Photofragmentation dynamics study of $ArBr_2$ ($v = 16, \ldots, 25$) using two theoretical methods: trajectory surface hopping and quasiclassical trajectories

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Two semiclasssical methods are applied in order to study the vibrational predissociation of the $ArBr_2$ ($v = 16, \ldots, 25$) complex [1]. Trajectory Surface Hopping **(TSH)** [2, 3, 4] and Quasiclassical Trajectory Method **(QCTM)** [5]. For the first case, the dynamics of the system is evolved on a potential energy surface (PES) corresponding to quantum molecular vibrational states. The possibility of hopping to other vibrational surfaces is also included, which can then lead to van der Waals bond dissociation. We have also incorporated the kinetic mechanism (see Fig. 1) into the TSH method for a better understanding and comparison of the evolution of the complex. On the other hand, the second case consists of propagating the dynamics on a single potential energy surface. We have compared our theoretical results, observables as lifetime, rotational distribution, and rotational energy among others, with previous theoretical and experimental work [6, 7].

Index Terms: molecular dynamics, trajectory surface hopping method, quasiclassical trajectory method

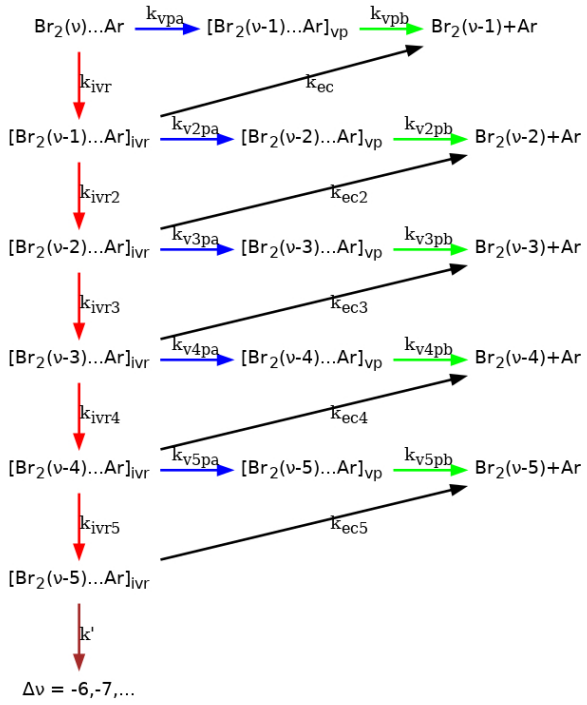

Figure 1: *Scheme of kinetic mechanism for $ArBr_2$ photofragmentation dynamics.*

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