

# Pericyclic Reactions: FMO Approach

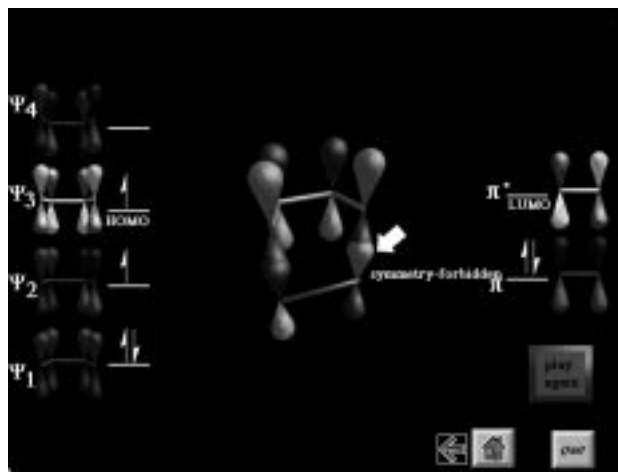
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## Abstract

Pericyclic Reactions: FMO Approach is a program for Macintosh computers in which the frontier molecular orbital approaches to electrocyclic and cycloaddition reactions are animated. The bonding or antibonding interactions of the frontier molecular orbital(s) determine whether the reactions are thermally or photochemically allowed or forbidden.

Pericyclic reactions that involve a redistribution of bonding and non-bonding electrons in a cyclic, concerted manner is an important class of organic reactions. Since the publications of the Woodward-Hoffmann rules on the conservation of orbital symmetry (1) and the frontier molecular orbital theory (FMO) by Fukui first described in the late 1960s (2), the underlying principles of these processes at the molecular level have become fully understood. Many modern organic chemistry textbooks include pericyclic reactions as a major topic. They are usually covered in detail in a typical introductory organic chemistry course.



Screen from Pericyclic Reactions: FMO Approach.

Among the two fundamental approaches to pericyclic reactions, the FMO approach has gained some popularity at the undergraduate teaching level. It is simpler and can be based on a pictorial approach. A detailed understanding of molecular orbital theories and symmetry is not required.

When learning the mechanisms of organic reactions, our students have often expressed a wish that they could see how the electrons "jump" and the orbitals "move" in the microscopic world. Pericyclic Reactions: FMO Approach has partially fulfilled the students' request. With its color 3-D graphics and animation, Pericyclic Reactions: FMO Approach can greatly enhance the teaching and learning of the FMO approach to the pericyclic reactions. The stereochemical outcomes of these highly stereospecific reactions can be seen clearly as the reaction process is animated on the computer screen. Based on the previous protocols (3) on the Apple II computer, we designed Pericyclic Reactions: FMO Approach using Macromedia Director (4) to teach the two most important pericyclic reactions: electrocyclic and cycloaddition reactions. Pericyclic Reactions: FMO Approach can be used in intermediate or advanced organic chemistry courses.

## Instructor Notes

When learning the mechanisms of organic reactions, students have often wished that they could see how the electrons “jump” and the orbitals “move” in the microscopic world. We found that our software package has partially fulfilled the students’ dream. A picture (and animation) is worth a thousand words, and seeing is believing. The software can be used in intermediate or advanced organic chemistry courses.

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## Citations

1. Woodward, R. B.; Hoffmann, R. *The Conservation of Orbital Symmetry*; Academic Press: New York, 1971.
2. Fukui, K. *Tetrahedron Lett.* **1965**, 2009; 2427.
3. Lee, A. W. M. *Educ. Chem.* **1988**, 25, 112.
4. *Macromedia Director*, version 4.0.3; Macromedia, Inc.: San Francisco, CA, 1994.