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*The organizing committee: Prof. Safronenko O.I., Senior lecturer Belayeva N.A.*

**INVESTIGATION OF PHOTOCROMICAL PROPERTIES OF SPIROPYRANS OF THE  
COUMARIN SERIES**

**Speaker:** 1<sup>st</sup> year PhD student Burtseva A.A.

**Language consultant:** Prof. Safronenko O.I.

**Research Supervisor:** Assoc. Prof. Metelitsa A. V., Dr. of Science in Chemistry

Spiropyrans containing coumarin moiety, annulated to the 2*H*-pyran ring at the 6,5-position were prepared and their structure, spectral kinetic and photochromic properties were studied by means of UV/Vis spectroscopy. Spiropyrans containing coumarin moiety exhibit positive photochromism under normal conditions and are characterized by exceptionally high values of colorability. Both, the strong electron donating and electron withdrawing 5-R substituents in the indoline moiety, provide for the noticeable decrease of colorability. Negative solvatochromism of merocyanine isomers of the synthesized spiropyrans indicates their dipolar structure, which is manifested by the reduction of the rate constants of recyclization upon increasing solvent polarity.

**APPLICATION OF THE CYANO DIELS-ALDER REACTION FOR FUSED PYRIDINE  
SYNTHESIS**

**Speaker:** 1<sup>st</sup> year PhD student Vyalykh Yu.V.

**Language consultant:** Prof. Safronenko O.I.

**Research Supervisor:** Assoc. Prof. Suzdalev K.F.

[4<sup>-</sup>+2] Cycloaddition strategies for the construction of pyridine derivatives that proceed *via* Diels-Alder reaction are described. Unactivated nitriles as 2*π*-cycloaddition components and organolithium dienes as activated 4*π*-components have been found to react in mild conditions forming 2-substituted pyridines as the main products. Lithium diisopropyl amide effect on 2-methyl-3-acylindoles and 1-methyl-2-acylbenzenes leads to the proton elimination from 2-methyl group and gives the corresponding activated anionic dienes. Addition of nitrile causes a reaction affording dihydropyridines, which often undergo a spontaneous water elimination and give the corresponding pyridine derivatives. DFT calculations in B3LYP/6-311++G\*\* basis show that the reaction of nitriles with the above described anionic species represent a non-concert cycloaddition. An energy barrier value essentially depends on the presence of lithium cation. This method was used to obtain a series of carbolines and isoquinolines.

**STRUCTURED CRYSTAL MOLECULE SYSTEM SIMULATION BY DFT METHODS:  
STRUCTURE AND PROPERTIES**

**Speaker:** 1<sup>st</sup> year PhD student Zaytsev S.A.

**Language consultant:** Prof. Safronenko O.I.

**Research Supervisor:** Prof. Minyaev R.M.

New nanomaterials created by theoretical simulation are considered. They can be obtained by replacing a carbon atom in graphane onto tetrahedral fragments of carbon, boron and aluminium.

Observed surfaces are single-layered and double-layered. Furthermore it can contain both one and two atom types. To establish compounds stability phonon spectrums were calculated. It is shown that phonon curves fall into the negative area of values. So, phonon spectrum points at some material demonstrate instability. The calculated band structure shows that all systems are good semiconductors. To understand the nature of the bond the natural bond orbitals (NBOs) were calculated. NBOs have shown that B–B bonds in tetrahedral are 3 center-2 electron, thus they are electron-unsaturated. Carbon bonds are the classical 2center-2electron. Aluminium NBOs have not been calculated due to the complicated nature of the metal. Investigation of some physical properties shows that their surfaces have lower density than water.

### **PHYSICO-CHEMICAL STUDY AND ELECTROPHORETIC DETERMINATION OF THE THIONES BASED ON THE S AND S, N-CONTAINING HETEROCYCLIC COMPOUNDS**

**Speaker:** 1<sup>st</sup> year PhD student Ivolgina V.A.

**Language consultant:** Prof. Safronenko O.I.

**Research Supervisor:** Prof. Chernovyants M.S.

Heteroaromatic thioamides derivatives possess numerous biological effects including antioxidant, antimicrobial, antiviral, antituberculous activities. They are used for gipertirooze and leukemia treatment. The physico-chemical studies of heteroaromatic thioamides (dithiones and monothiones) are provided. The protolitic properties, antioxidant activity, binding ability with BSA (bovine serum albumin) and the development of a rapid, simple and practical method for the determination of newly synthesized drugs (5-mercapto-3-phenyl-1,3,4-thiadiazolidin-2 potassium salt, thiophene-2-thiol, 5-(4-pyridyl-1,3,4-oxodiazol-2-thiol, 5-amino-1,3,4-thiadiazole-2-thiol)) by capillary electrophoretic method are considered. The focus is made on the methods widely used in pharmaceutical and clinical practice to identify and assess the thyrostatic agents. The analytical characteristics of individual methods to assess thyrostatic agents can be used in manufacturing at the quality control stage.

### **INFLUENCE OF CYCLIC LACTAMS AND THEIR STRUCTURAL ANALOGUES ON THE KINETICS OF Cu (II) IONS, MORPHOLOGY OF SURFACE AND PROPERTIES OF COATINGS**

**Speaker:** 1<sup>st</sup> year PhD student Mauer D.K.

**Language consultant:** Prof. Safronenko O.I.

**Research Supervisor:** Assoc. Prof. Skibina L.M.

Behavior of cyclic compounds in copper sulfate electrolytes is directly related to their structure. The nature of the heteroatom in the cycle, the size of the cycle, and the presence of side carbonyl groups has been investigated. It was shown that efficiency coefficient of the additive increases with an increase of volume concentration in the presence of nitrogen-containing heterocycles. However, such dependency was not observed in the presence of oxygen-containing heterocycles. Calculation of kinetic parameters of the process has confirmed that the kinetics of a cathodic reaction is mainly determined by the nature of the heteroatom in the cycle. The analysis of the chronopotentiometry and impedance data showed that the complexes formed on the surface layer block the electrode surface, increase the  $\Psi$  'potential and impede the discharge of metal ions. Their inhibitory effect increases with increasing ligand concentration. The ability to control effectively the deposition rate, morphology and coating properties was shown to be the result of changes in the nature, structure and volume concentration of the additives studied.

## THE STUDY OF MAGNETIC EXCHANGE IN COPPER COMPLEXES WITH HYDRAZONES

**Speaker:** 1<sup>st</sup> year PhD student Komarov I.V.

**Language consultant:** Prof. Safronenko O.I.

**Research Supervisor:** Prof. Lukov V.V.

The study of magnetic exchange in binuclear and polynuclear complexes of transition metals with hydrazones, oximes and related systems are provided. A correlation between the electronic and geometrical structures of complexes and characteristics exchange effects is discussed. A systematic analysis of magnetostructural correlations in such complexes is performed. The relationship between the symmetry of the coordination environment and the symmetry of the easy axis of magnetization are discussed.

## REACTIONS OF NITROFUROXANOQUINOLINE WITH N, N-DIMETHYLANILINE: REDUCTION, SUBSTITUTION, ANNULATION

**Speaker:** 1<sup>st</sup> year PhD student Temnyakova A.S.

**Language consultant:** Prof. Safronenko O.I.

**Research Advisor:** Prof. Kurbatov S.V.

It is known that nitrobenzofuroxans are highly electrophilic and low aromatic compounds. They take part in rare reactions for aromatic compounds of nucleophilic addition, substitution, and cycloaddition with formation of new condensed derivatives. Furthermore, benzofuroxans exhibit a wide spectrum of biological activity, such as antimicrobial, fungicidal, antiaggregatory and anticonvulsant ones. These compounds are of particular interest as sources of exogenous nitric oxide (II), which is known to be involved in the regulation of blood pressure, neurotransmission and immune response. Nitrofuraxanoquinoline (NFQ) exists as an inseparable mixture of 1,3 N-O isomers and in subsequent cycloaddition reactions it also forms mixtures of 1,3 N-O isomers of cycloadducts, which at times makes it difficult to interpret their NMR spectra. In this context, the nitrofuraxanoquinoline (NFzQ) system, a deoxygenated analogue of NFQ, is a more attractive synthon, since the furazanic cycle is a priori devoid of 1,3 N-O isomerism. The synthesis of NFzQ by the reduction of NFQ is reported. Since reagents commonly used for this type of reactions (PPh<sub>3</sub>, P(OEt)<sub>3</sub>, PCl<sub>3</sub> and HN<sub>3</sub>) hamper the separation of products mixtures, N,N-dimethylaniline was successfully used as a reducing agent. A mixture of four products is formed in the reaction with NFQ, one of which is NFzQ. The structure of the compounds obtained was confirmed by <sup>1</sup>H and <sup>13</sup>C NMR.

## SYNTHESIS, STRUCTURE, PROPERTIES AND COMPLEXING ABILITY OF FERROCENOYLHYDRAZONE 1-PHENYL-3-METHYL-4-FORMYL-5-HYDROXYPYRAZOLE

**Speaker:** 1<sup>st</sup> year PhD student Tkacheva Yu.O.

**Language consultant:** Prof. Safronenko O.I.

**Research Supervisor:** Prof. Scherbakov I.N.

The synthesis of a new potentially dibasic tridentate ligand system is described. It is the ferrocenoylhydrazone of 1-phenyl-3-methyl-4-formyl-5-hydroxypyrazole. The ligand was studied by IR, NMR and electron spectroscopy. According to the theoretical data, the compound has three basic tautomeric forms. IR, NMR spectroscopy and quantum-chemical calculation data suggest that the main form is pyrazolone-hydrazone. The dependence of the hydrazone absorption spectra upon the pH of the solution was studied. It is shown that in both acidic and alkaline media the shape of the spectrum changes due to protonation and deprotonation of the molecule, respectively. There is no protonation of the ferrocene fragment. Complex compounds of the ligand system with copper,

nickel and zinc were obtained. The complexes were investigated by IR, NMR spectroscopy, and their magnetic moments were measured. Based on the data obtained, a tetragonal planar structure is assigned to the copper(II) complex, and the nickel(II) and zinc(II) complexes are octahedral.

### **DYE-SENSITIZED SOLAR CELLS (DSSC)**

**Speaker:** 1<sup>st</sup> year PhD student Adamkovich V.V.

**Language consultant:** Prof. Safronenko O.I.

**Research Supervisor:** Prof. Scherbakov I.N.

Constant growth of energy consumption is directly related to the rapid growth of technologies and their miniaturization. The active search for alternative renewable energy sources has led to the development of photovoltaic technology of direct energy conversion of solar radiation into electric current.

To increase the overall light-electric conversion efficiency sensitizers are actively explored. The first generation of photosensitizers involves complexes of Ru with organic ligands. New generation DSSC use dyes that do not contain Ru in cells, this a very rare and expensive metal. There is an intensive development of methods for obtaining purely organic dyes and complexes of transition metals, to be used as photosensitizers. By selecting ligands and studying various photosensitizers different in the structures of complexes, it is possible to obtain sensitizers with high absorption efficiency over a wide range of wavelengths, good resistance to cyclic electron transfer reaction and other necessary qualities, which in turn will improve the efficiency of DSSC.