REVIEW

from Prof. DSc Sonia Varbanova Ilieva,
Faculty of Chemistry and Pharmacy, Sofia University “St. Kl. Ohridski"
of the materials submitted for the competition for the academic position of **'Associate Professor'**
at the Laboratory of Structural Organic Analysis (SOA),
Institute of Organic Chemistry with the Center of Phytochemistry (IOCCP), BAS
in higher education professional field 4.2. Chemical Sciences (Organic chemistry)

In the competition for the academic position 'Associate Professor' announced in the State Gazette, issue 40/16.05.2025, **Chief Assistant Dr Simeon Stoyanov Stoyanov** from the Laboratory of Structural Organic Analysis, IOCCP, BAS is the only candidate.

General presentation of the materials

The electronic and hard copy materials submitted by Chief Assistant Dr Simeon Stoyanov Stoyanov **meet all the requirements** of the Law for the Development of the Academic Staff in the Republic of Bulgaria and the relevant regulations for its implementation (including those of BAS and IOCCP). The applicant meets and exceeds the criteria (minimum requirements) of IOCCP-BAS for the academic position "Associate Professor".

Dr Stoyanov has published a total of 32 scientific papers (122 citations, h index 6) and for the participation in this competition he has submitted **26 scientific publications**, which do not repeat the ones presented for obtaining PhD degree. Submitted publications are distributed among the relevant Q factors as follows: 6 - Q1; 8 - Q2; 3 - Q3; 7 - Q4; 2 - without impact factor.

In the competition, Dr Stoyanov presents himself with the following parameters:

Indicator A – **50** points from the doctoral degree;

Indicator B – **166** points from 9 publications:3 - Q1; 2 – Q2; 1 – Q3; 3 – Q4 (required minimum 100 points);

Indicators Г – **273** points from 15 publications:3 - Q1; 6 – Q2; 2 – Q3; 4 – Q4 (required minimum 220 points);

Indicator Д (citations) – 238 points (required minimum 70 points)

An extended habilitation report on the scientific contributions of the candidate is presented in both Bulgarian and English. The report discusses in a concise and clear manner the main scientific developments in which Dr Stoyanov has participated, presented in **14** of the publications with which the candidate is involved in the competition. The applications of vibrational infrared spectroscopy and quantum-chemical calculations for studying the structure and stability of anionic derivatives containing cyano-, carbonyl-, and nitro-groups are presented. The work on this topic represents a continuation and development of the research included in S. Stoyanov's doctoral dissertation. At the end of the report, brief prospects for the candidate's future work are outlined.

Brief biographical information

S. Stoyanov graduated as a Master of Sciences in Organic and Analytical Chemistry at the Faculty of Chemistry, Sofia University “St. Kl. Ohridski” in 2001. In 2004, he joined the Institute of Organic Chemistry with the Centre of Phytochemistry (IOCCP) at the Bulgarian Academy of Sciences (BAS) as a chemist. In 2005, he was enrolled as a full-time PhD student in the Laboratory of Structural Organic Analysis at IOCCP. In 2009, he defended his doctoral dissertation on the topic "IR Spectral and Structural Changes Induced by the Conversion of Nitriles to Anions and Radicals," after which he continued his scientific work in the Laboratory of Structural Organic Analysis as an assistant and later as Chief Assistant (2011 – present). His scientific research is both fundamental and applied, focusing on organic chemistry, molecular spectroscopy, and quantum chemistry. It is dedicated to the synthesis, purification, and characterization of organic compounds and anionic derivatives using IR spectroscopy and quantum-chemical calculations. Therefore, Dr Stoyanov's accumulated professional and scientific experience is fully aligned with the announced competition.

The documents related to the competition show that S. Stoyanov has completed four short-term specializations – training in spectroscopy and theoretical chemistry, related to his scientific work. He has participated in a number of national and international scientific forums with 2 oral presentations and over 30 posters, as well as in 14 national scientific projects.

General characterization of the applicant's scientific activities

The candidate's overall scientific activity is in the field of organic chemistry, which fully corresponds to the field and professional area of the announced competition. The scientific publications submitted for participation in the competition reflect S. Stoyanov’s work in the following research areas: (i) synthesis of anionic derivatives of organic compounds, simulation and interpretation of their vibrational spectra; (ii) study and characterization of antioxidants; (iii) analysis of cultural heritage objects through the combined application of spectroscopic techniques.

The synthesis and characterization of carbanions, aza-anions, and oxyanions is not a trivial task due to a number of factors. A methodology has been developed for their study, based on the combined use of experimental IR spectra and quantum-chemical calculations. This approach has enabled the interpretation of the structures of a number of anions for which data in the literature is either lacking or very limited. In the Laboratory of Structural Organic Analysis, a specialized electrolysis cell has been developed for the electrochemical generation of radical anions in a DMSO or DMSO-d6 medium with a tetrabutylammonium salt. It is designed in such a way that the cathodic and anodic products are separated, allowing observation of only the spectrum around the cathode.

The interpretation and assignment of vibrational spectra of anionic derivatives is complicated by several factors: the main characteristic regions of anions and radical anions broaden and shift significantly compared to those of neutral molecules, resulting in substantial band overlap. Additionally, the bands of aromatic skeletal vibrations often compete with or exceed in intensity those of functional groups. Due to these and other factors that hinder spectral analysis, a combined experimental-theoretical approach has been developed in the laboratory for interpreting the vibrational spectra of anionic derivatives. This

approach is based not only on experimental spectra but also on quantum-chemical calculations and normal coordinate analysis using density functional theory (DFT), considering solvent effects and ion aggregation.

The theoretical studies include conformational and structural analysis of the investigated molecules and, in some cases, clarification of mechanisms of biological activity. The functional and basis set used in the quantum-chemical calculations have been validated through comparative analysis of results from ab initio calculations and by varying the basis set in terms of accuracy and computational time. To achieve good agreement between experimental and theoretically calculated vibrational frequencies, a specific scaling approach has been developed in the laboratory. This involves regression analysis and the derivation of a scaling equation by which the theoretical frequencies of the anion/radical anion are adjusted. S. Stoyanov has made a major contribution to these developments, as confirmed by the publication of a single-author article (4B in the report) in a well-established and reputable international journal (J. Phys. Chem. A).

As a result of collaborative work with colleagues from the Laboratory of Structural Organic Analysis, the Institute of Organic Chemistry with Centre of Phytochemistry (IOCCP), the University of Chemical Technology and Metallurgy (UCTM), the Faculty of Chemistry and Pharmacy at Sofia University, and others, the results of the following scientific studies have been published:

- Spectral and structural changes induced by the conversion of substituted benzophenones into ketyl radicals.
- Vibrational spectra and structure of carbanionic derivatives:
  - Carbanions of 1,1,3,3-tetracyanopropane: the influence of closely positioned carbanion centers on the frequency of the nitrile group;
  - Formation and isomerization of the carbanionic adducts of 2-{5,5-dimethyl-3-[(2-phenyl)vinyl]cyclohex-2-enylidene}malononitrile;
  - IR spectra and structure of the carbanion of phenindione (an anticoagulant of pharmaceutical relevance). It was found that the conversion of the molecule into a carbanion is accompanied by a fundamental change in the shape of the compound, as the tetragonal configuration of the central carbon atom transforms into a trigonal one, resulting in a planar structure of the carbanion.
- Vibrational spectra and structure of oxyanion and azanionic derivatives:
  - Oxyanion of apocynin (a compound used in traditional medicine). In order to clarify its antioxidant mechanism of action, the ability to scavenge reactive radicals was evaluated;
  - Oxyanion and dianion of acetoben (a compound present in antiviral medications);
  - Azanions and dianions of salophen (known for antirheumatic, antipyretic, analgesic, and antiseptic effects).
- Vibrational spectra and structure of anionic and radical anionic derivatives of nitroaromatic compounds (nitro-containing radical anions can lead to the formation of superoxide, reactive oxygen species, and ultimately oxidative stress). The research focused on anions and radical anions of benzimidazole derivatives, benzimidazolethiones, nimesulide, and flutamide.

I believe that Dr Stoyanov has played an active role in both the conceptual and practical development of the scientific works presented in the habilitation report. This is evidenced by the fact that he is the lead (corresponding) author in 6 of the 14 scientific publications discussed in the report.

Some of the publications not included in the candidate's habilitation report are related to the study and characterization of antioxidant and radical-scavenging substances. I believe that S. Stoyanov's contribution to these studies is associated with quantum-chemical calculations and IR spectral investigations.

Another area that stands out in the publications not included in the habilitation report is an analytical study aimed at clarifying the technological characteristics of the murals in the Church of the Assumption of St. Ivan Rilski at the Rila Monastery, in order to identify the painting materials and techniques used. These studies have a distinctly applied nature and are of significant importance for the preservation and restoration of endangered works of art.

The scientific research in which Dr Stoyanov has participated is interdisciplinary in nature, as confirmed by the above and the essence of the published scientific works. The conducted studies and published results have distinctly scientific and scientific-applied contributions, which can be formulated as demonstrating with new means essential new aspects of already existing scientific fields, problems, theories, and hypotheses; creating new methodologies for analysis; and obtaining new facts.

S. Stoyanov has been a co-supervisor of a Master's thesis in 2018. He participated as an assistant in conducting the International Summer School on IR Spectroscopy and X-ray Diffraction at IOCCP in 2013. Of course, it should be noted that according to the Law on the Development of the Academic Staff in the Republic of Bulgaria, the presence of teaching and pedagogical activity is not included in the minimum requirements for occupying the position of Associate Professor.

CONCLUSION

According to the submitted materials and scientific papers, the above analysis of their importance and scientific contributions, I am convinced in my **positive assessment** and firmly recommend to the Scientific Jury to prepare a report-proposal to the Scientific Board of IOCCP-BAS for the selection of **Chief Assistant Dr Simeon Stoyanov Stoyanov**, for the academic position of **'Associate Professor'** at IOCCP-BAS in the professional field 4.2. Chemical Sciences (Organic Chemistry).

19/09/2025 Reviewer:

Prof. Sonia Ilieva