

# Quantum stereodynamics of Li+HF reactive collisions: the role of reactants polarization on the differential cross section

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A complete quantum study for the state-to-state  $\text{Li}+\text{HF}(v, j, m) \rightarrow \text{LiF}(v', j', \Omega') + \text{H}$  reactive collisions has been performed using a wave packet method, for different initial rotational states and helicity states of the reactants. The state-to-state differential cross section has been simulated, and the polarization of products extracted. It is found that the reactivity is enhanced for nearly collinear collisions, what produces a vibrational excitation of HF, needed to overcome the late barrier. It is also found that  $\text{LiF}(v' = 0)$  products are preferentially forward scattered, while vibrationally excited  $\text{LiF}(v'=1 \text{ and } 2)$  are backward scattered. These results are interpreted with a simple reaction mechanism, based on the late character and bent geometry of the transition state, originated by a covalent/ionic crossing, consisting in two steps: the arrival to the transition state and the dissociation. On the first step, in order to get to the saddle point some HF vibrational excitation is required, what favors head-on collisions and therefore low values of  $m$ . In the second step a fast dissociation of H atom takes place, which is explained by the ionic  $\text{Li}^+\text{F}^-\text{H}$  character of the bent transition state: the  $\text{FH}^-$  is repulsive making that H departs rapidly leaving a highly rotating LiF molecule. Thus, when H departs forward it pushes backward the LiF molecule producing a vibrational excitation. When it dissociates backward it pushes the LiF molecule forward, the same direction of its motion, producing less vibrational excitation. For the higher energy analyzed, where resonances slightly contribute, the orientation and alignment of products rotational states referred to reactants frame (with the  $z$ -axis parallel to  $\mathbf{k}$ ) is approximately constant with the scattering angle. The alignment is close to -1, showing that  $\mathbf{j}'$  is perpendicular to  $\mathbf{k}$ , while starting from initial states with well defined orientation, as states with pure  $m$  values, the final rotational are also oriented. It is also found that when using products frame (with the  $z'$ -axis parallel to  $\mathbf{k}'$ ) the alignment and orientation of products varies a lot with the scattering angle just because the  $z'$  axis changes from being parallel to anti-parallel to  $\mathbf{k}$  when varying from  $\theta=0$  to  $\pi$ .