made easily available worldwide. The present experiment included extraction of oil from spent ground coffee. The production of energy from renewable and waste materials is an attractive alternative to the conventional agricultural feedstocks such as corn and soybean. Coffee grounds after oil extraction are ideal materials for garden fertilizer, feedstock for ethanol, and as fuel pellets. The analyzed coffee samples belonged to Arabica and Robusta varieties. Coffee oil was extracted with *n*-hexane using Soxhlet apparatus. The temperature was about 70°C. The yield of coffee oil was about 10–15%. An increase in reaction time did not significantly affect the yield. FT-IR spectra and GC were used to determine the present fatty acids. The oils extracted from spent ground coffee were successfully converted to alkyl esters of fatty acids by transesterification with both methanol and ethanol in the presence of alkaline catalyst.

10-P5. Synthesis of new analogues of pyrrole-based agent BM 212 with potential antitubercular and anti-inflammatory activity

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Today, tuberculosis is no more considered as a disease of the past. According to the World Health Organization, about 2 billion of the world's population is affected by *Mycobacterium tuberculosis*. Each year 8 million people around the world develop active tuberculosis, and 2 million die from it. The need of effective treatment of the widely spread inflammatory diseases is another current health concern.

Encouraged by recently published results about the excellent anti-tuberculosis activity of pyrrole derivatives LL-3858 (Sudoterb) and BM 212, we synthesized 15 analogues of the mentioned agents. Introduced structural variations, such as morpholine- and acetyl- (at position 3), and dichlorophenyl- and dimethoxyphenyl- (at position 3) moieties, made possible the evaluation of their effect on the activity during the next steps of pharmacological tests.

Some common structural features close to that of the tricyclic COX-2 inhibitors suggest that the evaluation of the same series of compounds as potential anti-inflammatory agents could be an additional field of interest for the new derivatives of pyrrole.

11-P1. My group work in the chemistry laboratory

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The purpose of this special summary lesson was, firstly, to enhance students' interest in chemistry and, secondly, to enrich and deepen their knowledge and skills to reveal the relationship between studied substances and their role in impairing or maintaining the ecological balance in nature.

A part of the annual review is allocated to the summary lesson and it is held within training class VII. We establish a set of tasks with environmental content and offer them regularly to the students as a means of additional environmental knowledge, thus stimulating their creative thinking and suggesting ecological behaviour. We share and discuss with students a non-standard form of an overview lesson, which we divide into three parts:

(i) I read the following assignments;
(ii) I drew up tasks;
(iii) I solved the problem.

In the first part of the lesson, the students read their share facts and data related to environmental issues, while respecting fixed regulations, to present the information briefly, clearly and accurately. In the second part of the lesson, we organize the students in groups to compile problems of environmental interest. Each group prepares tasks in writing and there is a copy for each student. In the last part of the lesson, representatives of the various groups mount posters on the blackboard with written assignments. The purpose is for 10 minutes students must decide the most possible number of tasks and provide the most original answers.

The summary lesson so organized and conducted allows us to systematize and summarize the environmental knowledge and skills of the students and to promote intellectual capacity and positive reasons for learning.

11-P2. Alchemical period

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Alchemy is the name of scientific chemistry for its period in ancient Egypt and the Middle Ages until the 17th century: primarily Arabia and West Europe. Its main goal was the search for miraculous 'philosopher's stone', which can turn metal into gold and gives longevity and eternal life.

During the second century AD, an Academy of Alchemy occurred in Alexandria. The lessons were 'sacred secret art' to imitate precious metals. In the 7th century BC, Arabs appeared on the world arena. Archaize authorities, Arab caliphs, began to patronize science and the first Arabic chemists appeared in the 8th-9th century. The Arabs converted the word khimia into al-khimia. The most talented and renowned Arab alchemist, Jabir Ibn Hayyan, is known later in Europe under the name Geber. Another prominent Arab alchemist, Al-Razi (Razes), dealt with medicine and alchemy. The most famous chemist dealing with alchemy was Ibn Sina, known as Avicenna. Due to the decline of the Arab Empire, the centre of scientific thoughts again moved to Europe. The first one is a prominent European alchemist, Albert Magnus, also known as Albert the Great. In the stories of his contemporaries, however, he is presented as a magician.

The idea of alchemy and alchemists is associated with mysticism and superstition, which are among the features of the Middle Ages. In the period from 9th to 16th century European alchemy offered several major scientists and thinkers who left deep traces in history of science. They were sincerely convinced that the alchemy is the truth; they laboured tirelessly and selflessly to have committed countless trials and found a number of elements, chemical compounds and processes, which laid the foundations of modern chemistry.

11-P3. Chemical education between two countries: the town of Dobrich

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The interest to a certain subject should directly be associated with the difficulties, which students find in learning and the subjectivity of the staff. It is even harder to reveal the ‘human face’ of the subject of chemistry, because the present curriculum and the circumstances at school involve mainly theoretical learning, which is difficult for students. That distances them from entering and ‘liking’ the school matter.

This work offers a solution of the problem by non-formal knowing the history of the chemical education in the homeland: the town of Dobrich. The school institutions have submitted to the rules of two different countries: Kingdom of Bulgaria and Kingdom of Romania. That is why the main moments of the analysis comprise chemical education in the town of Dobrich during the Rumanian occupation: chemistry textbooks, professionalism of the teachers, and operative curricula. Special attention is given to the influence of the Rumanian educational system on the knowledge and skills that students have obtained and taking exams in Rumanian language for getting a grade and diploma.

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