OPINION

from Assoc. Prof. Dr. Bistra Atanasova Stamboliyska, Institute of Organic Chemistry with Centre of Phytochemistry (IOCCP), Bulgarian Academy of Sciences (BAS)

on the materials presented for the competition for the academic position of an Associate Professor at IOCCP – BAS in higher education field 4.0. "Natural Sciences", professional field 4.2. "Chemical Sciences", scientific specialty „Theoretical Chemistry,"

Dr. Nadezhda Markova is the only candidate in the competition for the academic position of „Associate Professor", announced in the State Gazette, issue 79 of 08.10.2019 and on the website of IOCCP - BAS

General presentation of the procedure and the applicant

The presented set of documents and materials for review meets the requirements of the Rules for the conditions and procedure for acquiring scientific degrees and for occupying academic positions at IOCCP - BAS. In the category "Publications in specialized scientific publications equivalent to monographs" 5 scientific papers were presented - 4 of which are published in Q1 ranked journals and 1 - in Q2 ranked journals. These publications collected 120 points with the minimum required 100 points according to the Rules of IOCCP-BAS. The competition documents also include habilitation work, based on these 5 publications. In the second category, "Other original research publications", 13 publications were presented, of which 1 - in Q1, 5 - in Q2, 4 - in Q3, and 3 - in Q4. These publications collect 201 points with a minimum required of 200 points. Attached is a list of 100 citations in scientific journals, referenced in the world databases Web of Science and Scopus. The points collected on this indicator are 200 at the minimum required 70. The analysis shows that Dr. N. Markova exceeds in all indicators the national and additional minimum requirements of IOCCP - BAS for occupying the position of "Associate Professor".

Nadezhda Markova graduated with a master degree in chemistry from the Shumen University Konstantin Preslavski in 2000. From 2002 to 2005, she was a PhD student of Prof. V. Enchev at IOCCP. She received his doctoral degree in 2006 after successfully defending a PhD thesis "Theoretical investigations on Tautomeric Equilibria in Organic Molecules Taking into account the Specific Solvent Effects". From 2006 until now he is the Assistant Professor at IOCCP.

General characteristic of the applicant's activity

Dr. Nadezhda Markova's scientific research has been published in 34 papers, 27 of which - in the specialized journals referenced and indexed in international databases. These publications have been cited 314 times in the literature, which is indicative of the level and relevance of the research carried out. According to Scopus the Hirsch Index is 7. The contribution of Dr. Markova to the conducted research is indisputable. In 11 of the presented articles she is the first author and in 4 she is the corresponding author. The research results were presented in international and national forums with 40 poster and 18 oral presentations. To participate in the competition, 18 articles published in reputable scientific journals are presented.

The habilitation thesis "Water as a medium and catalyst in tautomeric reactions" summarizes the data on the proton transfer mechanism in biologically important molecules, as nucleobases and nucleosides as well as their analogues. An important contribution was the creation of a theoretical model for the study of tautomeric equilibria in liquids based on a molecular-dynamic and

quantum-chemical approach. With this model, tautomeric equilibria for azauracils, nucleosides inosine and guanosine, and the acyclic analogue of guanosine - acyclovir in aqueous solution have been successfully investigated. The reactions were carried out in one step and by an asynchronous concerted mechanism. Based on quantum-chemical calculations, theoretical and experimental ^{1}H, ^{19}F, and ^{13}C NMR and Raman spectra, it was shown that in aqueous solution at pH = 7.8-10 there were an equilibrium between different tautomeric forms of the energetically more stable anion of 5-fluorouracil, N3.

The papers outside the habilitation work have been devoted to elucidating the mechanism of organic reactions as well as the structure of organic and coordination compounds.

The effect of the electric field and electronic state of organic molecules on the mechanism of intramolecular proton-transfer reaction have been studied. A new model tautomeric system was proposed in this upon variation of the electric field strength it is possible to stabilize different tautomeric forms of the molecule. Thus these compounds have potential use in the design of new molecular electronic devices. A new compound showing unusually strong Stokes shifts was synthesized. A double proton transfer in two sequential reactions in the first excited singlet state occurs. It has been found that the presence of daunorubicin (pH 10-11) in the polymerization mediumn affect both the degree of polymerization and the compactness of the resulting nanoparticles.

By appropriate computational and spectral methods it was possible to evaluate the structure of amide derivatives of cinnamoyl amino acids, spirohydantoins of naphthalimides, the two isomers of amino-thiazolidine and the tautomeric forms of 2-urea-1,3-indadione. It has been found that the tautomeric form in solution is different from that one in solid state for two newly synthesized compounds (2- (methylthio) -1,3-diazaspiro [4.4] non-2-en-4-one and 2- (methylthio) -1,3-diaza-spiro [4.4] non-2-ene -4-thion). It has been suggested to call this phenomenon desmocatatropy. The structures of N-(4-benzalaniline)-15-crown-5 and N-(4'-benzalaniline)-15-crown-5 and their alkali and alkaline earth metal complexes have been studied. The Li^{+}, Na^{+}, Mg^{2+} and Ca^{2+} cations fit to cavity size of the crown while the K^{+}, Sr^{2+} and Ba^{2+} cations, whose size is greater than the macrocycle cavity diameter, protrude from the macrocycle.

A significant part of the research work is related to active participation in international and national projects. The candidate was the leader of one project „Science and business", Ministry of Education and Science, Operational Programme Human Resources Development, co-financed by European Social Fund. At the moment Dr. Markova is coordinator of two projects funded by the Nation Science Found of Bulgaria and participates in 5 international and 4 national scientific projects.

Dr. Nadezhda Markova has an active teaching activity. She has been a supervisor of one Master degree and one Bachelor degree theses of a student from the Sofia University; a consultant in a PhD thesis of a student from South-West University – Blagoevgrad and in a PhD these of a student from Agrarian University – Plovdiv; mentor of nine students within the framework of the "Student Practices" Operational Programme Science and Education for Smart Growth of the Ministry of Education and Science.

Personal impressions

I know Dr. Nadezhda Markova as an in-depth researcher who has successfully applied quantum-chemical methods to solve various problems related to elucidating the mechanisms of organic reactions. She is keenly involved in the teaching of students and young scientists. I am impressed by her ability to organize and coordinate interdisciplinary teams as a project leader.

CONCLUSION

In the announced competition, Dr. Nadezhda Markova presents a sufficient number of high quality scientific papers, published after the materials used in the defense the PhD thesis. The large number of citations is a clear proof of the relevance of the research carried out and its use by the scientific community. Dr. Nadezhda Markova's scientific qualification in the field of theoretical chemistry is undoubtedly.

After the evaluation of the materials and scientific papers presented in the competition, analyzing their importance and their scientific contributions, I give my positive assessment and recommend to the Scientific Jury to prepare a report-proposal to the Scientific Council of IOCCP-BAS for the selection of Dr. Nadezhda Markova at the academic position of ”Assistant Professor“ in the professional field „Theoretical Chemistry”.

16.09.2019 г.

Reviewer: