



California Science Center
CALIFORNIA STATE SCIENCE FAIR
2001 PROJECT SUMMARY

| | |
|--|---|
| Your Name (List all student names if multiple authors.) Timothy A. Dong | Science Fair Use Only S0403 |
| Project Title (Limit: 120 characters. Those beyond 120 will be ignored. See pg. 9) Rate Constants of the Oxidation of Substituted Phosphines with Singlet Oxygen | Division _ Junior (6-8) <u>X</u> Senior (9-12) |
| Preferred Category (See page 5 for descriptions.) 4 - Chemistry | |
| Abstract (Include Objective, Methods, Results, Conclusion. See samples on page 14.) Use no attachments. Only text inside these boxes will be used for category assignment or given to your judges. | |
| <p>Objective: This project had two objectives. First, to determine the effect of stereochemistry on the reactivity of phosphines with singlet oxygen; and second, to determine the mechanism by which phosphine oxidation proceeds.</p> <p>Materials and Methods: This project utilized an excited form of dioxygen, singlet oxygen, to measure the reactivity rate of sterically hindered tris(ortho-methoxyphenyl)phosphine and non-sterically hindered tris(para-methoxyphenyl)phosphine, two isomers identical except for the placement of the methoxy group. Rate constants were measured in solvents of varying polarities to provide clues as to the polarity of the intermediate involved in phosphine oxidation. Nuclear Magnetic Resonance provided the integration data used to calculate the reactivity rate of the phosphines. The molecule triphenylphosphine was also studied.</p> <p>Results: The reactivity rate decreased by nine times from the para- to the ortho-isomer #- demonstrating that steric hindrance plays a large role in phosphine oxidation. Experiments conducted in various solvents show that non-polar solvents yielded higher reactivity rates than polar solvents. In addition, at low phosphine concentrations, the experiment yielded oxidized insertion products (insertion of an oxygen atom between a phosphorus and carbon atom) as opposed to the typical phosphine oxide. The insertion product was more readily formed in non-polar solvents than in polar solvents following oxidation, demonstrating that the formation of the insertion product also proceeds via the non-polar, phosphadioxirane intermediate. The higher rate constant of the para-isomer compared to triphenylphosphine demonstrates that increased electron density about the phosphorus atom increases its reactivity with singlet oxygen.</p> <p>Conclusion: The steric factor and the electron density about the phosphorus atom play a major role in regulating the rate constant at which phosphines react with singlet oxygen. The mechanism involved in phosphine oxidation was shown to be the non-polar phosphadioxirane, as opposed to the polar zwitterion. By varying the solvent used and the concentration of the phosphine present prior to oxidation, the yield of the insertion product and the standard phosphine oxide can be controlled.</p> | |
| Summary Statement (In one sentence, state what your project is about.) I studied the mechanism of phosphine oxidation and the effect of stereochemistry on it. | |
| Help Received in Doing Project (e.g. Mother helped type report; Neighbor helped wire board; Used lab equipment at university X under the supervision of Dr. Y; Participant in NSF Young Scholars Program) See Display Regulation #8 on page 4. Used lab and equipment at CSULA. Father helped make board. | |