Quantum Reactive Scattering Study of the Mu+ Li$_2$, D+ Li$_2$, and T+ Li$_2$ Isotopic Reactions

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INTRODUCTION

This work presents an exact quantum investigation of the reactive scattering process X+Li$_2$→LiX+Li, with X=D, T, and Mu in the ground state with total angular momentum equal zero. This study has been carried out with a developed potential energy surface (PES)[1], which has been fitted from the *ab initio* energies determined with a full CI calculation for the 6-311G(2df,2pd) basis set and also through a pseudo potential representing the Li atom.

METHODS

Analytical representations of the X+Li$_2$ PES, with X=D, T and Mu, were obtained using a Bond Order (BO) polynomial expansion for both two and three-body terms, in agreement with the standard many-body method. Due to the fact that the considered reaction is highly exothermic (about 33.66 kcal/mol), a great number of rovibrational states and quadratures has been taken into account (even for low energies) in order to accurately describe its dynamical properties. The time-independent nuclear Schrödinger equation has been solved by means of the ABC program[2]. This code is ideally suited to calculating detailed state-to-state quantities - such as the state-resolved differential cross-sections - in which the quantum states of the reactants, as well as those of the products, are specified at the same time. ABC simultaneously expands the wave functions of all three possible chemical arrangements in the Delves hyper-spherical coordinate system.

RESULTS AND DISCUSSION

Reaction probabilities (RP) as a function of the translational energy of reactant (Deuterium) for the purely rotational excitation of the molecule Li$_2$ (considered in the vibrational states v=0, 1, 2, and 3) are shown in the figure below. From this figure
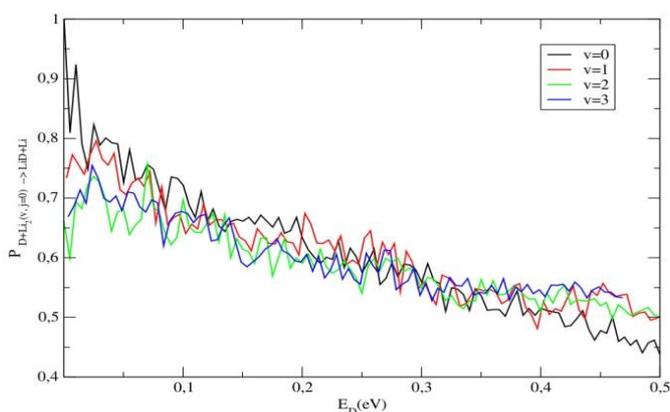
one can note that the system's reactivity is higher when the Deuterium translational energy is low. The same trend was observed for the RP for the purely vibrational excitation of the molecule Li$_2$. Furthermore, we observed that greater the reduced mass of the diatomic product, the greater the reactivity of the system. This result is consistent with the fact that the greater the mass of the diatomic product, the greater the ro-vibrational coupling states between reactant and product.

ACKNOWLEDGMENTS

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[2] Skouteris D., Castillo J. F., Manolopoulos D. E. Computer Physics Communications, v.133, p.128, (2000).