

Rotation-vibration inelastic collision rates of polyatomic molecules

The James Webb Space Telescope (JWST) is scheduled for launch in 2018. It is designed to observe spectra of molecules in the near- and mid-infrared with unprecedented sensitivity and resolution. Such spectra contain information on the temperature, density, and chemical composition of the environments of the molecules, which is essential for understanding the formation of stars and planets. Extracting the information from the observed spectra, however, requires a detailed understanding of the collisions of the molecules with the abundant helium atoms and hydrogen atoms or molecules that populate or depopulate their rotation-vibration quantum states.

The JWST will observe rotationally and vibrationally excited carbon dioxide, acetylene, and methane, in particular in warm (≈ 1000 K) regions near stars. Historically, quantum scattering calculations employing ab initio potential energy surfaces have been the main source of collisional data for diatomic molecules. The exponential scaling of quantum problems with the number of degrees of freedom makes such calculations for polyatomic molecules extremely challenging. In this PhD project you will develop the computational methods and approximations needed to solve this problem and provide the crucial data to the astrophysicists. This project is funded by the Dutch Astrochemistry Network II. You will have the opportunity interact with astrochemists and astrophysicist in the network and to collaborate with experimental molecular physicists at the Radboud University Nijmegen who perform advanced collision experiments that provide tests of our methods.

Requirements (PhD project)

We are looking for a chemist or physicist (M.Sc. or equivalent level) with affinity for molecular quantum dynamics and computational chemistry. A good knowledge of English, both written and oral, is required.

Conditions of employment

When filling a PhD position at the Radboud University Nijmegen, you will get a contract for 4 years. During the first year the gross salary is approximately 2000 euro per month, increasing to about 2400 euro during the fourth year.

Please send your application letter and CV to Prof. Dr. Gerrit C. Groenenboom (gerritg@theochem.ru.nl).