Reaction Rate of HX+Y systems, with X, Y = H, F, Cl or Br and X≠Y

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INTRODUCTION

The knowledge of the thermodynamic properties of chemical species is of fundamental importance for studies such as combustion processes, the study of reactions occurring in the atmosphere as the greenhouse effect, knowing how quickly a drug works in the body, industrial problems such as the discovery of catalysts to accelerate the synthesis of a product, desorption of water from soybean, among others.

Since these applications, knowing the rate of these reactions, it is essential to know the speed with which they occur. Was writing a program in C language to calculate the reaction rate[1-4], with the correction of small curvature tunneling, correction using transmission coefficient Wigner and Eckart, and then the rate constant is presented in the Arrhenius form. We had, also, include the rovibrational levels[5-6], when necessaire, of the reactants and products in our calculation.

METHODS

We study a series of reactions HX + H = H_2 + X, HX + H = H + HX, HX + Y = X + HY and HX + Y = H + XY, where X, Y = F, Cl, or Br, with X ≠ Y. The geometries are optimizes at MP2/6-61g(d), MP2/6-311++g(d,p) and MP2/aug-cc-pvtz and the energies are calculated in CCSD(T) and in a series of bases set, the difference in geometries and frequencies will be discussed.

RESULTS AND DISCUSSION

We compare the reaction rate to the type species HF+X, with X = Cl or Br, including the rovibrational levels for the reactants, as shown in Figure 1. And to type reactions HX+H = H_2+X, with X = F, Cl or Br, was calculate the reaction rate, and we compare with experimental data, as shown in Figure 2.

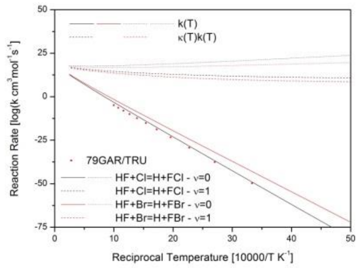

Figure 1. Reaction Rate for HF+X, with X = Cl or Br.

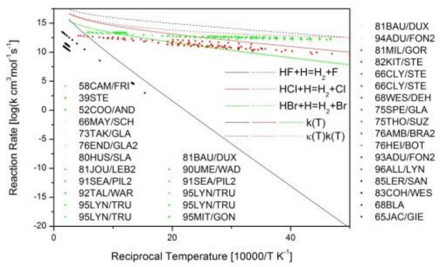

Figure 2. Reaction Rate for HX+H = H_2+X.

CONCLUSIONS

Our goal was to develop a code to determine the reaction rate for systems in general. Our code allows us to determine various reaction rates at once, provided all information about the reactions we want to analyze. Some changes still need to be implemented to make the most generic possible program, including other tunneling corrections to provide a better description of these effects at low temperatures, where it becomes critical.

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