DESCRIPTION FOR THE GENERAL PUBLIC

Objectives of the project

The object of the proposed studies is the simplest molecule, i.e., the hydrogen molecule. From physical point of view, such molecule is a system of two bound particles, which may rotate and oscillate. It has to be remembered, however, that this system is a microscopic object, which is not driven by the classical mechanics but by the quantum mechanics. Therefore instead of thinking about classical rotations and vibrations one should rather think about rotational-vibrational states (or shorter rovibrational states). The fundamental difference between the classical and quantum approaches is that the quantum bound states may have only some strictly allowed discrete values of energy. The most common way of studying such states is molecular spectroscopy, which in principle is nothing more than observing which frequencies are absorbed by the molecules. The values of these frequencies (known as positions of molecular lines) give the information about the internal structure and dynamics of the molecule. A much deeper information can be obtained if studying not only the line positions but also their shapes. In this project we will study a molecular hydrogen perturbed by the helium atoms (we will use the mixture of hydrogen and helium dominated by helium). The analysis of the line shapes will allow us to study not only the internal structure of the hydrogen molecules, but also the physics of the collisions between the hydrogen molecules and helium atoms. Note that within the quantum mechanics the collisions, in fact, should be regarded as a scattering of the matter wave and then the state of the whole system (in our case hydrogen molecule + helium atom) is called the scattering state. The first goal of this project is a comparison, at unprecedented level of accuracy, of the experimental shapes of molecular lines of hydrogen perturbed by helium with the theoretical predictions from first principles. The second goal is to use the developed and experimentally verified by us model to generate a complete dataset of parameters describing the line shapes for the system of molecular hydrogen perturbed by helium.

Research to be carried out

In the project we will carry out both the ultra-accurate measurements of the line shapes as well as the ab initio calculations. Within the experimental part an ultra-high finesse cavity will be used (i.e. the system of two highly reflective mirrors with very small losses). Such cavity traps the light for a long time, which causes that the overall optical path may reach several or even over a dozen kilometers. In effect, the response of the molecules is significantly enhanced, which allows the molecular line shapes to be accurately studied. The source of light is a very narrow (spectrally) and stable laser referenced to optical frequency comb (optical frequency comb is a laser system allowing the frequency of light to be measured with the accuracy reaching over a dozen significant digits), which makes the influence of the apparatus effects on the line shape negligible and ensures high repeatability of the measurements. Within the theoretical part of the project the scattering of the hydrogen molecules on the helium atoms will be handled with the Schrödinger equation, which solution will allow us to describe how the collisions perturb the internal state of the molecule as well as its translational motion which, in turn, will allow us to study the influence of the collisions on the light-molecule interaction and hence simulate the spectral line shapes.

Reasons for choosing the research topic

The result of the project will be the first comparison of the shapes of molecular lines determined from quantum calculations from first principles with ultra-accurate experimental spectra. The comparison of theory and experiment at the unprecedented level of accuracy will directly contribute to the development of science. Moreover a proper treatment of the shapes of molecular lines is crucial for many branches of optical metrology based on molecular spectroscopy. In particular, it is required for the studies of the atmospheres of Earth and other planets. The results on H_2-He, proposed within this project, will be applied to the studies of the atmospheres of gas giants (i.e. the planets like Jupiter) and in long-term perspective it could be also applied to the studies of the exoplanets. Moreover the results of this project will constitute a bridge between the quantum chemistry and the ultra-accurate molecular spectroscopy, which will allow the theoretical potential energy surfaces to be tested experimentally. Finally, the dataset generated within this project will be incorporated into the most popular database of spectral lines HITRAN as a model example of handling the collisional effects.