1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: Spectral line shapes calculations for atmospheric and fundamental study

1.1. Project goals

- application of realistic potentials for description of atomic and molecular collisions
- calculations of molecular spectral line shapes considering realistic description of collisions
- application of optical molecular transition for atmospheric and fundamental study

1.2. Outline

Understanding and realistic description of atomic and molecular spectral line shapes is crucial for many areas of science including of study on: Earth atmosphere and climate changes, exoplanets and search for extraterrestrial life, fundamental test of quantum electrodynamics and search for new interactions beyond standard model. The modern approaches [Ciurylo1997] developed in the end of 20th century for description of spectral line shapes go beyond Voigt profile and simulatonusly includes several effects such as: Dicke narrowing, speed-dependent effects, collision time asymmetry and line intensity variation, line-mixing. They are now incorporated in new generation of spectral data basis like HITRAN [Wcislo2016].

The cutting edge of this research is development of *ab initio* approaches for calculations of spectral line shapes [Ciurylo2001, Wcislo2013PRA, Slowinski2020]. Up to now rather simple potentials [Ciurylo2001, Wcislo2013JQSRT] where used for description of velocity-changing collisions leading to Dicke narrowing. The main goal of this project is to develop efficient approaches to include more realistic interaction between molecules. Realization of this task will required advanced mathematical and programing skills, deep understanding of physical problems, knowledge of statistical physics, algebraic methods, perturbation theory, quantum mechanics, numerical methods and application artificial intelligence technology. Having efficient way of realistic line shape calculations one could verify influence of proper description of molecular collisions on molecular spectra and confront them with existent models. Finally, developed approach could be used for data analysis of experimental spectra important for atmospheric spectra and fundamental research [Slowinski2020, Cygan2025].

1.3. Work plan

- development of description of velocity-changing collisions with realistic interactions (M1-M24)
- development of effective approach for spectral line shape calculations considering realistic description of collisions (M12-M36)

- confrontation of calculations with available experimental spectra and its application for atmospheric and fundamental study (M24-40)
- writing, submitting and defending the thesis (M36-M48)

1.4. Literature *(max. 7 listed, as a suggestion for a PhD candidate preliminary study)*

[Ciurylo1997] R. Ciuryło, J. Szudy, J. Quant. Spectrosc. Radiat. Transfer 57, 411 (1997).

[Ciurylo2001] R. Ciuryło, D. A. Shapiro, J. R. Drummond, A. D. May, Phys. Rev. A 65, 012502 (2002).

[Cygan2025] A. Cygan, S. Wójtewicz, H. Jóźwiak, G. Kowzan, N. Stolarczyk, K. Bielska, P. Wcisło, R. Ciuryło, D. Lisak, Sci. Adv. 11, eadp8556 (2025)

[Slowinski2020] M. Słowiński, F. Thibault, Y. Tan, J.Wang, A.-W. Liu, S.-M. Hu, S. Kassi, A. Campargue, M. Konefal , H. Jóźwiak, K. Patkowski, P. Żuchowski, R. Ciurył, D. Lisak, P. Wcisło, Phys. Rev. A 101, 052705 (2020).

[Wcislo2013JQSRT] P. Wcisło, R. Ciuryło, J. Quant. Spectrosc. Radiat. Transfer 120, 36 (2013).

[Wcislo2013PRA] P. Wcisło, A. Cygan, D. Lisak, R. Ciuryło, Phys. Rev. A 88, 012517 (2013).

[Wcislo2016] P. Wcisło, I. E. Gordon, H. Tran, Y. Tan, S.-M. Hu, A. Campargue, S. Kassi, D. Romanini, C. Hill, R. V. Kochanov, L. S. Rothman, J. Quant. Spectrosc. Radiat. Transfer 177, 75 (2016).

1.5. Required initial knowledge and skills of the PhD candidate

- The applicant has to have finished a master degree within the last 4 years prior to recruitment in physics or a closely related field
- An excellent academic record
- Experience through coursework and/or a research project in atomic and molecular physics
- Experience through coursework and/or a research project in quantum mechanics and statistical physics
- Experience in programing and application of numerical methods
- It is highly beneficial if the master thesis has been done in atomic, molecular or optical physics

1.6. Expected development of the PhD candidate's knowledge and skills

experience, knowledge and skills that are important in the high-tech industry and academia: molecular spectroscopy, atom-light interaction, statistical physics, transport phenomena, programming and other