

ATTITUDE OF REVIEWER
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Member of the Academic Jury set to render a decision on the competition for filling the academic position of an Associate Professor in the Professional Field 4.2. Chemical Sciences according to the Classifier of the Areas of Higher Education and the Professional Fields (Scientific Specialty "Organic chemistry")

1. Evaluation of the documents in the procedure

For participation in the announced competition, documents were received from a single candidate ch. assistant professor Vera Ventsislavova Deneva, Ph.D., from the Institute of Organic Chemistry with the Center for Phytochemistry (IOCCP), BAS. The set of materials presented by Dr. Deneva is in accordance with the Rules for the Development of the Academic Staff of the IOHTCF, and meets the criteria of the IOCCP-BAS for occupying the academic position of "associate professor".

The candidate has presented a list of a total of 26 scientific articles, of which 16 have been selected for participation in the competition, which are published after PhD thesis and are taken into account in the final evaluation. The specified publications are on the subject of the competition and are accepted for review, with 6 of them presented as an equivalent number of articles for a habilitation thesis (criterion **C**) and 10 as participating in the competition according to criterion **D**. The distribution of scientific works by quartiles is as follows: Q1: 12 and Q2: 4 nos., noting that two of the journals (*Spectrochimica Acta Part A* and *Foods*) are listed as Q2 according to Scopus and the candidate, but fall into Quartile 1 according to the Web of Science definition, and should to be considered as such. Dr. Deneva presents 118 citations are presented, significantly exceeding the required minimum (35 pieces), and making a good impression that the specified citations are only on the articles submitted for participation in the competition. The candidate holds *h*-index of 10 (Scopus), thus exceeding the requirements of the IOHCF for the academic position of associate professor.

A number of additional materials are also presented - a list of participation in 13 scientific research projects, one of which the candidate is the head of, data on participation in conferences, specialization abroad and a certificate for the Ivan Evstratiev Geshov award for youngest scientists.

Dr. Deneva received her master's degree in organic chemistry from Sofia University "St. Kliment Ohridski", Faculty of Chemistry (currently Faculty of Chemistry and Pharmacy) in 2009, and the same year she started her doctoral studies at the Institute of Organic Chemistry with the Center for Phytochemistry. After defending her thesis in 2012, she successively held the academic positions of assistant professor in 2012-2017 and senior assistant professor from 2017 to the present.

2. General characteristics of the candidate's research activity

According to the submitted materials, the candidate's research interests are in the field of the application of spectroscopy in the visible and ultraviolet regions for investigation of the

tautomeric properties of various organic compounds. The studies are summarized in three directions, united around the classes of studied compounds - tautomeric systems based on azo dyes (publications 1-6, **criterion C**), systems based on Schiff bases (publications 1-3, **criterion D**) and other tautomeric systems (publications 4-8, **criterion D**). Finally, two papers with other studies are also presented.

The contributions in each direction can be summarized as follows:

In the first direction:

- The tautomeric properties in several systems based on 4-(phenyldiazenyl) naphthalen-1-ol were studied, along with the possibility of controlling the equilibrium by means of protonation and complexation with alkaline earth metals. In a subsequent publication, based on existing structures and theoretical calculations, a design of a new sensor for the detection of alkaline earth metals is proposed using the same platform and tweezer-like ionophores containing amide group as substituents that support complexation.

- The tautomeric equilibria of two series of azo dyes containing a pyrazole ring were studied in solution and solid state, and it was found that varying the substituent at position 5 allowed shifting the tautomeric equilibrium entirely to the aza- or hydrazo-forms.

- Using UV-VIS and NMR spectroscopy, the behavior of three rotary switches - ethyl-2-(2-(quinolin-8-yl)hydrazono)-2-(pyridin-2-yl) acetate and two 4-hydroxy coumarin derivatives was investigated. Based on experimental results and quantum chemical calculations, a switching mechanism was proposed for each of the studied compounds.

In the second direction:

- The tautomeric equilibrium of phthalimide-derived Schiff based with salicylic and 2-hydroxynaphthyl residues was studied. A dependence between the size of the hydroxyaromatic substituent and the used solvent on the tautomeric properties of this type of system was established.

- Two examples of Schiff bases derived from 7-hydroxy quinoline were examined, and one of the compounds was found to be a promising candidate for bistable switch triggered by 365 nm irradiation.

- Using molecular spectroscopy and quantum chemical calculations the photophysics and dynamics of proton transfer in N-(benzo[d]thiazol-2-yl)picolinamide and N-(benzo[d]thiazol-2-yl)isonicotinamide were elucidated, and it was confirmed that the preferred mechanism is excited-state proton transfer from the amide to the benzothiazole nitrogen.

Other tautomeric systems:

The publications summarized in the third direction cover studies of tautomeric and conformational equilibria in solution, and in some cases also in the solid state, for various organic compounds - derivatives of 10-hydroxybenzo[h]quinoline, rotor switch based on substituted quinoline, derivatives of pinene-bipyridine and pinene-phenanthroline, the antiviral drug favipiravir, as well as a series of compounds with potential OLED properties.

The last two publications reflect the use of spectral techniques for determining active components in natural products and determining the quality of Bulgarian wines.

Given that most of the reviewed articles, aim at characterization of tautomeric equilibria of selected compounds, clarification of the factors that influence it and investigation of the

possibilities of its controlled shift, I believe that the scientific contributions can be referred to the category of "proving with new means of substantial new aspects of already existing scientific fields, problems, theories and hypotheses". A positive reference for the relevance of the research and its quality is the level of the journals in which the results were published - 14 of the journals fall into the first quartile and only two of the publications are in journals with the Q2 category. The originality of the research is well accepted by the scientific community, as evidenced by the number of citations – 118 independent citations from publications in international peer reviewed journals. Regrettably, the habilitation thesis does not outline the candidate's personal contributions clearly enough, but the fact that Dr. Deneva is the first author in 6 of the articles and the second author in other 5 allows me to assume that the candidate has a substantial involvement in the research.

3. Critical remarks and recommendations

My main remarks to the candidate are related to the clarity of the habilitation thesis and the structure of the presented material. Personally, I expected a more detailed habilitation report, especially in the part with the publications under criterion C, which in my opinion should be more clear with respect to the scientific contributions of the candidate to the greatest extent, especially given the interdisciplinary nature of the articles. I consider as a difficulty in the analysis of the materials also the discrepancy in reference numbering in the thesis, the lists of publications and the attached full-text copies. In conclusion, I would ask the applicant to give examples of the systems he is currently working on or plans to research in the immediate future, as I find the outlined perspectives for future research relatively broadly defined.

The recommendations described above do not detract from the scientific value of the considered materials, and I believe that they would rather help the candidate in future presentations of his results.

CONCLUSION

The candidate in the competition has submitted a sufficient number of scientific works published after the materials used in the defense her PhD thesis, and the results achieved in the scientific and research activity correspond to and in some cases exceed the specific requirements of the Rules of the IOCCP-BAS. After reviewing the materials and scientific works presented in the competition, analyzing their significance and the scientific contributions contained in them, I give my positive assessment and recommend the Scientific Jury to prepare a report-proposal to the Scientific Council of IOCCP-BAS for conferment of the academic position "Associate Professor to Dr. Vera Deneva in professional direction 4.2. "Chemical Sciences", scientific specialty "Organic Chemistry" for the needs of the "Organic Synthesis and Stereochemistry" laboratory.

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