Evolution of Physical Organic Chemistry:

Advances in Computations, Pericyclic Reactions, and Pericyclases

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The birth of physical organic chemistry – the use of physical principles to interpret properties of organic molecules, including mechanisms and rates of their transformations, began with Louis Hammett and Robert Taft's linear free energy relationships in the mid-20th century. These concepts brought order to the available data of the time. With the development of computers and instrumentation, physical organic chemistry grew in scope. Photoelectron spectroscopy, computational chemistry and advanced kinetic measurements by Stan Brown are good examples of the evolution of physical organic chemistry in the late 20th and early 21st centuries. Computations bring the tools of quantum mechanics to understand and predict structures and mechanisms of transformations. My lecture will describe the power of computational methods in 2025. I will describe studies of pericyclic reactions, Woodward-Hoffmann allowed and forbidden processes and how to alter these rules, reactions that can form two or more products through ambimodal transition states, and the discovery of enzymes that we have named pericyclases, that catalyze pericyclic reactions.