REVIEW

of a thesis submitted for awarding the scientific degree „PhD“ in

4.1-Physical sciences according to the procedure pursued in

Faculty of Physics of Sofia University “St. Kliment Ohridski”

This review has been prepared by:

associate professor Hristo Iliev, Faculty of Physics, Sofia University “St. Kliment Ohridski” as a member of the jury according to order **RD 38-273/03.06.2024** of the Rector of Sofia University.,

Thesis title: Ultrafine structure of selected states in diatomic molecules

Thesis author: Velizar Rosenov Stoyanov

I. General description of the submitted documents

1. Data for the submitted documents

The applicant **Velizar Rosenov Stoyanov** has submitted 16 documents in total including dissertation in English, abstract in English and Bulgarian, as well as the required by the internal rules for the faculty of Physics tables for the fulfillment to the requirements scientific degree „PhD“.

He has also submitted a curriculum vitae, a diploma for a completed higher education with a "master's" degree an order for enrollment in the doctoral program, an order for the extension of the period of the doctoral program, a declaration of authorship, an application for pre-defense, a certificate of the successfully passed exams and the deduction of the candidate with the right of defense, protocol for verifying the originality of a dissertation work, as well as copies of the two publications contained in the dissertation work.

The documents submitted by the applicant for the defense comply with the requirements of the laws and the regulations for the terms and conditions for acquiring scientific degrees and occupying academic positions at Faculty of Physics of Sofia University “St. Kliment Ohridski” as well as the national requirements as defined in the corresponding lows (ЗРАСРБ, ППЗРАСРБ, and ПУРПНСЗАДСУ).

2. Applicant data

The applicant Velizar Stoyanov has been born in 1995 in Kyustendil. He graduated from the high school of science and mathematics "prof. Emanuil Ivanov" in 2014. In the period between 2014 г. to 2018 г. he is a student in the Faculty of Physics specialty, "Quantum and Cosmic Theoretical Physics". From 2019 to 2020, he is a master's student in "Theoretical and Mathematical Physics" again at the Faculty of Physics of Sofia University “St. Kliment Ohridski” and immediately after his graduation in 2020 he become a full-time doctoral student in professional direction 4.1- Physical sciences, specialty: "Physics of atoms and molecules" at the Department of "Optics and Spectros-

copy", Faculty of Physics of SU Sofia University “St. Kliment Ohridski”. As a professional experience it is worth mentioning his work as a technician in IBPhotonics Ltd. in the period between 2017 г. and 2018 г. while he was still a student. From 2020 to 2021, while he was a doctoral student, he was also appointed as a physicist in the Research Sector at Sofia University “St. Kliment Ohridski”. From 2022 to 2023, he was appointed as a first-level researcher under the program "Young scientists and post-doctoral students", Faculty of Physics of Sofia University “St. Kliment Ohridski”. From 2023 until now, he has been appointed as a young scientist under the "Sofia University - Marker for Innovation and Technology Transfer (SUM-MIT)" project.

3. General evaluation of the scientific achievements of the applicant

The publications used in the dissertation includes a paper from group **I** published in peer revied journal with impact factor (JCI - Q2) and a full text conference proceeding from group **III** with impact rank (SJR). These two publications results in 30 pts in total, deliverables form group Г, which corresponds to the minimal national requirements, but also cover the additional requirements of the faculty of physics, ate least one of the publications to be in a journal with impact factor. In both publications the applicant is the first author with a major contribution. In the documents applicants state that he has participated in three conferences with a poster presentation, but the list of the publications included in the dissertation covers only the papers and no evidence for the conferences has been found. After an official request for the chair, the list was send to the jury.

To the moment of preparation of the current review, no citation of the works used in the dissertation has been spotted. I have found no evidence for the publications had been used in previous procedures for academic positions and no evidence for the plagiarism

After the review of the documents and because of what has been said above I believe that:

a) the scientific publications included in the dissertation meet the requirements of the laws and the regulations for the terms and conditions for acquiring scientific degrees and occupying academic positions at Faculty of Physics of Sofia University “St. Kliment Ohridski” (ЗРАСРБ, ППЗРАСРБ, and ПУРПНСЗАДСУ);

b) scientific publications included in the dissertation work do not repeat those from previous procedures for acquiring a scientific title and academic position;

c) no plagiarism has been proven in accordance with the law in the submitted dissertation work and in the abstract on it.

4. Characteristics and assessment of the candidate's teaching activity

The applicant dos does not submit proof for teaching activity, but from my personal experience I know he is actively involved in the work with the students working and preparing their diploma works in the laboratory.

5. Content analysis of the applicant's scientific and scientific-applied achievements contained in the materials for participation in the competition

Diatomic alkali metal molecules have been and still are of interest in numerous experimental and theoretical studies. From an experimental point of view, they are attractive due to their relatively

easy preparation (alkali metals have relatively low melting and vaporization temperatures) and due to the fact that there are available laser sources that cover a large part of their optical spectrum. From a theoretical point of view, they are much more complex quantum mechanical systems than those of individual atoms, but at the same time much simpler than those of large and complex molecules, which gave a possibility for the direct application of various theoretical models and their comparison with experimentally obtained spectra.

The dissertation work of Velizar Stoyanov is dedicated to the study of selected energy levels in the diatomic molecule of KRb, and two different isotopes were studied: $^{39}K^{85}Rb$ and $^{39}K^{87}Rb$. The selected states are not chosen because of their simplicity, but on the contrary, because they interact with each other which leads to the presence of fine and ultra-fine structure, the study of which is the main task of the presented work. A theoretical model based on an effective Hamiltonian was developed, which successfully describes the experimentally obtained results for the broadening of the lines in the case of $^{39}K^{85}Rb$ and their splitting into four separate lines in the other isotope $^{39}K^{87}Rb$.

In technical point of view, the thesis is 178 pages long, written in very good English and includes 31 figures with clear graphs and illustrations, 5 tables and 104 references. The dissertation is formally divided into two parts, a theoretical study and an experiment with subsequent analysis of the obtained results. Organized in 9 chapters, the first two of which are introductory, giving a precise and clear idea of the objectives of the dissertation and the tasks set. **Chapters 3, 4** and **5** systematically present the theoretical model, used later along with numerical methods, to analyze the experimentally obtained spectra. A very good impression is made by the systematic and clear presentation of the theoretical model and the main experimental methods used, with the obvious goal of being complete, coherent and accessible to the reader, despite the complex matter. This makes the work complete from an experimental and theoretical point of view, which in the future can help the citation of the dissertation.

Chapter 6 examines in detail the main spectroscopic methods used in the dissertation, namely saturation spectroscopy and double optical resonance spectroscopy. In **chapter 7** the experiment is presented, and the main experimental results are given. **Chapter 8** compares experimental results with theoretical predictions using numerical simulations. **Chapter 9** provides a summary.

In my opinion, the main contributions in the dissertation can be systematized as follows:

1. An experimental setup including a molecule source, a laser source and spectroscopic equipment was built, and four different spectroscopic methods have been used.
2. A complete theoretical model was built based on the so-called effective Hamiltonian, including the fine and hyperfine structure of the energy levels. The model shows good agreement with the experimentally obtained results for the position and the spectral width of the lines.
3. The fine and ultrafine structure of two isotopes of the KRb molecule between two specific states $B^1\Pi$ and $c^3\Sigma^+$ in the range of the rotational quantum number $20 < J < 60$, where a strong entanglement and interaction between the two energy levels was investigated.

4. In the case of the isotope $^{39}K^{87}Rb$, experimental spectra were obtained with good resolution for the ultrafine structure of 6 separate lines showing the splitting of 4 separate components, and these experimental results were compared with the theoretical model, including their positions and intensities.
5. For the other isotope $^{39}K^{85}Rb$, experimental fine structure results are obtained, and the positions of the identified lines are compared with the theoretical results. The ultrafine structure of the spectral lines predicted by the theoretical model was not observed in the experimentally obtained spectra, but only broadening of the individual lines. The reasons for this are discussed in detail in the dissertation.
6. For the two isotopes, the nuclei that make the main contribution to the spin-orbital interaction and, accordingly, the ultrafine structure of the spectral lines, have been identified.
7. Obtained molecular constants and estimated their uncertainties for the two isotopes of the molecule $^{39}K^{85}Rb$ and $^{39}K^{87}Rb$. Their physical meaning is also discussed.
8. The results in the dissertation are reflected in two publications, one in the Journal of Quantitative Spectroscopy and Radiative Transfer (JQSRT) and one in the Journal of Physics: Conference Series. In all works, the candidate is the first author and has a major contribution.

6. Critical notes and recommendations

As a drawback of the work, I can say that in some places for the seek of complete and systematic presentation, it is hard to find and distinguish the personal scientific achievements of the applicant. For example, in the very systematically presented theoretical part of the thesis, it was hard to find which parts are new, developed and proposed by the applicant and which parts are common knowledge.

It is good practice and style if the figures and the tables appear in the text near the places where they are mentioned. For example, in chapter 8.1 where $^{39}K^{87}Rb$ is discussed fig. 8.1 and 8.2 as well as tables 8.1 and 8.2 can be found in the next chapter where the other isotope $^{39}K^{85}Rb$ has been discussed, which is a bit confusing.

I also have some questions to the applicant:

1. In the theoretical model it is clearly stated that a general assumption when diagonalizing the matrices is that the Fermi-contact interaction is weak. That is, the off-diagonal components are negligible and have no significant contribution. This should be true in a larger part of the studied range, but not where the two studied energy levels intertwine, around J=40 – 50. Are there serious deviations of the theoretical model in this area and is there room for improvement of the model?
2. Does the theoretical model presented in this way allows calculation of important parameters of the system, such as lifetimes of the excited states, cross sections for spontaneous and possibly for stimulated emission? Such a theoretical results could be compared with experimental results from fluorescence spectroscopy for example.

3. What accounts for the significant difference in the width of the lines for the two isotopes and, accordingly, the absence of ultrafine structure in the case of $^{39}K^{85}Rb$?

7. Personal impressions of the candidate

I have known Velizar Stoyanov since 2017 when he was working on his bachelor's thesis in the laboratory of laser physics and applications, where at that time part of my scientific research was also taking place. Even then, Velizar made a good impression with his calm, systematic approach to any task, experimental or theoretical, and showed the ability to work independently on specific problems. My main impressions from that time is that Velizar is independent, hardworking and very careful in his experimental work. Now, several years later, from his dissertation work, I see that he copes very successfully with quite non-trivial theoretical problems, such as that of diatomic molecules, thus combining in himself the skills of a good experimenter and theorist, which is a rare and valuable combination.

Conclusion

After a detailed review of the abstract, the thesis and all the other submitted documents, based on the analysis of their significance and the scientific contributions contained in them, **I confirm that the scientific achievements of Velizar Rosenov Stoyanov meet the requirements** of the laws and the regulations for the terms and conditions for acquiring scientific degrees and occupying academic positions at Faculty of Physics of Sofia University “St. Kliment Ohridski” (ЗРАСРБ, ППЗРАСРБ, and ПУРПНСЗАДСУ). In particular, the candidate satisfies the minimum national requirements in the professional field and no plagiarism has been found in the dissertation, abstract and scientific works submitted for the competition.

I am giving my positive assessment of the dissertation work of Velizar Rosenov Stoyanov.

II. GENERAL CONCLUSION

Based on what has been said, I gave my recommendation to the scientific jury to **award the scientific degree "PhD" in 4.1 Physical sciences to Velizar Rosenov Stoyanov**.

September 04, 2024. Prepared by: .....

(Assoc. Prof. Hristo Iliev)