Effect of Hydrogen Sulfide on the Depletion of Ozone Layer, Kinetics and Mechanism

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Introduction

Hydrogen sulfide is one of the important pollutants in the atmosphere. Its effect on the ozone layer is one of the major issues that attracted the concerns of many scientists who are working on the atmospheric chemistry. Despite the important rule of the reaction of H2S + O3 on the chemistry of atmosphere, no accurate data on the kinetics and mechanism of the title reaction is reported in the literature.

Method of Calculations

The geometries and relative potential energy surfaces are calculated by means of Gaussian03 at different levels of theory. The reaction consisted of several minimum wells and saddle points. As shown in the following suggested mechanism, the major end products are O_2, H_2O, H_2S_2, and SO_2.

$H_2S + O_3 \rightarrow HSO + HO_2$

$HO_2 + O_3 \rightarrow HO + 2O_2$

$HO + H_2S \rightarrow H_2O + HS$

$HS + O_3 \rightarrow HSO + O_2$

$2HS + M \rightarrow H_2S_2 + M$

$HSO + O_3 \rightarrow HS + 2O_2$

$HSO + O_3 \rightarrow HO + SO + O_2$

$SO + O_3 \rightarrow SO_2 + O_2$

Our study indicates the possibility of some other steps like $H_2S + O_3 \rightarrow HSO_2 + HO$ that its relative importance will be investigated during this work. Some intermediates like HO_2, HSO_2, HSO, HO, and SO produce in this mechanism that are important species in reacting with the other species exist in the atmosphere. A primary potential energy surface for one of the branches of the reaction of $H_2S + O_3$ is shown in Figure 1.

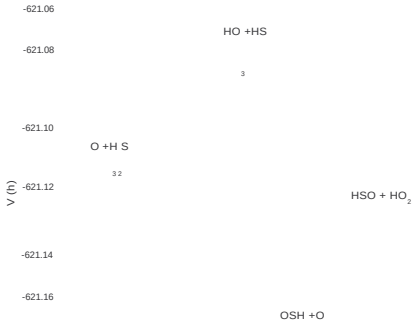
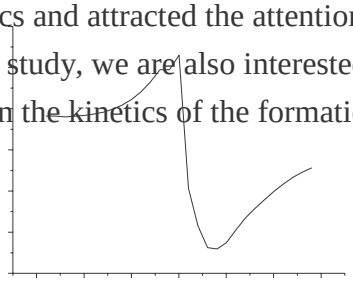


Figure 1. Potential energy surface for reaction $H_2S + O_3$.

Kinetic parameters of different paths were calculated by POLYRATE and GAUSSRATE programs. The effect of tunneling process for these reactions consisting hydrogen transfer were investigated.

One of the interesting aspects in this reaction is the existence of the potential wells. The effect of this kind of potential wells is one of the challenging issues in the kinetics and attracted the attention of many researchers in this field. In this study, we are also interested to study the effect of these potential wells in the kinetics of the formation of different products.



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