Name(s)

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Project Number

S0906

Project Title

Study of Atmospherically-Relevant Reactions between Dinitrogen Pentoxide with Organic Acids and Chlorine Ions in Water

Abstract

Objectives

This project aimed to explain why the presence of organic acids is able to suppress the reaction between dinitrogen pentoxide and chlorine ions. It was hypothesized that formate ions, which were used to model organic acids, are more likely to react with dinitrogen pentoxide than chloride ions, because the reaction with formate ions requires less activation energy to occur.

Methods

The reactions between dinitrogen pentoxide and either formate ions or chlorine ions were studied in three different trials, with the presence of either zero, one, or six water molecules. This project used the quantum chemistry programs QChem and GAMESS in conjunction with a supercomputer at UC Irvine. The programs were used to optimize molecular structures, calculate potential energies, search for transition states, and more. For each trial, various reaction pathways were proposed and analyzed in the search for the most favorable reaction pathway. Thermodynamic calculations were then performed to calculate the activation energy.

Results

With zero and one water molecule, both formate ions and chlorine ions react spontaneously with dinitrogen pentoxide. In the presence of six water molecules, a full reaction pathway was found for both formate ions and chlorine ions. Thermodynamic calculations showed that the activation energies for the reaction between either formate or chlorine and dinitrogen pentoxide were 2.3 kcal/mol and 3.7 kcal/mol respectively.

Conclusions

The hypothesis was supported by the data, as the activation energy for the reaction with chlorine ions was 61% higher. This project can be applied to other organic acids, as the formate ion represents the carboxyl group common on organic acids. The reaction between dinitrogen pentoxide and chloride ions contributes to ozone destruction, but the work done in this project can be used to find possible solutions.

Summary Statement

In this project, computational methods were used to explain why the presence of organic acids suppresses the reaction between dinitrogen pentoxide and chlorine in water.

Help Received

This project was conducted in the Gerber Lab at UC Irvine, and my mentors were Professor R. Benny Gerber and Dr. Natalia Karimova, a postdoctoral student. My mentors taught me how to use the programs, introduced me to the tools at my disposal, discussed my project with me, and helped with troubleshooting.