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Rovibrationally Inelastic Atom-Molecule Collision Cross Sections from a Hard Sphere Model JACOB LASHNER, BRIAN STEWART, Wesleyan University — Hard-shell models have long been used to elucidate the principal features of molecular energy transfer and exchange reaction in the A + BC system. Nevertheless, no three-dimensional hard-shell calculation of inelastic collision cross sections has been reported. This work aims to fill that void. A particular motivation comes from our experimental results, which show the importance of equatorial impacts in the vibrational excitation process.

Working with the simple hard-sphere model, we incorporated secondary impacts, defined as those in which A strikes C after striking B. Such collisions are important in systems such as Li_2 - X, in which vibrational energy transfer occurs principally through side impacts. We discuss the complexity this adds to the model and present fully three-dimensional cross sections for rovibrational excitation of an initially stationary molecule in the homonuclear A + B_2 system, examining the cross section as a function of the masses and radii of the atoms. We show how the features in the cross section evolve as these parameters are varied and calculate the contribution of secondary (near-equatorial) impacts to the dynamics. We compare with recent measurements in our laboratory and with the results of quasiclassical trajectories.

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