

REVIEW

by prof. Ivayla Nedialkova Pantcheva-Kadreva, PhD
on a competition for acquiring the academic position “associate professor”,
Field of higher education 4. Natural sciences, mathematics and informatics,
professional field: 4.2. Chemical Sciences (Organic chemistry)
for the needs of the NMR Spectroscopy Centre
at the Institute of Organic Chemistry with the Centre of Phytochemistry (IOCCP) - BAS

The only candidate for acquiring the academic position "associate professor" announced in the State Gazette (issue 37 of 17.05.2022) is the chief assistant professor Yavor Nikolaev Mitrev, PhD, from the Laboratory of NMR Spectroscopy at IOCCP-BAS. According to the regulatory requirements Dr. Mitrev submitted electronically all the necessary information and was allowed to participate in the procedure.

1. Brief introduction of the candidate

Yavor Mitrev graduated at Sofia University “St. Kliment Ohridski”, Faculty of Chemistry, aa BSc (2004) and MSc (2006) in Chemistry. From 2007 to 2011 he was a PhD student at the at the Department of Organic Chemistry – Faculty of Chemistry, Sofia University, under the supervision of prof. Mariana Palamareva, DSc, and obtained his PhD degree defending a thesis titled “Synthesis, spectral and chromatographic properties of new 6H-6-oxo-dibenzo[c,h]chromes”.

Work experience: Since 2005 Yavor Mitrev is a member of the scientific team of IOCCP-BAS (Laboratory "NMR Spectroscopy") and successively held the positions of chemist (2005), assist. prof. (2010) and chief assist. prof. (2012 – up to now). The main activities he performs beyond those related to his research work in the field of NMR spectroscopy include the maintenance of the available spectrometers and the engagement in the NMR service.

2. Research activity of the candidate

Publication activity: Ch. assist. prof. Yavor Mitrev published 22 papers, referenced and indexed in the Scopus database, adequately cited in the scientific literature (138 citations excluding self-citations, Hirsch index 6).

Scholarships: Yavor Mitrev conducted a long-term post-doc at the University of Geneva (Switzerland), where he developed new approaches for experimental work in the field of NMR.

Project activity: Ch. assist. prof. Yavor Mitrev, PhD, is a member of the scientific teams of 9 scientific projects, being a head of one of them, funded by BAS, National Science Research Fund and Operative Programs.

Dissemination of the results: Within 2015-2021 Dr. Mitrev attended 14 scientific forums (10 international and 4 national) giving 6 oral and 9 poster presentations, 70% of which were personally presented by the candidate.

3. Evaluation of the materials presented for the competition and their compliance according to the running legislation in the Republic of Bulgaria

General performance

Dr. Mitrev submitted 16 scientific publications, all in refereed and indexed journals. According to the recent Regulations the publications are distributed as follows: 11 – Q1, 2 – Q2, 1 – Q3 and 2 – Q4 with an impact factor ranging from 0,2 to 7,8. The contribution teams include researchers from IOCCP-BAS, Bulgarian Universities (SU "St. Kl. Ohridski", SEU "N. Rilski") and BAS (Institute of Polymers, Institute of Mineralogy and Crystallography, Institute of optical materials and technologies, IEMPAM), as well as research groups from and outside the EU. The studies were carried out within two scientific research infrastructures - IOCCP-BAS and the University of Geneva. Yavor Mitrev's scientific production for the last three years (2019-2021) is impressive, publishing 8 (50%) of the full-text scientific communications submitted for the review.

Dr. Mitrev has summarized the main results he achieved after acquiring the PhD Degree in a habilitation report entitled "Applied and methodological NMR investigations", where the future prospects for the scientific research are also outlined. The numbering of the publications discussed in the present review follows that presented in the report.

Indicator A-1

The candidate has defended a PhD thesis based on three scientific contributions that do not repeat the publications presented in the current competition.

Indicator C-4

The candidate presents 5 scientific publications, equivalent to a habilitation thesis, which do not duplicate the materials used in other contests for holding an academic position and acquiring a scientific degree. Four of them are in journals within the first quartile and one – in the fourth. Dr. Mitrev is the sole author of one of the publications [3], the others are co-authored by research groups from Switzerland [1, 2], Bulgaria [2, 4, 5], Portugal [4] and

Hungary [5]. The topic of three of the publications [1-3] is entirely in the field of NMR spectroscopy and relates to the development of new experimental approaches for analysis purposes (Section I of the habilitation paper). The remaining two papers [4-5] are interdisciplinary, with an emphasis on the application of solid-state NMR spectroscopy (Section II).

The following innovations should be noted in the first direction:

- A rapid NMR method was developed to distinguish hexabromocyclododecane from alternative bromine-containing polymers applied as flame retardants using HSQC-heterocorrelation and specific filtering techniques [1];
- An analytical technique for NMR titration in water was developed, based on the preparation of NMR-invisible gels containing the analyte and the formation of a concentration gradient of the titrant into the gel. In addition, an experimental approach for accelerated “interleaved” data acquisition was developed, reducing significantly the quantitative analysis time using the spatially selective one-dimensional spectroscopy [2].
- For the purposes of the spatially selective NMR spectroscopy, new program products have been developed for accelerated registration of interleaved acquisition spectra and a number of specific conditions have been optimized for the study of distribution processes in two-phase systems possessing different magnetic susceptibility [3].

In the second direction, modified silicates (potential CO₂ scavengers [4] or owing catalytic activity [5]) have been characterized by solid-state NMR spectroscopy. The structural features of the studied mesoporous materials and the monitoring of the processes that take place under the effect of various factors require the application of non-traditional NMR techniques - a challenge that Dr. Mitrev and prof. Shestakova (IOCCP) excellently solved. Due to their work, one of the materials (MCM48 modified with 1-methylpiperazine [4]) emerged as a promising carbon dioxide adsorbent, and the specific structural changes in beta-type zeolite aluminosilicate matrices [5] occurring upon use of a certain modifier (Ni, Pt, Ru and their combinations) were determined.

The candidate's contributions can be summarized as follows:

- 1) **NMR methodology** – new specific procedures and programs for solving a particular research aim have been developed;
- 2) **solid-state NMR application** – a combination of techniques was applied to analyze solid-state mesoporous materials.

Indicator D-7

According to the indicator D, 11 articles are presented, seven of which are in journals in the first quartile, two - in the second, and one each - in the third and fourth, resp. The main part of the publications has highly interdisciplinary impact and they are devoted to the synthesis and chemical/biological characterization of compounds with different structures and properties [6-14]. The last two contributions [15-16] relate to specific problems in the field of organic chemistry. The co-authoring is an impressive: two of the publications are entirely written by Bulgarian scientists ([9, 13]); researchers from Bulgaria [6-14, 16], China [6-8] Russia [6], Czech Republic [6], Germany [6, 12, 15], Greece [6], Turkey [10, 11], Spain [14], Portugal [15, 16], Switzerland [15], Austria [15], Poland [15] took part in the rest of the papers. The research topic in this group of articles is very diverse, but the unifying link in all publications is the application of NMR spectroscopy, which, combined with other appropriate analytical techniques, has been successfully used to evaluate the behavior of target compounds in solution. Logically, in the habilitation report (Section III), Dr. Mitrev emphasizes the NMR studies performed, and stress on the points where the use of non-traditional approaches is required beyond the application of routine analysis techniques. Here it is appropriate to note that, apart from the already mentioned contributions (Indicator C-4), Yavor Mitrev masters and successfully applies the **NMR spectroscopy as analytical tool in solution**:

- A systematic NMR structural study of adamantane, rimantidine and memantine derivatives possessing potential antiviral and neuroprotective properties was carried out [6-9];
- Zn(II) phthalocyanine dyes have been characterized using various techniques to suppress the interfering signals [10, 11];
- The configuration (chalcone [12], stilbenes [13]) and tautomeric (folic acid [14]) forms of the compounds in solution were determined using one- and two-dimensional NMR spectroscopy;
- The glycerol / dimethylsulfoxide and 5-hydroxymethyl furfural systems were studied applying the diffusion NMR technique.

Indicator E-11

In the scientific database Scopus 138 citations have been noticed on all publications of Yavor Mitrev (22 articles). The candidate submitted a list of 97 citations on 11 of the peer-reviewed materials for the participation in the present competition. 22 (20%) of these citations refers to the recent production of Dr. Mitrev (in the last three years), which is a strong evidence for the relevance of its scientific research.

Indicator G (specific according to IOCCP-BAS Regulations)

The Hirsch-index of the candidate refers to the overall impact of his publications. At the point of completing the review ch. assist. prof. Yavor Mitrev, PhD, owns an H-index of 6 (Scopus), which is in agreement with the IOCCP minimal requirements (H-factor ≥ 5 , excluding the self-citations of all co-authors).

4. Concluding remarks

The scientific research output of Dr. Yavor Mitrev reveals that he is a researcher with in-depth knowledge in the field of organic chemistry and the application of NMR spectroscopy for: 1) qualitative / quantitative analysis of single (isolated) compounds and/or their mixtures, 2) studying the system behavior in solution and in solid state; 3) solving methodological problems developing new procedures and approaches. The options offered by modern NMR spectrometry constantly increase, but they require also a permanent user's improvement, a fact that is highly valid in the case of the candidate Yavor Mitrev. The quality of the presented materials is indisputable – 70% of its articles are published in recognizable journals in the first quartile such as *Chem Comm*, *Nanomaterials*, *Molecules*, *J Mol Liquids*, *Phys Chem Chem Phys*, etc. The obtained results are mainly referred by foreign scientists (99%). The membership of Y. Mitrev in various scientific projects is adequate to his professional specialization; he was a head of a scientific project, which confirms his ability to independently plan, conduct and summarize the scientific research. On the other hand, its ability to be a team-worker is also evident, considering its contribution in the most of the scientific communications. The results visibility was completed at scientific forums directly related to the running research topic.

According to the recent regulations for the acquisition of the academic position “associate professor” in 4.2. Chemical Sciences, the scientific production of Yavor Mitrev meets the national minimum requirements as well as the specific criteria of IOCCP-BAS:

Group	Indicator	Points – Y. Mitrev	Points required by IOCCP
A	1	50	50
C	4	112	100
D	7	242	220
E	11	194	70
G		6	≥ 5

The overall performance of Yavor Mitrev supports his application for the position of associate professor; based on its expertise he is ready to take his own professional direction of

future development. Undoubtedly, the habilitation will offer further additional opportunities for supervising PhD students, attracting project funding and deepening even more the active international cooperation – activities in which I sincerely wish Dr. Mitrev success.

In conclusion, the scientific contributions of Dr. Yavor Nikolaev Mitrev in the field of NMR spectroscopy give me a reason to strongly support his election as an “associate professor” in the professional field 4.2. Chemical Sciences (Organic chemistry) for the needs of the “NMR spectroscopy Center” at the Institute of Organic chemistry with Center of Phytochemistry – BAS.

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prof. Ivayla Pantcheva, PhD

Reviewer