Photofragmentation dynamics study of NeI_2 ($v = 13, \dots, 23$) using two theoretical methods: Trajectory Surface Hopping and Quasiclassical Trajectories

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The vibrational predissociation of the NeI_2 triatomic system ($v = 13, \dots, 23$) has been studied when the diatom (I_2) is found in an excited electronic state (B). Figure 1 displays the I_2 and the NeI_2 potentials [1].

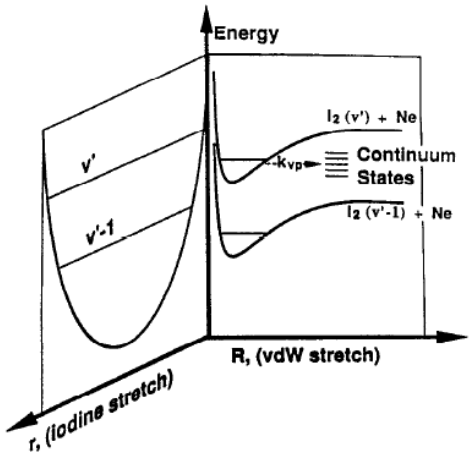

Figure 1: *Vibrational predissociation scheme is shown in two perpendicular planes with a common axis (Energy). Perpendicular axes corresponds to the stretch motion: r for the diatomic motion (I_2) and R for the motion of the rare gas with respect to the diatomic center of mass. On the diatomic plane vibrational levels are shown considering it isolated. On the other hand, the I_2-Ne potentials in the van der Waals plane.*

For this study we have used, the Quasi-Classical Trajectory Method (QCT), which consists of considering that nuclear motion is decoupled from electronic motion. It is known how approximation Born-Oppenheimer or adiabatic approximation. This allowed us to analyze nuclear dynamics as the nuclei motion in the force field imposed by electrons. Classical equations for the nuclear motion are solved considering one unique potential energy surface (PES) where the system is able to evolve during the whole dynamics. How starting point, we have properly chosen the initial conditions (classically) which ensure the description of the quantum energy state at the beginning of our simulation.

A second stage for this investigation implies using a second theoretical method: Trajectories Surface Hopping Method (TSH) under a diabatic representation, where has been demonstrated to be in good agreement with this kind of system [2-4]. In this case, the different PES, as well as their couplings, will be determined by the average potential of the van der Waals interaction. Likewise, we will make use of the "fewest switches" algorithm proposed by Tully [5], in order to obtain a good balance between quality of the results and computational efficiency.

We want compare both methods taking into account different observables of the NeI_2 dynamics, such as lifetime, rotational energy and maximum rotational angular momentum of the diatom, dissociation channels, rotational distribution of the dissociation fragments, among others.

In addition, we have compared the results obtained with previous theoretical [6] and experimental [1] results for these same levels, obtaining a good agreement.

Index Terms: vibrational predissociation, potential energy surface, surface hopping.

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