STANDPOINT

by Prof. Dr. Ivelina Mircheva Georgieva

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of the materials for participation in the competition for the academic position

"Associate Professor"

at the Institute of Organic Chemistry with Center of Phytochemistry (IOCCP), BAS

in the field of higher education 4. Natural Sciences, Mathematics, Computer Science

Professional field 4.2. Chemical Sciences, scientific specialty "Organic Chemistry"

for the needs of the Structural Organic Analysis Laboratory (SOA)

In the competition for the academic position of Associate Professor, announced in the State Gazette, issue 40 of 16.05.2025 and on the website of IOCCP-BAS, only one candidate participated: Chief Assistant Professor Simeon Stoyanov Stoyanov, PhD;
Stoyanov, Simeon S.; ORCid: 0000-0003-4356-5960; Scopus ID: 8504442200

*General presentation of the procedure and the applicant***.** The presented set of materials (on electronic format) for participation in the competition is in accordance with the requirements of the Law on the Development of the Academic Staff in the Republic of Bulgaria, the Regulations for its implementation at the BAS and the recommended criteria of the IOCCP-BAS on PF 4.2. Chemical Sciences. The verification of the specified requirements for occupying the academic position "Associate Professor" showed that Simeon Stoyanov fulfills the necessary minimum in all groups of indicators, GI (A, C, D, E, G) and collected **727 points.** with a total required minimum of 440 points.

Simeon Stoyanov completed his higher education at the Faculty of Chemical and Pharmacy, Sofia University with a Master's degree in Organic and Analytical Chemistry in 2001, and in 2010 at the IOCCP-BAS, he acquired the educational and scientific degree of "Doctor" in PF 4.2 Chemical Sciences, specialty "Organic Chemistry". With a PhD degree, the candidate fulfills indicator **"A" (50 points).** In his consistent career development in the field of Organic Chemistry, as Senior Assistant Professor (2008-2010) and Chief Assistant Professor since 2011 at the Structural Organic Analysis Laboratory at IOCCP, Dr. Stoyanov has over 10 years of work experience in the specialty. During his scientific career, the candidate has specialized in three European scientific institutions: Faculty of Technology, University of Novi Sad, Serbia and Montenegro, Summer School, 2004; in Amsterdam, the Netherlands, Training with the MOE (Molecular Operating Environment) software package, 2013; Leibniz Institute of Polymers, Dresden, Germany, Training with Raman Spectrometer, 2015 and trained in the course "Supercomputer Applications in Natural Sciences", Sofia, 2011.

Scientific and research activities. In his research activities so far, Dr. Stoyanov is a co-author in **32 scientific articles** (according to the attached list) and **24** according to the SCOPUS and Web of Science databases (with data from 2008). At the time of drafting the document, the total number **of citations** of the publications is **105**, **H-index 5** (SCOPUS) (without self-citations of all co-authors), which meets the requirements of IOCCP-BAS, H-index ≥ 5.

In this competition, Dr. Stoyanov participates with **26 original scientific publications**, which exclude those from his doctoral thesis (6). The articles correspond thematically to the competition's specialty "Organic Chemistry" and have been published in prestigious refereed journals such as *Spectrochimica Acta A* (IF = 4.6), *Journal of Physical Chemistry A* (IF = 2.8), *Journal of the Electrochemical Society* (IF = 3.3), *Vibrational Spectroscopy* (IF = 3.1), *Molecules* (IF = 4.6), etc., which is a recognition of the merits of the scientific research with the participation

of Dr. Stoyanov. The scientometric indicators of the candidate are as follows: **24** articles for participation in the competition are published in indexed scientific journals and distributed by quartiles (for the year of publication) - **6** in **Q1, 8** in **Q2, 3** in **Q3** and **7** in **Q4** and two publications are in non-refereed journals. With his publication activity, Dr. Stoyanov fulfills the minimum criteria: 1) under GI "**C**" for habilitation work on **9** scientific articles (required 100 p./completed **166 p.**), in **8** of the scientific papers on this list, Dr. Stoyanov is the first author; 2) under GI "**D**" for scientific papers (**15**) (required 220 p./completed **273 p.**); 3) under GI "**E**" for **119** citations (in SCOPUS (105 in total) and other database (14)) on all publications (without self-citations of co-authors) (required 70 p./ fulfilled **238 p.**).

In fulfillment of the requirements of the competition for Associate Professor, Dr. Stoyanov has presented **a habilitation thesis** on the topic *"**Application of vibrational spectroscopy to the study of structure and stability of anionic derivatives containing cyano-, carbonyl- and nitro groups. Experimental and theoretical approach.**"* At the discretion of the candidate, 14 publications from the list for the competition are included in this reference. Dr. Stoyanov's scientific interest is aimed at obtaining and characterizing organic anions and corresponding radical anions in solution, based on polynitrile, benzophenones, carba-, oxy- azanion and nitroaromatic derivatives. The studied compounds are intermediates in a number of organic syntheses and biochemical reactions or pharmaceutical forms, which in a dynamic biological environment are transformed into reactive radicals. Knowledge of the geometric, energetic, kinetic and thermodynamic characteristics and properties of anionic and radical-anionic intermediates is of utmost importance and aims to identify them in chemical and biochemical processes, which helps to clarify their biological activity and mechanism of action.

Dr. Stoyanov's main contribution to the research approach to anionic organic compounds in solution is the skillful combination of synthetic methods for preparation, special experimental IR spectroscopic techniques, and quantum chemical calculations. The most important results of the research work can be summarized as follows:

1) Synthetic procedures for the preparation of anions (mono-, di-, tri-) with the selection of reagents and solvents have been developed. The following have been studied:
- the role of the solvent (polar, aprotic, nonpolar) in the formation of anions (aggregates or solvate-separated);
- the effect of the solvent on the geometric structure and vibrational properties of the anions;
- the vibrational behavior of the solvent, including deuterated ones, in order to avoid overlapping or distinguishing its bands from those of the studied anions.

The advantages and disadvantages of a series of solvents have been evaluated and the most suitable ones (e.g. dimethyl sulfoxide) have been selected that are slightly corrosive to CaF_2 cuvettes and stabilize the anions. Techniques have been developed for electrochemical preparation of radical anions in a DMSO solvent and tetrabutylammonium salt, in a quasi-hermetic medium using a special electrolysis cuvette.

2) Non-trivial spectroscopic techniques (Infrared, Raman and isotopically labeled solutions) and cuvettes with special windows for record the vibrational bands of anions and radical anions, existing only in solution and characterized by a certain solubility, reactivity and short life, are applied. Despite the special techniques, the obtained spectroscopic data are not unambiguous, due to the complex dynamic processes of anions in solution.

3) By modeling the studied systems, following the experiment and simulating the vibrational spectra, in-depth and reliable information about the geometric structure of anions and radical

anions in solution and their characteristic vibrational properties was obtained. The computational protocol, in particular DFT functionals and basis sets, has been validated with respect to the models in solution (mono-, di-, tri-anions, radical anions and possible isomers) and to the their vibrational frequencies. Through comparative approaches, the adequacy of solvation models to simulate the influence of the solvent (global - PCM, global and microsolvation - ONION), as well as the accuracy of the method for geometric parameters and vibrational spectroscopic data (frequency and intensity of IR bands) were assessed. It has been found that the inclusion of diffuse functions is necessary for the more accurate description of the geometric and electronic structure of anions and radical anions, and they reduce the anharmonic correction. With the help of model calculations of possible geometric structures and the corresponding vibrational frequencies and comparison with experimental spectra, the most probable structures of anions and radical anions in solution were predicted and their observed vibrational spectra were reliably interpreted. On the basis of the predicted structures (neutral, anionic and radical-anionic) and calculated IR frequencies, structure – IR spectrum relationships were deduced and geometric, electronic (distribution of electron density) and spectroscopic changes during deprotonation and radical reaction were traced.

Dr. Stoyanov's scientific activity is closely related to the implementation of 14 projects: two infrastructure projects of the Bulgarian Academy of Sciences and the Ministry of Education and Science, nine of the National Science Fund - Ministry of Education and Science and three of University of Chemical Technology and Metallurgy (UCTM) -Sofia. To disseminate the scientific results, Dr. Stoyanov has participated in 32 international and national scientific forums. He was the supervisor of a successfully defended master's degree from the UCTM, 2018 and led the training of postgraduate students at the International Summer School on IR Spectroscopy and XRD Applications, 2013.

Comment: According to the Rules of Procedure for the Acquisition of Scientific Degrees and for Occupying Academic Positions at the Institute of Organic Chemistry with the Center of Phytochemistry, the Bulgarian Academy of Sciences and "Art. 36(3) 13. List of citations participating in the competition, which are not submitted in other competitions for occupying academic positions and acquiring scientific degrees", formally 10 citations should be excluded from the list of citations from the competition. This does not affect the fulfillment of GI "E".

In conclusion, the high evaluation of the research with the participation of Dr. Stoyanov, published in indexed scientific journals, his research contributions and active participation in projects prove that he is a highly qualified and established scientist in the field of anionic derivatives of organic compounds - preparation and characterization with experimental and theoretical approaches of vibrational spectroscopy. The research is in full compliance with the scientific specialty "Organic Chemistry" of the competition for "Associate Professor". The presented analysis of the competition materials gives me reason to vote positively with a convinced **"yes"** and I recommend to the Scientific Jury to propose to the Scientific Council of the IOCCP-BAS that the Chief Assistant Professor **Dr. Simeon Stoyanov Stoyanov to be elected to the academic position of "Associate Professor" at IOCCP-BAS** in the professional field 4.2. Chemical Sciences, scientific specialty "Organic Chemistry".

05.09.2025 **Who prepared the standpoint:**

Prof. Dr. Ivelina Georgieva