



*"ANGEL KANCHEV" UNIVERSITY OF RUSE
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*РУСЕНСКИ УНИВЕРСИТЕТ "АНГЕЛ КЪНЧЕВ"
СЪЮЗ НА УЧЕНИТЕ - РУСЕ*



*56th Annual Science Conference of Ruse University
INDUSTRY 4.0. BUSINESS ENVIRONMENT. QUALITY OF LIFE.*

*56-та годишна конференция на Русенския университет
ИНДУСТРИЯ 4.0. БИЗНЕС СРЕДА. КАЧЕСТВО НА ЖИВОТ.*

SESSIONS SCHEDULE & ABSTRACTS ПРОГРАМА & РЕЗЮМЕТА

**2017
BULGARIA
Ruse
Razgrad
Silistra**

FRI-LCR-1-CT(R)-06

FORMAMIDE-BASED PREBIOTIC CHEMISTRY: ONE-POT SYNTHESIS OF NUCLEOBASES AND AMINO ACIDS

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Abstract: In scenario framing the origin of life, the generation of precursors in abiotic conditions remains the major initial hurdle. Understanding the formation of biogenic molecules in abiotic conditions is a prerequisite in the origin-of-life studies. Determining the conditions allowing an efficient one-pot synthesis of the largest possible panel of biogenic compounds may shed light on the plausible scenario in which the processes that started life might have occurred. We report experiments describing the syntheses taking place from formamide. The formamide-based synthetic system proved to be particularly robust. Large panels of different compounds were observed – nucleobases (adenine, cytosine, uracil), amino acids (glycine, alanine), hypoxanthine, pterine, purine, urea and urocanic acid. Mechanism of reactions affording nucleic bases and amino acids were simulated by high-level *ab initio* quantum chemical methods.

Keywords: prebiotic chemistry, formamide, amino acids, nucleobases, *ab initio*

Acknowledgements: Funding of this work by the National Science Fund, under Grant DN09/7/2016 is gratefully acknowledged.

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SAT-LB-P-2-CT(R)-03

TAUTOMERISM OF INOSINE IN WATER: IS IT POSSIBLE?

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Abstract: Inosine, 9-[2R,3R,4S,5R]-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-3H-purin-6-one is a purine nucleoside that has hypoxanthine linked by the N9 nitrogen to the C1 carbon (β-N-glycosidic bond) of ribose. It is an intermediate in the degradation of purines and purine nucleosides to uric acid and in pathways of purine salvage. Inosine is commonly found in tRNAs and is essential for proper translation of the genetic code in wobble base pairs. The water-assisted proton transfer process in inosine was investigated using ab initio MP2 and SCS-MP2 quantum chemical approaches. It was found that in the gas phase and in water solution, the most stable tautomer for inosine is the 6-keto followed by the 6-enol form. Available X-ray data suggest that inosine can exist in two conformer forms according to the ribose ring position – syn- and anti-conformation. The proton transfer for both conformer forms of inosine keto and enol tautomers was considered. Potential energy surfaces of the "bare" finite solute-solvent clusters containing inosine molecule and five water molecules were explored, while within the second approach these clusters were embedded in "bulk" solvent treated as polarizable continuum (C-PCM/SCS-MP2/6-31+G(d,p) level of theory).

The rate constant is sufficiently large to generate the 6-enol tautomer. The analysis of the reaction profiles shows the proton transfer processes occur through the asynchronous concerted mechanism.

Keywords: tautomerism, ab initio, inosine

Acknowledgements

Funding of this work by the National Science Fund, under Grant DN09/7/2016 is gratefully acknowledged. The calculations were partially performed on the computer system MADAIRA installed at the Institute of Chemistry, Bulgarian Academy of Sciences with the financial support of the National Science Fund.

SAT-LB-P-2-CT(R)-04

HIGH DENSITY POLYETHYLENE COMPOSITES CONTAINING WOOD FLOUR

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Abstract: The aim of this paper was to investigate of using wood flour as fillers of thermoplastic polypropylene. Those natural fillers are low-cost, environment – friendly and renewable raw nature. Polymer matrix of high density polyethylene was used to prepare composites with different amounts (1, 3, 5, 10, 20, 30, 40 and 50 mass%) of wood flour.

The results of mechanical properties showed that the tensile strength decreased and the Young's modulus increased with the amount of filling than that the pure PEHD. The MFI decreased with amount of filling. The samples was analysed with TGA method and the results showed that the composites containing wood flour had a better thermal stability.

Keywords: composite, high density polyethylene, wood flour, tensile strength properties, thermogravimetric analysis.

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CERTIFICATE

of participation awarded to

**Venelin Enchev, Nadezhda Markova, Nina
Stoyanova, Miroslav Rangelov, Ivan Angelov,
Ivayla Dincheva**

for participation at the

**CONFERENCE
WITH INTERNATIONAL PARTICIPATION**

**03.11. – 04.11.2017
Razgrad Hotel Cartoon**

the report

**"Formamide-based prebiotic chemistry: one-pot synthesis
of nucleobases and amino acids "**

**Organization committee:
Assoc.Prof. DSc. St. Damyanova**

04.11.2017



Razgrad, Bulgaria