

## ISSUE CONTENTS LIST WITH GRAPHICAL ABSTRACTS

SPECIAL ISSUE DEDICATED TO THE 70<sup>TH</sup> ANNIVERSARY  
FROM THE FOUNDATION OF THE FIRST ACADEMIC INSTITUTIONS  
AND TO THE 55<sup>TH</sup> FROM THE FOUNDATION OF  
THE ACADEMY OF SCIENCES OF MOLDOVA

### PREFACE

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#### THE 6<sup>TH</sup> INTERNATIONAL CONFERENCE "ECOLOGICAL & ENVIRONMENTAL CHEMISTRY" 2017

March 2-3, 2017, Chisinau, Republic of Moldova

Conference topics:

- A. Ecological Chemistry
- B. Environmental Chemistry and Engineering
- C. Green Chemistry
- D. Ecological & Environmental Aspects in Chemical Research and Education

Deadline for the *Abstracts submission* is October 1<sup>st</sup>, 2016.



### REVIEW PAPER

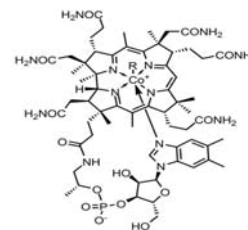
PHYSICAL CHEMISTRY AND CHEMICAL PHYSICS

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#### THE NATURE OF THE Co-C BOND CLEAVAGE PROCESSES IN METHYLCOB(II)ALAMIN AND ADENOSYLCOB(III)ALAMIN

Tudor Spataru, Francisco Fernandez

No grounded mechanisms for Co-C vitamin B<sub>12</sub> coenzyme bond breaking process and subsequent reactions have been found up to now. The influence of the mixing orbitals e.g. Pseudo-Jahn-Teller and similar effects on the reactions paths of bond-cleavage mechanisms of vitamin B<sub>12</sub> co-factors must be taken into account. Afterward, the updated mechanisms of vitamin B<sub>12</sub> bio-processes can be determined.



### FULL PAPER

ECOLOGICAL CHEMISTRY

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#### ECOLOGICAL POTENTIAL OF SURFACE WATERS IN NATURAL SCIENTIFIC RESERVE "LOWER PRUT"

Maria Sandu, Anatol Tarita, Raisa Lozan, Natalia Zgircu, Elena Mosanu, Tatiana Goreacioc, Alexandru Zlotea, Anna Comarnitchi, Iulia Sidoren, Sergiu Turcan, Adrian Tarita

The research results have marked a low value of the self-purification capacity for Belevu Lake water, between 0.12 and 0.19, which is of 1.2-2 times smaller than the one from Prut River (0.25), correlating positively with the values of BOD<sub>5</sub>, COD-Cr and the time of biochemical oxidation of ammonium ions. The evolution of stage  $\text{NH}_4^+(\text{NH}_3) \rightarrow \text{NO}_2^-$  in the process of nitrification in lake water in November 2014 takes place about 25 days and the process  $\text{NO}_2^- \rightarrow \text{NO}_3^-$  - more than 35 days, the duration about 2 times higher than in lake water stages from 2015 and 2.8-3.0 times higher than that of the model with water from Prut River.

### FULL PAPER

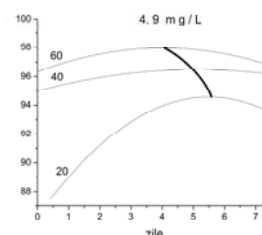
INDUSTRIAL CHEMISTRY

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#### EFFECT OF ALUMINIUM SULPHATE AGING ON COAGULATION PROCESS FOR THE PRUT RIVER WATER TREATMENT

Larisa Postolachi, Vasile Rusu, Tudor Lupascu

Aluminium sulphate is one of the most widely used coagulants for water treatment and has been proven to be an effective coagulant for the removal of certain contaminants, turbidity and colour. Aluminium sulphate used during the coagulation process is hydrolyzed in the water, forming polynuclear complexes. Aged aluminium solutions show different coagulation behaviour than that of freshly prepared solutions. Obtained results reveal that using of optimal *aging* solution of coagulant improves the coagulation process.



## FULL PAPER

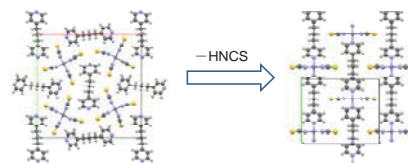
## INORGANIC AND COORDINATION CHEMISTRY

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**THE FORMATION MECHANISM OF ASSEMBLED COMPLEXES BRIDGED BY 1,3-BIS(4-PYRIDYL)PROPANE**

Haruka Dote, Hiroki Yasuhara, Satoru Nakashima

Several types of crystals having different color appeared in the synthesis of assembled complex of mixed crystals with three metals.  $[\text{H}_2(\text{bpp})][\text{M}(\text{NCS})_4]$  changed to 1D chain polymer  $(\text{M}(\text{NCS})_2(\text{bpp}))$  by releasing HNCS from the cation and anion in a reaction vessel.



## FULL PAPER

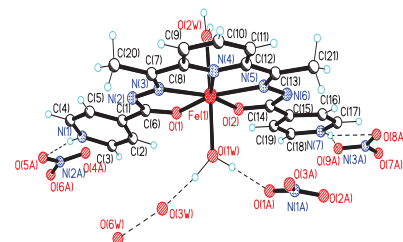
## INORGANIC AND COORDINATION CHEMISTRY

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**STRUCTURE AND SOME BIOLOGICAL PROPERTIES OF Fe(III) COMPLEXES WITH NITROGEN-CONTAINING LIGANDS**

Ion Bulhac, Alexandra Deseatnic-Ciloci, Paulina Burosh, Janetta Tiurina, Olga Bologa, Cezara Bivol, Steliana Clapco, Ana Verejan, Svetlana Labliuc, Olga Danilescu

Four coordination compounds of iron(III) with ligands based on hydrazine and sulfadiazine:  $\text{FeCl}_3 \cdot \text{digsemi} \cdot 2\text{H}_2\text{O}$  (I) (digsemi-semicarbazide diacetic acid dihydrazide,  $[\text{Fe}(\text{HL})\text{SO}_4]$  (II) (HL - sulfadiazine),  $[\text{Fe}(\text{H}_2\text{L}^1)(\text{H}_2\text{O})_2](\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$  (III) ( $\text{H}_2\text{L}^1$  - 2,6-diacetylpyridine bis(nicotinoylhydrazone) and  $[\text{Fe}(\text{H}_2\text{L}^2)(\text{H}_2\text{O})_2](\text{NO}_3)_3 \cdot 1.5\text{H}_2\text{O}$  (IV) ( $\text{H}_2\text{L}^2$  - 2,6-diacetylpyridine bis(isonicotinoylhydrazone) were synthesized. The spectroscopic and structural characterisation as well as their biological, properties are presented.



## FULL PAPER

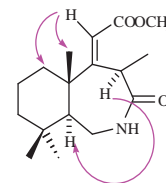
## NATURAL PRODUCT CHEMISTRY AND SYNTHESIS

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**SYNTHESIS OF NEW DRIMANE AND HOMODRIMANE LACTAMS BY BECKMANN REARRANGEMENT OF SOME KETOXIMES**

Elena Secara

Synthesis of new drimane and homodrimane lactams, derivatives of octahydro-1H-benzo[d]azepine and octahydro-1H-benzo[c]azepine, from norambreinolide is reported. These compounds were prepared by Beckmann rearrangement of the corresponding ketooximes.



## FULL PAPER

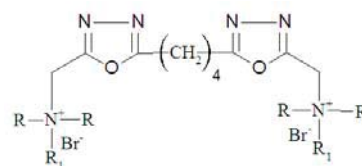
## ORGANIC CHEMISTRY

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**SYNTHESIS AND ANTIMICROBIAL EVALUATION OF SYMMETRICAL DIQUATERNARY AMMONIUM SALTS BEARING BIS-1,3,4-OXADIAZOLE RINGS MOIETIES**

Sofiane Daoudi, Tahar Benaissa, Djallal Eddine Adli, Nisserine Hamini-Kadar

This study describes the synthesis of some novel compounds containing bis-1,3,4-oxadiazole bearing quaternary ammonium salt moieties. The newly synthesized compounds were evaluated for their antibacterial activity against various gram-positive and gram-negative strains of bacteria, and the antifungal activities were tested against three phytopathogenic fungi namely, *Fusarium oxysporum*, *Fusarium commune* and *Fusarium rodelens*.



## FULL PAPER

## PHYSICAL CHEMISTRY AND CHEMICAL PHYSICS

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**STUDIES OF THE SUBSTITUTION EFFECTS ON THE ELECTRONIC PROPERTIES FOR BIPHENYL AND DERIVATIVE MOLECULES BY USING DFT METHOD**

Rajaa Khedir Al-Yasari

DFT method has been carried out to study the substitution effects of  $\text{NO}_2$  group on the electronic (ionization potential, electron affinity, electronegativity, hardness, softness and electrophilicity index) and IR spectral properties of biphenyl and derivative molecules by using the B3LYP functional and the 3-21G basis set, as well as the optimization structure. The calculated values of HOMO and LUMO energies, as well as predicted by ChemBioDraw program  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra for the studied compounds are in a good agreement with experimental data.



## FULL PAPER

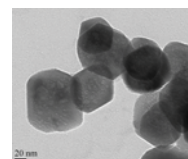
## PHYSICAL CHEMISTRY AND CHEMICAL PHYSICS

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**ELECTRON MICROSCOPY OF ANIONIC SURFACTANT-DIRECTED SYNTHESIS OF MAGNETITE NANOPARTICLES**

Sharali Malik, Ian James Hewitt, Annie Katherine Powell

We have synthesized a variety of magnetite nanoparticles which appear to have biogenic signatures and could give insights into how the nanomagnetite particles form in biological systems, and how they are associated with Alzheimer's disease. We have also synthesized mesoporous magnetite nanoparticles which have potential use in the targeted drug delivery.



## FULL PAPER

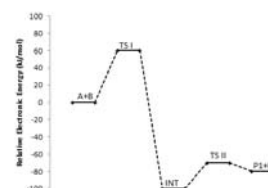
## PHYSICAL CHEMISTRY AND CHEMICAL PHYSICS

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**DFT (B3LYP) COMPUTATIONAL STUDY ON THE MECHANISMS OF FORMATION OF SOME SEMICARBAZONES**

Abdulfatai Siaka, Adamu Uzairu, Sulaiman Idris, Hamza Abba

Thermodynamic and kinetic mechanisms of forming six semicarbazones have been investigated computationally by DFT B3LYP method. All the reactions proceed *via* two transitions and include two consecutive steps: bimolecular and unimolecular. The computed transition steps have varying equilibrium constants values, enthalpy of activation and Gibbs energy of activation, depending on the semicarbazone involved.



## FULL PAPER

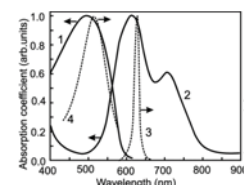
## PHYSICAL CHEMISTRY AND CHEMICAL PHYSICS

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**PHOTOELECTRIC PROPERTIES OF HETEROSTRUCTURES BASED ON PEPC AND MEH-PPV FILMS DOPED WITH ZINC OCTABUTYLPHTHALOCYANINE**

Nicolay Davidenko, Irina Davidenko, Oleg Korotchenkov, Victor Kravchenko, Elena Mokhrinskaya, Andrey Podolian, Sergey Studzinsky, Larisa Tonkopiyeva

Planar organic heterostructures were prepared using poly-N-epoxypropylcarbazole films and poly[2-methoxy-5-(2'-ethylhexyloxy)-1,4-phenylenevinylene] by the method of successive deposition adding 2,3,9,10,16,17,23,24-zinc octabutylphthalocyanine. Photoelectric, photodielectric and photovoltaic properties of the heterostructures were studied.



## FULL PAPER

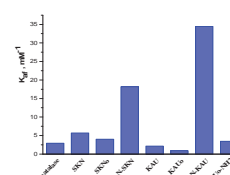
## PHYSICAL CHEMISTRY AND CHEMICAL PHYSICS

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**BENZOYL PEROXIDE DECOMPOSITION BY NITROGEN-CONTAINING CARBON NANOMATERIALS**

Daryna Haliarnik, Oleg Petuhov, Olga Bakalinska, Tudor Lupascu, Mykola Kartel

The catalytic activities of nanoporous carbon materials, their modified forms and enzyme catalase was determined by calculation of Michaelis constants according to the kinetics of substrate decomposition. It is found that the catalytic activity of studied samples correlated with surface basicity and presence of quaternary nitrogen groups in structure.



## FULL PAPER

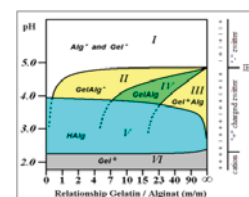
## SUPRAMOLECULAR CHEMISTRY

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**PHASE DIAGRAM OF GELATINE-POLYURONATE COLLOIDS: ITS APPLICATION FOR MICROENCAPSULATION AND NOT ONLY**

Alexei Baerle, Olga Dimova, Irina Urumoglova, Pavel Tatarov, Larisa Zadorojnai

Phase state and the charge of colloidal particles in the gelatine-polyuronate system were studied. A method for comparative evaluation of molecular weight of colloids by means of viscosimetric measurements and electrophoresis was developed. It is shown that the Diagram {Phase state = f (composition, pH)} contains six well-defined regions. The diagram explains and predicts the behaviour of protein-polysaccharide colloids, which are included in beverages or forms the shells of oil-containing microcapsules.



## INSTRUCTIONS FOR AUTHORS

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