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

Project title: Quantum scattering calculations for atmosphere relevant molecular systems

1.1. Project goals

- *Ab initio* quantum scattering calculations for diatomic molecules that are relevant for the atmospheres of Earth and other planets (such as CO-N_2)
- Application of the quantum scattering calculations for determination of the generalized spectroscopic cross sections and collision-perturbed spectra simulations
- Tests and development of approximated quantum-scattering calculation techniques that can enable accurate calculations at high temperatures (up to 1000 K)

1.2. Outline

Remote measurement of the composition of atmospheres of Earth and other planets are based on spectroscopic measurements. It turns out that the experimental accuracy achievable today requires the collisional line-shape effects to be properly handled in the atmospheric spectra interpretation [Miller2005]. The scientific missions aimed at monitoring Earth greenhouse gases from both space- and ground-platforms require increasingly accurate line-shape parameters over the wide range of temperature range. For instance, the Orbiting Carbon Observatory-2 NASA satellite mission [Miller2007] has a target relative uncertainty of 0.3% in the retrieval of the column-integrated carbon dioxide molar fraction. NASA and ESA defines similar goals for other projects such as TCCON, ASCENDS mission, as well as MERLIN mission. Such measurements require accurate radiative-transfer codes for modeling the atmospheric absorption from lower troposphere through the upper stratosphere. These spectroscopic models are based on accurate line-by-line spectroscopic databases and require accurate values of the beyond-Voigt line-shape parameters, which are not available yet (almost at all). Availability of the accurate reference line-parameters becomes also important for the studies of the atmospheres of other planets. For instance an accurate list of the pressure broadening and shift coefficients for electric-quadrupole H_2 and -dipole HD lines is required for the spectroscopic studies of the atmospheres of giant planets [Lellouch2010], in particular the determination of the D/H ratio (both He- and self-perturbed). Furthermore, the accurate values of the line-shape parameters also become crucial for exoplanets studies [Tennyson2017]. Today they already play an important role since the line broadening directly determines the opacity of the exoplanetary atmospheres. In the near future, when the use of the line-by-line inverse retrieval codes [Waldmann2015] would become a routine in exoplanets' spectra analysis the importance of the reference line-shape parameters will be even larger. This PhD project constitute a significant step toward construction a comprehensive *ab initio* dataset of

reference spectra [Stolarczyk2020] for such atmospheric studies. The PhD student will perform *ab initio* quantum scattering calculations for the atmosphere-relevant systems and use the resulting scattering S-matrices to determine the generalized spectroscopic cross sections. The cross sections will be used to calculate the beyond-Voigt line-shape parameters and, hence, provide accurate reference spectra.

1.3. Work plan

- Preparation and expansion (over a set of appropriate basis functions) of the potential energy surfaces
- Performing the scattering close-coupling calculations
- Calculating the generalized spectroscopic cross-sections
- Calculating the collision integrals and the beyond-Voigt line-shape parameters
- Implementation of the approximate solutions to the close-coupled equations

1.4. Literature *(max. 10 listed, as a suggestion for a PhD candidate)*

[Lellouch2010] E. Lellouch et al., A&A 518, L152 (2010)
[Miller2005] C.E. Miller,et al., C. R. Phys. 6, 876 (2005)
[Miller2007] C.E. Miller, et al., J. Geophys. Res. 112, D10314 (2007)
[Stolarczyk2020] N. Stolarczyk, ..., P. Wcisło, JQSRT 240, 106676 (2020)
[Tennyson2017] J. Tennyson, S.N. Yurchenko, Mol. Astrophys. 8, 1 (2017)
[Waldmann2015] I. P. Waldmann, G. Tinetti, et al., Astrophys. J. 802, 107 (2015)

1.5. Required initial knowledge and skills of the PhD candidate

Skills and experience in theoretical physics. Good knowledge of FOTRAN or C (also Matlab and Python). Excellent problem-solving and communication skills. Written and verbal communication skills and presentation skills. Teamwork ability. Good command of the English language.

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

Knowledge, skills and experience in molecular physics, computer coding and numerical methods. Knowledge of quantum-scattering theory, molecular interactions and molecular spectroscopy.