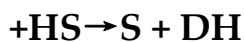## COMMUNICATION

Theoretical Calculation of Vector Correlations of the Reaction D (²S) +HS→S + DH

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Abstract: Quasi-classical trajectory calculations were performed to study the abstraction and exchange processes in the title reaction on an accurate ¹A′potential energy surface [J. Chem. Phys. 116, 4124 (2002)]. The alignment and orientation of the product DH and the polarized differential cross-section have been calculated at collision energies of 35 kcl/mol. Moreover, the effect of vibrational excitation on the alignment and the orientation of product molecule have also been obtained and discussed.

From the last two decades, the S (¹D, ³P) + H₂ reactions and its reverse reaction as well as the isotopic variants have received considerable interest due to their important role in combustion and atmospherica chemistry. Many dynamic properties such as integral cross sections and differential cross sections [1-3], product translational energy distribution and isotope branching ratio [4-7], potential energy surface [8-10], as well as the remarkable noadiabatic effect have been extensively studied [11-14]. Very recently, Guo and coworkers employed the QCT method to study the integrated cross-sections [15-16] and stereodynamics of abstract reaction D+DS on the ³A″potential energy surface (PES). The results indicated that the product rotational angular momentum vectors are not only aligned, but also oriented. Lv [17-18] et al studied the exchange reaction H + HS and D+DS rections on the ¹A′ potential energy surface (PES) by using the quantum time dependent wave packet (TDWP) and quasiclassical trajectory (QCT) calculations. However, to the best of our knowledge, up to now there is still no correlative work to study the stereodynamics properties of the D+HS

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reaction on ¹A′PES. In this paper we mainly focus our attention on energy dependence on stereodynamics properties of this reaction restricted on ¹A′PES.

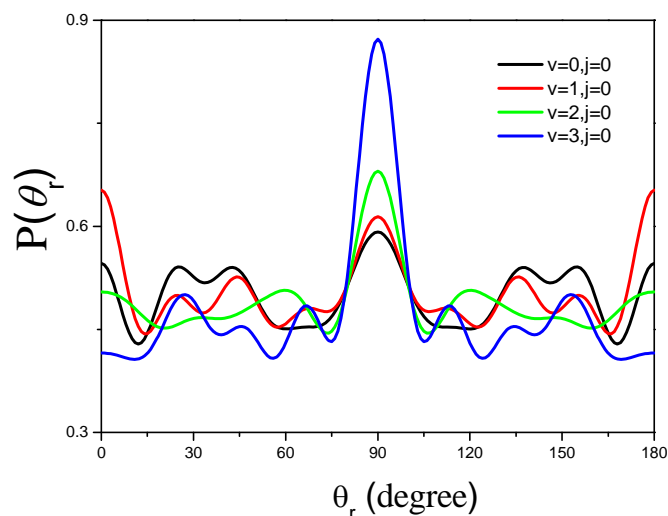**Figure 1**: The distributions of $p(\theta_r)$ of the DH product from the reaction D (²S) +HS (v=0,1,2,3 j=0)→S + DH at the collision energy of 35 kcal/mol.

The center-of-mass (c.m.) frame is utilized in our calculations. The CM frame is used in the present study. The z-axis is parallel to the reagent relative velocity vector k, while the xz-plane (also called the scattering plane) contains k and k' with k' on the x ≥ 0 half plane. The y-axis is perpendicular to the scattering plane, θ_r is the angle between k and j', Φ_r is the dihedral angle between the scattering plane and the plane containing k and j', θ_r is the angle between the k'. In the c.m. frame, the product rotational polarization can be depicted through angular distributions $P(\theta_r)$, $P(\Phi_r)$ and polarization-dependent generalized differential cross section (PDDCS). The product rotational polarization for the title reactions is investigated, using the stereo-QCT procedure which was developed by Han et al. [19-22]. Each reaction runs 100 000 trajectories and the integration step size is set as 0.1 fs to guarantee the conservation of total angular momentum and total energy. The calculations of the product rotational polarization with the initial rotational quantum number j=0 and initial vibrational quantum number v=0, 1, 2, 3. The collision energy is 35 kcal/mol and the initial collision length is 15Å for each reaction.

As we know, the distribution of $P(\theta_r)$ describes the $k-j'$ correlation and the distributions of $P(\theta_r)$ for product DH at collision energies of 35 kcal/mol are presented in **Fig. 1**. As can be seen from **Fig. 1**, the $P(\theta_r)$ distributed at all scattering angle from 0-180° and are symmetric with respect to 90° for v=0 and 1, which indicates there is no preferentially direction the product aligned. However, with the increasing vibrational quantum numbers, it is clearly see that the largest peaks of $P(\theta_r)$ are at 90° for v=2 and 3, which directly demonstrates that the