Theoretical Studies of HS+HX=H_2S+X, with X = H, F, Cl and Br

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INTRODUCTION

Chemical models are an important tool in helping us understand various physical and chemical processes in space, the full understanding of the physics and chemistry in molecular sources requires a detailed understanding of chemical kinetics and, in particular, reaction rate coefficients over a wide range of temperatures involving the chemical species in space. In the following year of the discovery of interstellar CH, others additional neutral diatomic hydrides have been discovered in the interstellar gas, such as: OH, H_2, HCl, NH, HF, and SiH, in addition to these neutral molecules, hydride molecular ions have, also, been discovered: CH+, OH+, SH+, and HCl+. These diatomic hydrides represent the simplest of interstellar molecules, and may provide key information about the interstellar environment.

METHODS

In this work, we will discuss the theoretical studies of HS+HX=H_2X+X and HS^++HS=H_2S+X^+, with X = H, F, Cl and Br reaction. The theoretical reaction rate will be compared with the experimental data, for the neutral cases and also the difference among the neutral with the charged cases

The geometries are optimized at MP2/aug-cc-pVTZ using the GAUSSIAN09 program and the energies are obtained at CCSD(T)/aug-cc-pVQZ.

RESULTS AND DISCUSSION

Table 1 present the optimized geometries of the transition state of HSHX systems,with X=H, F,Cl, Br, neutral or charged ones. It is possible to observe the increase of the HS distance in all cases and the decreases of the HX distances when compared the neutral and charged cases. For the HSH, SHX and dihedral angle there is not a patterned when compared the neutral and charged cases. Figure 1 compares the reaction rate of the neutral cases and presents the conventional and with tunneling correction the reaction rate.

Table1: Geometry structure of transition state of HS+HX

Neutral	H	F	Cl	Br
r_HS	1.3355	1.3346	1.3359	1.3370
r_HS	1.4492	1.3903	1.4415	1.5627
r_HX	1.0564	1.4494	1.6456	1.6241
a_HSH	90.245	93.152	91.437	91.0821
a_SHX	174.884	91.519	135.187	145.399
D	0.000	80.824	78.992	76.096
Charged	H	F	Cl	Br
r_HS	1.3643	1.3497	1.3457	1.3449
r_HS	1.4636	1.5485	1.6680	1.7877
r_HX	0.9481	1.1929	1.4364	1.5335
a_HSH	99.460	94.932	93.673	93.210
a_SHX	74.192	81.473	87.983	87.778
D	0.000	87.846	91.086	91.193

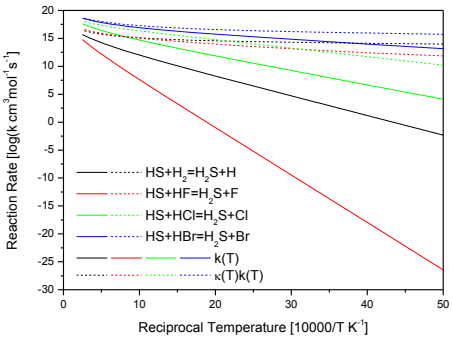

Figure 1. Reaction rate of HS+HX=H_2S+X, with X=H, F, Cl and Br.

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