



CALIFORNIA STATE SCIENCE FAIR
2002 PROJECT SUMMARY

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Project Title Oxidation of Substituted Phosphines with Singlet Oxygen: Intra- vs. Inter- Molecular Pathways	
<p style="text-align: center;">Abstract</p> <p>Objectives/Goals While the typical product in the reaction between singlet oxygen and phosphines is phosphine oxide, an additional product, referred to as the insertion product, has been found in the reaction of sterically hindered tris(ortho methoxyphenyl)phosphine with singlet oxygen. The objective of this project is to determine how solvent polarity and phosphine concentration affect the product distribution of these two products.</p> <p>Methods/Materials Following reaction between the ortho- phosphine and singlet oxygen, the product distribution was determined by proton and phosphorus Nuclear Magnetic Resonance. From the product distribution the ratio k_o/k_i was obtained, k_o referring to the rate constant of the oxide pathway and k_i referring to the rate constant of the insertion pathway.</p> <p>Results The k_o/k_i ratio was measured in solvents of varying polarity including benzene, methylene chloride, and chloroform, and found to be 52.1, 42.9, and 25.9 respectively. At concentrations of 10^{-3} M, the dominant product was found to be insertion product, while concentrations of 1.5 M yielded phosphine oxide as the dominant product.</p> <p>Conclusions/Discussion Since the value of k_o/k_i is higher in non-polar solvents than in polar solvents, formation of phosphine oxide is favored in more non-polar solvents while formation of insertion product is favored in more polar solvents. Increasing concentration of phosphine facilitates formation of phosphine oxide, a conclusion supported by a similar scientific study done in the past.</p>	
Summary Statement The reaction between phosphine and singlet oxygen involves two pathways, an intra- molecular pathway that results in formation of insertion product and an inter- molecular pathway that results in formation of phosphine oxide.	
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