Reg. No: 2015/18/E/ST2/00585; Principal Investigator: dr hab. Daniel Lisak

Spectroscopy is the most accurate method to study the fundamental properties of matter and its interactions with radiation. The complexity of the absorption or emission spectra of the molecules allow to obtain precise information on the investigated system and its physical state. Precise data on the frequency, intensity and shape parameters of molecular spectral lines are required in applications such as research on atmosphere of the Earth and other planets, modeling weather and climate change, spectroscopic determination of the temperature and pressure of the gas, detection of trace gases and pollutants, calibration of measuring devices and non-invasive medical diagnostics. Satellite and ground-based lidar systems for monitoring the Earth's atmosphere with high spatial resolution require precise spectroscopic data on selected molecular transitions. The parameters of spectral lines often must be known with the uncertainties of tenths of a percent. Obtaining such a precise reference laboratory data is difficult and requires taking into account a number of physical effects caused by light – matter interaction and interaction between the gas molecules - so-called collisional effects, affecting the shape and center frequency of absorption spectral lines. To fully exploit the potential of laser spectroscopy it is therefore essential to do basic research on the influence of physical conditions influencing molecular system (such as temperature, pressure, gas composition) on the observed absorption spectrum and to develop a parametrized models based on physically justified assumptions, describing the spectrum in an interesting range of variability of physical conditions.

The project aims to study experimentally the temperature and collisional dependencies of spectral lines for molecules important e.g. in atmospheric research and climate change, as well as to develop new cavity-enhanced spectroscopic methods, both Doppler-free methods with very high resolution, and the broadband methods using the optical frequency comb as a source for excitation of molecular transition. In particular, we plan to experimentally investigate dependence of collisional broadening and shifting of spectral lines on the speed of molecules and to verify the theoretical models describing the shape of the line. These data will allow the correct interpretation of other line shape effects, particularly the collisions changing velocity of molecules absorbing the radiation.

We plan to investigate the applicability of new methods of measuring the absorption spectrum from the width of the optical cavity modes and dispersion spectrum from shifts of the cavity modes, for the broadband spectroscopy based on the optical frequency comb (OFC). These new methods are based on measurement of the frequency and not the intensity of light, so that it is possible to obtain a very high accuracy of measurement and to eliminate systematic instrumental effects of broadband spectroscopy in the cavity due to the dispersion effect in the cavity.

Experimental studies of molecular spectra in the visible range (O_2) and near infrared (CH_4, CO, CO_2, C_2H_2) will be done by the frequency-stabilized cavity ring-down spectroscopy, which is constantly developing by us and is now the most accurate technique for measuring the low-intensity lines. To study the temperature dependence of the line shapes the optical cavity (containing the test gas) with precise temperature control will be built.

The above mentioned requirements for precision of molecular spectra description caused that new spectroscopic databases are switching to the description of the spectral lines beyond the Voigt profile approximation. Recently the HTP model was adopted as a new standard description of the shape of the spectral lines. It allows achieving the desired accuracy of below 0.1%, but the experimental determination of its parameters is difficult due to their correlations. Direct measurement of the speed-dependent effects enable investigation and correct interpretation of the spectra and provide critical data to the mentioned earlier applications as well as will enable verification of the theoretical methods of molecular physics. So far, almost all experimental data on advanced spectral line-shape analysis are limited only to room temperature. The determined dependence of the collisional line shape parameters on the temperature and molecular velocity will allows for verification of theoretical methods of calculating the line shapes developed in collaborating research groups.

Broadband spectroscopy with optical frequency comb in the optical cavity is now being rapidly developed. Its huge potential arises from high speed of measurement of broad spectrum without loss of high resolution. Therefore, it is the perfect tool to provide reference spectroscopic data and for metrology and detection of gases. Elimination of the instrumental effects by determining the spectrum from the frequency measurement, instead of the amplitude should allow achievement of accuracy similar to methods using continuous-wave diode lasers, while maintaining unmatched speed and easier transfer to the strongest molecular bands in the infrared.