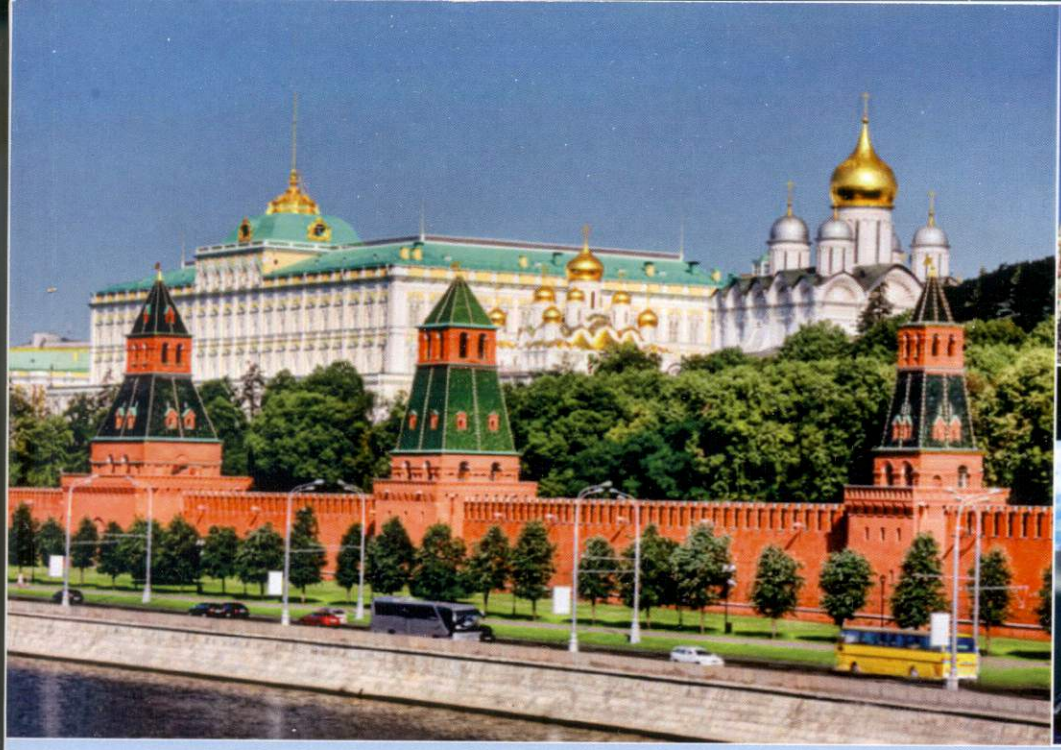

BOOK OF ABSTRACTS

International Congress on Heterocyclic Chemistry "KOST-2015"

dedicated to 100 years anniversary of professor Alexei Kost

KOST 2015
18–23.10.2015
Lomonosov Moscow State University

October 18-23, 2015
Lomonosov Moscow State University
Moscow, Russian Federation

16.10 - 16.25 (O-09)

Трансформации 2-тиогидантоинов и их производных в реакциях комплексообразования

E.K.Beloglazkina

16.25 - 16.40 (O-53)

НИТРОЗИРОВАНИЕ ЦИКЛОПРОПАНОВ: ПЕРСПЕКТИВЫ РЕАКЦИИ

Бондаренко О. Б.

16.40 - 16.55 (O-11)

Soft N-Donor Heterocyclic Ligands for Metal Extraction and Fluorescent Analysis

Borisova N.E.

16.55 - 18.30 coffee break / Poster Session 1 P001-P140

HALL B2 Chairman Prof. Valery Fokin

14.30 - 14.50 (I-02)

Intelligent reaction media for synthetic modifications of heterocyclic compounds

A.V. Aksenov

14.50 - 15.10 (I-31)

ФУНКЦИОНАЛЬНЫЕ МАТЕРИАЛЫ НА ОСНОВЕ НОВЫХ ПРОИЗВОДНЫХ ПОРФИРИНОВ И ФТАЛОЦИАНИНОВ: КЛЮЧЕВАЯ РОЛЬ ПРОЦЕССОВ САМОСБОРКИ

Горбунова Ю.Г.

15.10 - 15.25 (O-54)

Эффективные гетерогенные Pd-катализаторы на основе N,O-Полимерных носителей и 1,2-азольных лигандов для реакции Соногаширы в воде

Бумагин Н.А.

15.25 - 15.40 (O-13)

New multicomponent synthesis of polyfluoroalkylated imidazo[1,2-a]pyridines

Burgart Ya.V.

15.40 - 15.55 (O-56)

Реакции имидазо[4,5-e] тиазоло[3,2-b]-1,2,4-триазин-7-онов с карбонильными соединениями

Г.А. Газиева

15.55 - 16.10 (O-59)

Молекулярные конформационные переключатели на основе транс-3,4-дигидрокси - и транс-4-амино-3-гидроксипиперидинов.

Гришина Г.В.

16.10 - 16.25 (O-63)

Перегруппировка 6-имино-2,7-диоксабицикло[3.2.1] октан-4,4,5-трикарбонитрилов в производные 3-амино-1,6-диоксо-2,7-диазаспиро[4.4] нона-3,8-диен-4-карбонитрила

Иевлев М.Ю.

16.25 - 16.40 (O-30)

Efficient assembly of hetaryfuroxan scaffolds

N. N. Makhova

SOFT N-DONOR HETEROCYCLIC LIGANDS FOR METAL EXTRACTION AND FLUORESCENT ANALYSIS

Borisova N.E.[1], **Ivanov A.V.**[1], **Korotkov L.A.**[1], **Harcheva A.V.**[2], **Patsaeva S.V.**[2], **Kaminskaya T.P.**[2], **Reshetova M.D.**[1]

[1] *Chemical Dept. MSU* [2] *Dept. of Physics MSU*

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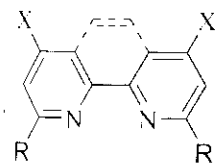
A new type of the ligands – soft-donor N,N',O,O'-teradentate compounds (A) based on 2,2'-bipyridyl and phenanthroline scaffolds are designed and synthesized. Such oxygen-donor side groups as: amidic (CONR2), phosphinoxy (POR2) and N-oxy (NOR2) are proposed for additional metal chelation. The DFT modeling (PBE0, B3LYP, cc-pv-TZ) show that the charges on N,N',O,O'-metal binding atoms aren't affected by the nature of the substituents at the anilidic side chain. The analysis of the structures of complexes of A with lanthanides show the presence of a number of minima on PES which are differ by positions of nitrate groups. The complexes of A with lanthanides were synthesized and X-Ray structures of them were determined. As well the thermodynamic basisity ($14.9>pK>15.6$) of the ligands and their binding constants with lanthanides ($7.5>lg\beta>5.5$) and several actinides ($9.2>lg\beta>5.1$) were measured. The main trends in relations which binds structure and properties of the ligands were shown. The target compounds shown their effectiveness as an extragents for 5f-elements separation: Am(III), U(IV), Th(VI), Np(V) from lanthanides. Intra a row of 4f-complexes with one ligand the DFT calculated degree of reorganization are correlate well with both the complexation energy and extraction. The luminescent properties of the complexes of A with lanthanides were investigated and the interrelation between the ligand's structure and quantum yield and life-time were determined in solution, solid state and thin films. The concentration quenching of luminescence depending on the structure of the anilidic side chains were found. The aggregation of the complexes at films formation was elucidated by AFM, such process probably responsible for the quenching of luminescence in the films of europium complexes.



A

Ligands based on 2,2'-bipyridyl

X	R
H, Br, NO_2	C(O)NEtAr
tt	$P(O)Ar_2$
Ligands based on 1,10-phenanthroline	
Cl, $O^nC_5H_{11}$, Ph	C(O)NEtAr, $C(O)NEt_2$
H	$P(O)Ph_2$
tt	$N(O)Alk_2$

The work was support by Ministry of Education and Science of RF (contract №14.604.21.0082 (RFMEFI60414X0082)).

DIAMIDES OF THE 2,2'-BIPYRIDYL-6,6'DICARBOXYLIC ACID WITH A NUMBER OF N-ETHYLAMINOPYRIDINES. NEW LIGANDS TO ASSOCIATE F-ELEMENTS.

A.V. Ivanov[1], A.V. Harcheva[2], Ts.B. Sumyanova[1], N.E. Borisova[1]

[1]*Moscow State University, Department of Chemistry*

[2]*Moscow State University, Department of Physics*

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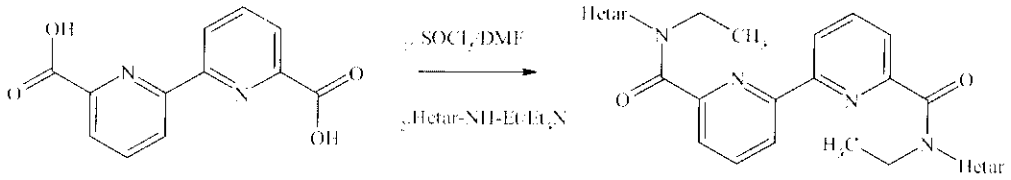
Lately 2,2'-Bipyridyl derivatives have been widely used for different metals binding [1,2]. The *tert*-diamides of 2,2'-bipyridyl-6,6'dicarboxylic acid represent an important class of these compounds and are applied to associate in a complexes and separate f-elements [3-5].

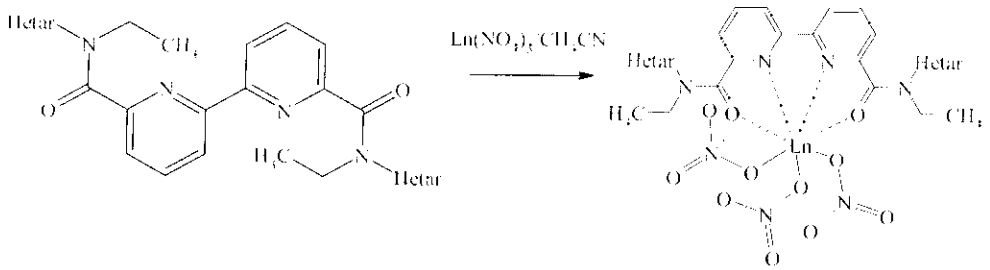
Diamides of the 2,2'-bipyridyl-6,6'dicarboxylic acid with a number of N-ethylaminopyridines have been prepared to continue our investigations:



Hetar=2-Py, 3-Py, 4-Py, 6-CH_3-2-Py, 6-$COOCH_3$-2-Py

Decrease of electronic density in N-ethylpyridines amino-group in comparison with N-ethylanilines leads to some trouble with their acylation and, as a result, reduces target compounds yields. The constants of basicity and the constants of a number of rare-earth elements binding are measured.

Complexes with lanthanides (III) nitrates have been obtained on the basis of synthesized ligands:



Ln=La, Sm, Gd, Eu, Tb, Dy

Luminescence properties of the prepared complexes have been explored.

The work was support by Ministry of Education and Science of RF (contract №14.604.21.0082 (RFMEFI60414X0082)).

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