ISSUE CONTENTS LIST WITH GRAPHICAL ABSTRACTS

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FROM THE FOUNDATION OF THE FIRST ACADEMIC INSTITUTIONS
AND TO THE 55TH FROM THE FOUNDATION OF
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PREFACE

NEWS AND EVENTS

THE 6TH 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 1st, 2016.

REVIEW PAPER

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 12 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 12 co-factors must be taken into account. Afterward, the updated mechanisms of vitamin B 12 bio-processes can be determined.

FULL PAPER

ECOLOGICAL CHEMISTRY

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 Beleu 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 BOD₅, COD-Cr and the time of biochemical oxidation of ammonium ions. The evolution of stage NH₄⁺(NH₃) → NO₂⁻ in the process of nitrification in lake water in November 2014 takes place about 25 days and the process NO₂⁻ → NO₃⁻ - 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

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.
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. \([\text{H}_2(\text{bpp})][\text{M(NCS)}_2]\) changed to 1D chain polymer (\(\text{M(NCS)}_2(\text{bpp})\)) by releasing HNCS from the cation and anion in a reaction vessel.

STRUCTURE AND SOME BIOLOGICAL PROPERTIES OF Fe(III) COMPLEXES WITH NITROGEN-CONTAINING LIGANDS
Ion Bulhac, Alexandra Deseatnic-Ciloci, Paulina Bourosh, 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: \(\text{FeCl}_3\cdot(\text{digsemi})\cdot2\text{H}_2\text{O}\) (I) (digsemi-secarbamylidic acid dipyrazidrile), \([\text{Fe(HL)}\text{SO}_4]\) (II) (HL - sulfadiazine), \([\text{Fe}(\text{HL}_2)\cdot(\text{H}_2\text{O})_3][\text{NO}_3]\cdot5\text{H}_2\text{O}\) (III) (HL - 2,6-diacylpyridine bis(nicotinoylhydrazone) and \([\text{Fe}(\text{HL}_2)(\text{H}_2\text{O})_2][\text{NO}_3]\cdot1.5\text{H}_2\text{O}\) (IV) (HL - 2,6-diacylpyridine bis(nicotinoylhydrazone)) were synthesized. The spectroscopic and structural characterisation as well as their biological, properties are presented.

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 ketoximes.

SYNTHESIS AND ANTIMICROBIAL EVALUATION OF SYMMETRICAL DIQUATERNARY AMMONIUM SALTS BEARING BIS-1,3,4-OXADIAZOLE RINGS MOIEITES
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, \(\text{Fusarium oxysporum}\), \(\text{Fusarium commune}\) and \(\text{Fusarium rodelens}\).

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 NO2 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 \(^1\)H and \(^13\)C NMR spectra for the studied compounds are in a good agreement with experimental data.
FULL PAPER  PHYSICAL CHEMISTRY AND CHEMICAL PHYSICS

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

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

PHOTOELECTRIC PROPERTIES OF HETEROSTRUCTURES BASED ON PEPC AND MEH-PPV FILMS DOPED WITH ZINC OCTABUTYLPHTHALOCYANINE
Nicolay Davidenko, Irina Davidenko, Oleg Korotchenkov, Victor Kravchenko, Elena Mokrinskaya, 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

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

PHASE DIAGRAM OF GELATINE-POLYURONATE COLLOIDS: ITS APPLICATION FOR MICROENCAPSULATION AND NOT ONLY
Alexei Baerle, Olga Dimova, Irina Urumoglova, Pavel Tatartov, 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