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SPECIAL ISSUE DEDICATED TO THE 10TH ANNIVERSARY OF CHEMISTRY JOURNAL OF MOLDOVA. GENERAL, INDUSTRIAL AND ECOLOGICAL CHEMISTRY

PREFACE

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ACADEMICIAN GHEORGHE DUCA – THE SCIENTIST WHO LIVES THE PRESENT BY LEARNING FROM THE PAST AND INVESTING IN THE FUTURE

EDITORIAL

OVERVIEW OF ECOLOGICAL CHEMISTRY CONFERENCES (1985-2016)

REVIEW PAPER

SUPRAMOLECULAR CHEMISTRY

RECENT TRENDS IN ALGINATE, CHITOSAN AND ALGINATE-CHITOSAN ANTIMICROBIAL SYSTEMS
Albert Ivanic

Present work outlines the main synthetic approaches for the preparation of antimicrobial systems based on alginate (1) and chitosan (2) polymers as well as identifies potential areas of their application. Various techniques used for preparation, applications and usefulness of these systems as carriers of antimicrobial compounds are also discussed.

FULL PAPER

ECOLOGICAL CHEMISTRY

ADSORPTION OF STRONTIUM IONS FROM WATER ON MODIFIED ACTIVATED CARBONS
Mihai Ciobanu, Victor Botan, Tudor Lupascu, Tatiana Mitina, Maria Rusu

Adsorption of strontium ions from aqueous solutions on active carbons CAN-7 and oxidized CAN-8 has been studied. Obtained results showed that the adsorption isotherms for strontium ions from aqueous solutions are well described by the Langmuir and Dubinin-Radushkevich equations, respectively. The surface heterogeneity of activated carbons CAN-7 and oxidized CAN-8 has been assessed by using Freundlich equation.

FULL PAPER

ECOLOGICAL CHEMISTRY

SEASONAL CHANGES OF MACRO- AND MICROELEMENTS CONTENT IN SOILS OF GREEN TEA FARMING FROM RIZE (TURKEY)
Fatih İslamoğlu, Özlem Buçan, Oktay Torul, Naciye Erdoğan

During of 2014 year, 60 soil samples at the point of 30 soil samples in the spring and 30 soil samples in autumn were taken from the locality of Findikli, Pazar and Sabuncular, where cultivation of green tea has been made in Rize (Turkey). The value of pH, organic matter content, and macro- and microelements amount were determined in sampled soils and the seasonal changes were investigated.

FULL PAPER

ECOLOGICAL CHEMISTRY

ANTIOXIDANT AND ANTIMICROBIAL PROPERTIES OF STEVIA LEAVES EXTRACTS AND SILVER NANOPISTICLES COLLOIDS
Irynà Laguta, Teteiana Fesenko, Oksana Stavinskaya, Oksana Dzjuba, Lesya Shpak

Stevia rebaudiana (Bertoni) extracts prepared from various types of raw material (leaves of plants grown ex situ and in vitro and callus culture) were found to contain different amounts of bioactive substances and differ from each other by antioxidant/reducing and antimicrobial properties and by activity in synthesis of silver nanoparticles colloids.
SYNTHESIS AND STRUCTURAL CHARACTERISTICS OF BIS(CITRATE)GERMANATES(IV) (Hbipy)2[Ge(HCitr)2]·2H2O AND [CuCl(bipy)2]2[Ge(HCitr)2]·8H2O

Inna Seifullina, Elena Martsinko, Elena Chebanenko, Olha Pirozhok, Viktoriya Dyakonenko, Svitlana Shishkina

The crystalline compounds (Hbipy)2[Ge(HCitr)2]·2H2O (1) and [CuCl(bipy)2]2[Ge(HCitr)2]·8H2O (2) (where H4Citr is citric acid, bipy is 2,2'-bipyridine) were obtained for the first time and their structures were determined by the single-crystal X-ray diffraction method. The two compounds were characterized by IR spectroscopy, thermogravimetric (TGA) and elemental analyses. In both compounds complex bic(citrat)germanate anion is formed, protonated 2,2'-bipyridine molecule and [Cu(bipy)2Cl]+ complex are cations in 1 and 2, respectively.

SYNTHESIS, SPECTRAL AND THEORETICAL CHARACTERIZATION OF 5,6-DICHLORO/DIMETHYL-2-(2´,3´/2´,4´/2´,5´/3´,4´/3´,5´-DIMETHOXYPHENYL)-1H-BENZIMIDAZOLES

Demet Gürbüz, Aydin Tavman, Adem Cinarli, Ismail Boz

5,6-Dichloro/dimethyl-2-(2´,3´/2´,4´/2´,5´/3´,4´/3´,5´-dimethoxyphenyl)-1H-benzimidazoles were synthesized and characterized experimentally and theoretically. The optimized molecular geometry, zero point energy, dipole moment, ESE and charge distributions were calculated by Gaussian 09 using DFT method. The calculated energy values with ZPE correction and DFT show that the methyl derivatives are more stable than the chloro forms.

EXTRACT OF BARBERRY AS ENTIRELY GREEN CATALYST FOR THE SYNTHESIS OF STRUCTURALLY DIVERSE 3,4,5-SUBSTITUTED FURAN-2(5H)-ONES

Nourallah Hazeri, Razieh Doostmohammadi, Belgehis Adrom, Mojtaba Lashkari, Malek Taher Maghsoodlou

An eco-friendly and environmentally benign synthesis of 3,4,5-substituted furan-2(5H)-ones employing Iranian seedless barberry or zereshk (Berberis integerrima ‘Bidaneh’, Berberidaceae) as a biocatalyst was developed. The merits of this method include the environmentally friendly reaction conditions, simple operation, broad substrate, satisfied yields and generate less waste than the conventional chemical reagents.

REMOVAL OF METHYLENE BLUE BY ADSORPTION ONTO RETAMA RAETAM PLANT: KINETICS AND EQUILIBRIUM STUDY

Dalila Badis, Zoubir Benmaamar, Othmane Benkortbi, Houcine Boutoumi, Houria Hamitouche, Amele Aggoun

The feasibility of using Retama raetam plant, for the cationic dye (methylene blue) adsorption from simulated aqueous solution, has been investigated as a low cost and an eco-friendly adsorbent. The methylene blue maximum adsorption occurred at pH 8 and the lowest adsorption occurred at pH 2. The apparent equilibrium was reached after 120 min. Adsorption modelling parameters for Freundlich and Langmuir isotherms were determined and, based on R², various error distribution functions.

TOPOLOGICAL ANALYSIS AND FREQUENCY DEPENDENT HYPERPOLARIZABILITY CALCULATIONS OF FDDNP: A DFT STUDY

Keivan Akhtari, Keyumars Hassanzadeh, Bahareh Fakhraei, Ghazal Akhtari

In this study, we have shown that FDDNP as a functional fluorescent biomarker has high performance in near-infrared region. The best predicted working wavelength belongs to Ti:sapphire laser (880 nm). The employed near-infrared (NIR) wavelengths reduce scattering and maximize tissue penetration.
DISPOSAL OF POISONOUS ORGANIC HALIDES BY USING THE ELECTROCHEMICAL METHOD: DFT SIMULATION

Tudor Spataru, Francisco Fernandez, Joseph W. Sista, Petru Spataru, Igor Povar

Geometry optimizations at the UBP86/6-311++G** level of electronic structure theory have been performed for DDT, β-hexachlorocyclohexane, and heptachlor organic polychlorides and their positive and negative ions. The geometry optimization of the obtained neutral intermediate molecules after the first and second reducing by two electrons show that the electrochemical dehalogenation of the organic polychlorides is sequential.

STRUCTURAL DISTORTIONS OF COORDINATED KETENE MOLECULE INDUCED BY THE PSEUDO JAHN-TELLER EFFECT

Natalia Gorinchoy

It is shown that the only reason of structural distortions of ketene molecule coordinated in the complexes VCp2-H2C2O (I) and Pt(PPh3)2-H2C2O (II) is the pseudo Jahn-Teller effect induced by the orbital charge transfers by coordination. The η2-(C-O) coordination and the in-plane distortion of ketene in the complex (I) is due to the PJTE induced by the back donation to its LUMO 3b2. The η2-(C-C) coordination mode, and the out-of-plane distortion of the molecule in the complex (II) is caused by two OSTs: from the HOMO 2b1 to the metal, and from the dxy-AO of Pt to the vacant 3b1 MO of ketene, thus being the result of the diorbital Pt-ketene interaction.

GC-MS ANALYSIS OF THE ESSENTIAL OIL OF SATUREJA SUBSPICAT. BARTL. EX VIS. OF MOLDOVAN ORIGIN

Ion Dragalin, Aculina Aricu, Nina Ciocarlan, Alexandru Ciocarlan, Victoria Codita

For the first time the results of GC-MS analysis of Satureja subspicata L. oil of Moldovan origin are reported. The chemical profile includes forty-four constituents and consists mostly (97.86%) of phenolic monoterpenes, monoterpen hydrocarbons, bicyclic sesquiterpenes and their oxygenated derivatives. A substantial quantitative and qualitative chemical differentiation of S. subspicata oil of Moldovan origin and reported oil of Croatian origin were found. The essential oil of S. subspicata L. plants cultivated in Republic of Moldova belongs to the carvacrol chemotype.