# ABSTRACT

The subject of this dissertation is a comprehensive study of the interplay between molecular collisions and spectroscopy. In particular, the dissertation provides key reference data, such as rate coefficients, collisional line-shape parameters, and the positions and intensities of hyperfine components of rovibrational transitions for various diatomic molecules. The work is firmly grounded in quantum theory: the reference data are determined using rigorous quantum scattering calculations performed on state-of-the-art potential energy surfaces. The results are discussed in the context of applications in astrophysics, terrestrial atmosphere research, and high-precision spectroscopy of molecular hydrogen.

In addition to providing practical reference data, this dissertation addresses fundamental challenges at the intersection of quantum scattering and line-shape theory. In particular, we investigate how subtle collisional effects manifest in astrophysical observations, we explore the role of the accuracy of potential energy surfaces in providing accurate reference data for remote sensing applications, and we demonstrate the feasibility of performing large-scale *ab initio* calculations for populating spectroscopic databases. Finally, we explore how hyperfine interactions and external magnetic fields affect precision measurements of molecular hydrogen, and we propose novel methods to push the experimental accuracy further, allowing for more stringent tests of quantum theory through spectroscopy of the simplest neutral diatomic molecule.