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## COMMUNICATION

# Quasi-Classical Trajectory Study of the Effects of Reactant Ro-Vibrational Excitation on the H($^2$S)+ClO($^2\Pi$) → OH($^2\Pi$)+Cl($^2$P) Reaction

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**Abstract:** The quasi-classical trajectory calculations have been performed to investigate the stereodynamics of the reaction H($^2$S)+ClO($^2\Pi$)→OH($^2\Pi$)+Cl($^2$P) on the ground electric state $1^1A'$ potential energy surface. The alignment and orientation of the product molecule and the differential cross sections (DCSs) for this reaction at the collision energy 1.0 eV on the different ro-vibrational states of ClO ($v$=0－2 and $j$=0－10) are reported. It is found that the product rotational polarization and DCSs are sensitive to the selected initial ro-vibratioanl quantum number. We discuss these phenomena in detail in our work. The calculated results probably indicate that, for this system, the two deep wells of the potential energy surface have a powerful influence on the degree of the product rotational polarization and the product angular distribution.

**AMS subject classifications**: 68U05, 74F25, 81v55

**Key words:** Stereodynamics, Quasi-classical trajectory method, Potential energy surface, Rotational alignment and orientation

## 1. Introduction

In recent years, the hypochlorous acid, HOCl, which corresponds to three dissociation channels, O + HCl, H + OCl, and Cl + OH, has gained considerable attention, since it plays an important role in atmospheric chemistry such as in ozone layer depletion. A lot of works have

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been performed in experiment and theory. The first experimental value of the rate coefficient for the global deactivation of $O(^1D)$ by HCl was obtained in the measurement of Davidson et al. more than 30 years ago [1, 2]. They reported $k_1=(1.4\pm0.4)\times10^{-10}$ $cm^3 \cdot molecule^{-1} \cdot s^{-1}$ independent of temperature over the range 200–350 K. In 1986, Wine et al. obtained a similar experimental value of $(1.50\pm0.30)\times10^{-10}$ $cm^3 \cdot molecule^{-1} \cdot s^{-1}$ at 297 K [3]. The experimental investigation of the highly vibrationally and rotationally excited state distribution of OH was carried out by laser induced fluorescence (LIF) [4]. Balucani et al. measured the angular velocity distribution of the ClO product from the reaction $O(^1D)$ + HCl at 12.2 kcal/mol collision energy in a crossed-molecular-beam experiment and estimated the branching ratio $\sigma_{ClO}/\sigma_{OH} \geq 0.34\pm0.10$ [5]. The first pioneering classical trajectory study of the title reaction using an analytical potential energy surface fitted to extensive ab initio calculations was published in 1984, which reveals the reactions proceed via long-living HOCl complexes before breaking up into products [6]. And then a new PES was fitted to the limited ab initio information [7]. Hernandz et al. calculated the potential energy surface of the $O(^1D)$+HCl reaction at an ab initio level[8]. And later, an improved PES was produced by Laganá et al. with supplement of the ab initio points [9].

As mentioned above, most experimental and theoretical studies so far have focused on $O(^1D)$ + HCl→OH + Cl, ClO + H reactions. However, little attention has been paid to the reaction H + ClO→OH + Cl on the single state PES. On other hand, previous investigations deal basically with the scalar properties. In order to gain a comprehensive understanding of the reaction H + OCl→OH + Cl, we should also study the vector properties, such as the velocity and momentum vectors, the rotational alignment and orientation of product molecules. In this paper, the influence of different ro-vibrational excitation states of reagent OCl has been studied. The fitted analytical potential is shown in **Figure 1**.

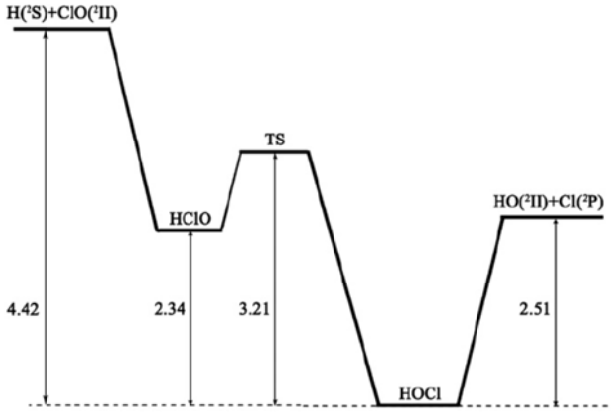


**Figure 1:** Schematic diagram of the $1^1A'$electronic ground state for the $H(^2S)$+$ClO(^2\Pi)$ reaction