Spectroscopy is the most popular method of molecular research. It consists of illuminating the molecules with the light which has different wavelengths and observing when the molecules absorbed or transmitted the light. The relation between the absorption and wavelength of the light is called a spectrum. For some groups of wavelengths more light is absorbed – these are the spectral lines. Analysis of their position (what wavelengths are absorbed?), strength (what fraction of the light was absorbed?) and their shapes allow to reconstruct the information about the structure of the molecule, its motion and interaction with the environment. The collisions with atoms and other molecules have a significant impact on the shape of the spectral lines, hence we can analyse the collisional effects by observing the molecular spectra in a laboratory. For a proper conclusions, however, the experimental data need to be compared with an accurate theoretical model, which includes the molecular collisions possibly in the most realistic way.

The main goal of this research is the theoretical description of the molecular collisions and considering their presence in the theoretical spectral line shapes models. In today's world we see, in the rigid objects collisions, all the interaction happens in the moment of their contact. In the molecular world, an counterpart of this situation is so-called "Billiard Balls" model, which assumes the full interaction only in the moment when the molecules "touch". It is one of the most precise contemporarily-used models of the molecular collisions. In the real world, however, we can imagine other situations, i.e., the collision of two magnets. From our experience we know that the magnets interact with magnetic fields they generate, what means they can "rebound" without touching. In the other case, the magnetic interaction accelerates the moment of the collision or even causes the magnets to stick together after the collision. In the microscopic world, where the shape and dimensions of the molecule are not well-defined, a key role is played by such "contactless" interactions.

The clue of this project is the description of the molecular collisions, taking into account both repulsive and attractive aspects of the interaction (we will use Lennard-Jonnes potential). It will allow us to describe the spectral line shapes more accurately and analyse the ultra-accurate experimental results more deeply.

An accurate numerical simulation, even of a single spectral line, is extremely demanding and time-consuming. One needs to solve the transport-relaxation equation which describes the motion of the molecule, as well as its interaction with the environment and inner states. We found a simple mathematical way to find a solution of this equation utilizing a multidimensional series expansion. Despite obtaining one solution, i.e., the value of the absorption coefficient for a given line and wavelength, this method allows us to simulate the shape of the entire spectral line and use this solution to model the shapes of other lines within the spectrum of the same molecule.

Realistic description of the molecular collisions, increased accuracy of the spectral line-shape models and methods of accelerating the line-shape calculations have significant impact on the entire domain of molecular spectroscopy. Analysis of the spectra is the only way to investigate the composition of the atmospheres of distant planets and exoplanets, it is also used to observe the atmosphere of the Earth, for instance to control the climate changes by observing the concentration of carbon dioxide. More accurate spectroscopic research allows us to increase the knowledge about the fundamental interactions between the most basic elements of the matter.