Project objective

The object of the current project is the carbon monoxide molecule and its interaction with argon atoms. From a physical point of view, such molecule is a system of two connected massive particles, which may vibrate and rotate. To describe the physical processes concerning the behavior of single molecules we cannot limit ourselves to classical physics, but have to make use of the quantum view. In this case, this means that the vibrations and rotations can only occur in very specific ways to which certain discrete energy states are ascribed. The most common way to observe the states is through molecular absorption spectroscopy, where energy in the form of electromagnetic field is is absorbed by the molecule and the amount of energy absorbed is measured. The relation between the frequency of the electromagnetic field and the degree of absorption takes a certain shape, which we call the spectral line shape. By analyzing the spectral line shapes, information about the internal structure and dynamics of the molecule, and its interactions with environment can be retrieved (in this case collisions with argon atoms) . The most accurate spectroscopic techniques use laser radiation of precisely known frequency. In this project we will use a laser emitting ultra-short pulses to generate so called optical frequency comb, which is equivalent to using tens of thousands single-frequency lasers. The main aim of the project is to obtain accurate theoretical predictions and broadband measurements of spectral line shapes of carbon monoxide perturbed by argon. As a result of recent measurements, an unexpected form of dependence of line shape positions on pressure was observed. The secondary aims of the project comprise explaining the irregularity and using the measurements obtained with an optical frequency comb for sophisticated line shape analysis.

Research

In the computational part of the project, the Schrödinger equation describing scattering of argon atom on carbon monoxide molecule will be solved. This solution will be used to retrieve information on the effect of collisions on the internal molecular states and on direction of its motion and its speed. This information will enable us to describe the way in which collisions effect the molecule-light interaction and to construct spectral line shapes of transitions of interest. The measurements will be performed by one of techniques, which uses the precise knowledge of frequencies contained in the optical frequency comb to obtain the spectral line shapes of many transitions at the same time. Because of the very small absorption of light in the investigated spectral range by the carbon monoxide molecules, an optical absorption enhancement cavity will be used. A cavity consists of two mirrors with very low transmission coefficient and very low losses. Electromagnetic waves whose wavelengths permit a build-up of standing waves between the mirrors are trapped in the cavity for a long time (few microseconds compared to two nanoseconds needed by the light to travel the cavity length distance in air). In this time light travels up to a dozen kilometers. This behavior enables measuring the absorption of very small amounts of carbon monoxide and enables us to ignore the effect of collisions of carbon monoxide molecules with each other on the line shapes.

Motivation

The results of the project will be the first theoretical predictions and the first accurate measurements of carbon monoxide spectral line shapes in the investigated spectral range. The calculations will represent one of very few obtained in fully quantum mechanical framework using a realistic interaction potential. For the measurements, a recently developed technique will be used, which has not been applied before for retrieving spectral line shapes with such accuracy. The development of the technique will augment the set of tools with which we can precisely interrogate the nature. The inclusion of both experimental and theoretical part in the same projects will allow for ongoing verification of results and allow for immediate investigation of any potential unexpected effects. The theoretical predictions will be essential to solve the puzzle of nonlinear dependence of the line position on pressure, whose explanation will enrich the scientific knowledge. The results will find applications in atmospheric research, whose aim, among other things, is to explain global climate changes, and in exoplanetary science. The project will verify the accuracy of a new potential energy surface, describing the interaction between carbon monoxide molecules and argon atoms. The same surface will be used in investigations on cold Ar-CO complex and intermolecular forces responsible for its bonding.