

An efficient algorithm to calculate rovibrational cross-sections

An efficient algorithm combining distorted-wave Born with an improved coupled-states to calculate rovibrational cross-sections for astrochemical applications

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Modeling the formation of stars and planets requires a full understanding of the anatomy and the chemical evolution of their parent protoplanetary disks. These systems are often not in a local thermodynamical equilibrium (LTE). Progress in high-resolution spectroscopy in both ground and space-based telescopes helps astronomers to detect and resolve IR bands of rovibrational transitions of molecules in different interstellar media. Interpreting the observed spectra requires a full knowledge of both Einstein coefficients and collision rates. In contrast to Einstein coefficients, rovibrational collision rates are not known completely in the literature. Therefore, astronomical models need accurate collision rates of rovibrational transitions of the important species such as CO_2 , C_2H_2 , etc., induced by collisions with H_2 and He, in a temperature range that extends from 10 to 1500 K.

Collision rates can be calculated theoretically and accurately by quantum scattering dynamics. Such calculations yield rovibrational state-to-state integral cross sections (ICSs) and differential cross-sections (DSCs), which can be compared to data from crossed-beam measurements in the laboratory under specific conditions but can also be applied to provide the rate coefficients for astronomical models. Accurate quantum-mechanical calculations for rovibrational transitions in molecular collisions can be made by the coupled-channels (CC) method using accurate potential energy surfaces. This method is enormously expensive, especially at higher collision energies. Several quantum-mechanical methods were developed in the literature to make the calculations cheaper by introducing approximations in the couplings between the collided molecules. One example is the coupled-states approximation (CSA), which neglects Coriolis coupling. Sometimes, cross-sections computed by CSA, however, can differ by an order of magnitude or more compared to the CC results. The second example is the coupled-states with including the nearest neighboring Coriolis couplings (CSA-NNCC). This method can compute very close results to the CC ones. However, the calculations of ICSs of rovibrational transitions induced in polyatomic molecules involving several vibrational modes, each with a different j -manifold, during collisions still expensive and not affordable.

Herby, we developed a new algorithm using the distorted-wave Born approximation (DWBA) combined with CSA-NNCC to calculate ICSs of rovibrational transitions of polyatomic molecules induced by collisions with He or H_2 . This algorithm is considerably faster and takes less memory than CSA-NNCC calculations; it treats the rotational anisotropy using CSA-NNCC and the vibrational coupling perturbatively. We present ICSs and rate

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coefficients from CC, CSA, CSA-NNCC, and DWBA-CSA-NNCC calculations for a wide range of temperatures required by astronomers and we demonstrate the accuracy of the new DWBA-CSA-NNCC compared to the rigorous CC calculations.