Name(s)	Project Number
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Project Title

Oxidation of Substituted Phosphines with Singlet Oxygen: Intra- vs. Inter- Molecular Pathways

Abstract

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.

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 ko/ki was obtained, ko referring to the rate constant of the oxide pathway and ki referring to the rate constant of the insertion pathway.

Results
The ko/ki 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.

Conclusions/Discussion
Since the value of ko/ki 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.

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.

Help Received

Father helped make board. Professor, graduate students, and science teacher provided guidance.