

PHD PROJECT DESCRIPTION

(4000 characters max., including the aims and work plan to be published online)

Project title: Advancing molecular spectroscopy: high-accuracy tools for atmospheric and fundamental research

1.1. Project goals

- Development of the cavity-enhanced spectrometer with the frequency axis linked to the primary frequency standard
- High-resolution study of near-infrared transitions of small molecules such as CO, CO₂, H₂ with the use of advanced theoretical line-shape models

1.2. Outline

High-quality data on molecular spectral line shapes are essential for applications in metrology, atmospheric science, astrophysics, and fundamental physics, many of which demand extremely high accuracy. For example, satellite monitoring of greenhouse gas concentrations by major space agencies (NASA, ESA) already requires sub-percent accuracy of laboratory reference data. Such measurements support research on climate change, climate zones shifting, and extreme weather. In fundamental physics, testing quantum electrodynamics (QED) and searching for the new physics beyond the Standard Model relies on extremely precise measurements of H₂ transition frequencies. In addition, modelling exoplanet atmospheres and searching for extraterrestrial life require comprehensive spectral data, including weak transitions from higher overtones in complex molecules.

This project aims to develop a state-of-the-art, high-resolution, ultra-sensitive spectrometer based on cavity-enhanced techniques. Methods such as cavity ring-down spectroscopy (CRDS) and cavity mode-dispersion spectroscopy (CMDS) will be employed to measure absorption and dispersion with exceptional precision.

While theoretical *ab initio* calculations can describe collisional effects in molecular spectra, accurate results are currently limited to simple systems like H₂. For more complex molecules such as CO and CO₂, reliable predictions - especially of line intensities - are still emerging and require experimental validation. This project will combine high-quality laboratory measurements with theoretical work in collaboration with world-leading groups from University College London and Université de Rennes, building on recent successes that have already achieved accuracy at the promille level.

Proper description of spectral lines also depends on advanced line-shape models that account for effects such as the speed-dependent collisional broadening and Dicke narrowing. Wherever possible, especially for simple systems like H₂, experimental results will be compared with first-principles quantum mechanical predictions, enabling highly precise tests of QED. The experimentally retrieved and theoretically supported line-shape parameters will ultimately be incorporated into major spectroscopic databases like HITRAN, improving tools used for spectral modelling worldwide.

1.3. Work plan

- Development of cavity enhanced spectrometer
- Measurements of molecular spectra
- Line-shape analysis of measured spectra

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

- [1] P. F. Bernath, *Phil. Trans. R. Soc. A.* **372**, 20130087 (2014).
- [2] G. Li et al., *Astrophys. J. Suppl. Ser.* **216**, 15 (2015).
- [3] W. Ubachs et al., *J. Mol. Spectrosc.* **320**, 1 (2016).
- [4] A. Cygan et al., *Opt. Express* **27**, 21810 (2019).
- [5] K. Bielska et al., *Phys. Rev. Lett.* **129**, 043002 (2022).
- [6] L. Gianfrani et al., *Riv. Nuovo Cim.* **47**, 229 (2024).
- [7] A. Cygan et al., *Sci. Adv.* **11**, eadp8556 (2025).

1.5. Required initial knowledge and skills of the PhD candidate

Knowledge of optics, electronics, atomic and molecular physics at the level corresponding to standard undergraduate university courses. Experience in construction of experimental optical systems and/or spectral line-shape analysis is welcome. Skills and experience in programming (Labview/Mathematica/C++/Fortran/Python) and numerical methods will be an additional advantage. Teamwork ability and high motivation for research work. Good command of the English language.

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

Knowledge, skills and experience enabling work in world-leading groups devoted to various aspects of quantum physics, optics and metrology. Knowledge, skills and experience in development of cavity-enhanced spectrometers and high-sensitive spectroscopic techniques. Knowledge of molecular spectroscopy, spectral line-shape theories and numerical methods. Preparation for writing scientific articles and setting experimental goals. Development of skills needed in international collaboration with experimental and theoretical groups.