Tytuł projektu

Badania z wysoką dokładnością natężeń słabych linii molekularnych pod kątem zastosowań atmosferycznych

Project title

Highly accurate line intensity studies of weak molecular transitions for atmospheric application

Dyscyplina /Area of science

Nauki fizyczne

PROJECT DESCRIPTION

Project goals

- To use spectroscopic techniques utilizing high finesse optical cavities to accurately determine spectral parameters of weak molecular transitions
- To determine the most accurate experimental line intensities
- To provide data experimental data for joined theoretically-experimental molecular linelists

Outline

Precise and accurate spectroscopic measurements are sources of knowledge on the Universe and condition of our atmosphere. They also enable research in micro scale, especially on atoms and molecules. However, in spite of long term investigations, there are no accurate enough models of molecular spectra, which might be used as reference data. Growing number of applications require permile accuracy on reference line intensities, which is confronted with order of magnitude higher uncertainties of line intensities typically available in commonly used spectral databases such as HITRAN. The PhD project will be part of the research project devoted to development of techniques of construction of spectral models far more accurate than ones presently available.

The spectrum of even small molecules, such as carbon monoxide, consists of hundreds or thousands of lines with intensities measurable in laboratory conditions. There are even more lines with intensities orders of magnitude lower. Many of these very weak lines belong to the so-called "hot bands". Line intensities in these bands are very low in laboratory temperatures, however they increase with temperature and become important in atmospheres of many stars and exoplanets.

A huge number of lines in spectrum causes that it is impossible to construct high quality spectrum models based only on experimental data. On the other hand, purely theoretical *ab initio* calculations do not achieve good accuracy for molecules larger than hydrogen. This problem can be solved by including a certain amount of highly accurate experimental data in theoretical calculations. Such an approach allows predicting the intensity of non-measured lines with high accuracy. However, the accuracy of laboratory data needs to be about order of magnitude higher from accuracy of line intensities stored in commonly used spectral databases such as HITRAN. The project will be realized

in collaboration with theoretical molecular spectroscopy group at University College London. The main task of the PhD student will be to acquire and analyze ultra accurate spectral data for molecules of atmospheric importance, such as carbon monoxide, carbon dioxide and water, in order to provide experimental line intensities.

Measurements will be performed with state-of-the art spectrometers built and continuously developed in our laboratory. They utilize three measurements techniques based on high finesse optical cavities. These are cavity ring-down spectroscopy (CRDS), cavity mode-width spectroscopy (CMWS) and cavity mode-dispersion spectroscopy (CMDS). CRDS has already been established as an ultrasensitive experimental technique. It relies on measurement of photon life time in an optical cavity, decreasing with increase of sample absorption. Two other techniques, CMWS and CMDS, are new techniques complementary to CRDS. CMWS is based on measurement of width of the cavity mode, which increases with increasing absorption, whereas CMDS relies on measurement of the cavity mode shift due to sample dispersion. We have recently shown that CMDS is highly linear in large dynamic range and free from systematic uncertainties which are present in CRDS and CMWS due to nonlinearity of the detection system.

Work plan

- 1. Introduction into cavity ring-down spectroscopy (CRDS), cavity mode-width spectroscopy (CMWS) and cavity mode-dispersion spectroscopy (CMDS) techniques
- 2. Spectral data analysis methodology, including multispectrum fit approach
- 3. Highly accurate experimental study of weak molecular transitions for molecules such as carbon monoxide, carbon dioxide and water.

Literature

D. Romanini et al., "Introduction to Cavity Enhanced Absorption Spectroscopy", in "Cavity-Enhanced Spectroscopy and Sensing", ed. G. Gagliardi, H.-P. Loock, Springer 2014

A. Cygan et al., Opt. Express 23 (2015) 14472

O. Polyansky et al., Phys. Rev. Lett 114 (2015) 243001

Required initial knowledge and skills of the PhD candidate

→ MSc in physics, chemistry or related field

- → knowledge of optics, electronics, molecular physics, laser spectroscopy and numerical methods at the level equivalent to basic university courses
- → programming skills in at least one programming language
- → knowledge of cavity-enhanced spectroscopy techniques and automation of measurements processes in LabView will be an additional advantage
- ➔ good English

→ teamwork skills and high motivation for research work

Zgłaszający projekt/ Author of the project	
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