Theoretical investigation of the influence of collision energy on the stereodynamics of Li+DF→LiF+D reaction

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Synopsis Calculations on the stereodynamics of the title reaction have been performed using the quasi-classical trajectory (QCT) method on the Aguado-Paniagua2-potential energy surface (AP2-PES) developed by Aguado et al. (J. Chem. Phys. 106 1013 (1997)) [1]. The product angular distributions which describe the vector correlations, $P(\theta_r)$, $P(\phi_r)$ and $P(\theta_r,\phi_r)$ are presented. The calculated results indicate that the vector properties are sensitive to the change of the collision energy.

Based on the isotopic effect on the stereodynamics for a reaction, we investigated the product vector properties of Li+DF→LiF+D reaction on the AP2-PES at three collision energies E=15 kcal/mol, E=22 kcal/mol and E=29 kcal/mol. In our calculations, the product angular distributions, $P(\theta_r)$ and $P(\phi_r)$ are presented using the QCT method [2]. The $P(\theta_r)$ distributions which characterizing the ***k*-*j'*** correlation is plotted in Figure 1. Here, ***k*** is the reagent initial relative velocity vector, ***j'*** is the product rotational angular momentum vector and the following mentioned ***k'*** is the product relative velocity vector. We can see at different collision energies, the peaks of $P(\theta_r)$ are close to $\theta_r = 90^\circ$ and symmetric with respect to the direction of 90° which implies that the product rotational angular momentum vector ***j'*** is strongly aligned along the direction perpendicular to the relative velocity direction. Furthermore, the peaks of $P(\theta_r)$ become higher and narrower as the collision energy increase, indicating that the product alignment get stronger at high collision energies.

Figure 2 illustrates the dihedral angle distributions $P(\phi_r)$ describing the correlations of ***k*-*k'*-*j'***. The $P(\phi_r)$ tended to be antisymmetrical with respect to the ***k*-*k'*** scattering plane, directly reflecting the strong polarization of angular momentum for the Li+DF→LiF+D reaction. The main peaks on different collision energies are almost at $\phi_r = 270^\circ$ and with increase of the collision energies, the peaks become stronger, implying that the rotational angular momentum vectors were not only aligned, but also preferentially oriented along the negative y-axis.

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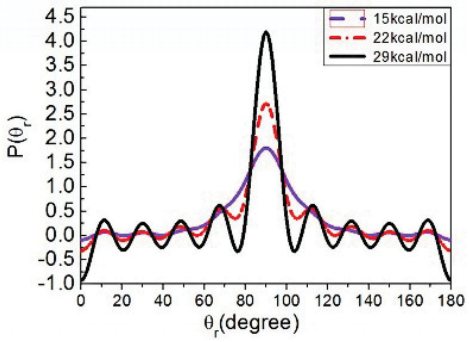

Figure 1. The distributions of $P(\theta_r)$ at collision energy E=15kcal/mol, E=22kcal/mol and E=29kcal/mol.

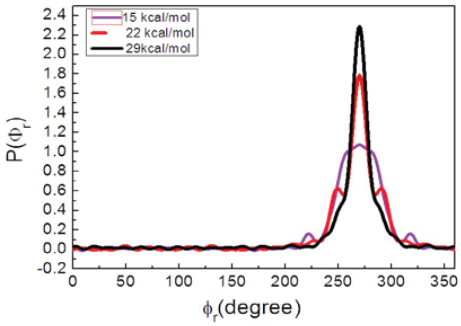

Figure 2. The dihedral angle distribution of $P(\phi_r)$ with respect to the ***k*-*k'*** plane plotted at collision energy E=15kcal/mol, E=22kcal/mol and E=29kcal/mol.

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References

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[2] K L Han, G Z He and N Q Lou 1996 *J. Chem. Phys.***105** 8699