Chapter 5
Spectroscopic Methods for Studying Reaction Mechanisms

Charuwan Thanawiroon
https://orcid.org/0009-0004-9076-3219
Ubon Ratchathani University, Thailand

Bancha Yingngam
https://orcid.org/0000-0001-7215-9123
Ubon Ratchathani University, Thailand

ABSTRACT

Spectroscopic methods represent key tools for identifying organic reaction mechanisms and obtaining information about molecular structures and transient intermediates. However, the broad repertoire of organic reactions, frequent difficulties in tracking compound intermediates, and challenges in the interpretation of spectral data can hamper progress and lead to misconceptions. This chapter aims to explain these methods alongside kinetic studies and isotope effects to comprehensively understand reaction dynamics. This chapter explains how nuclear magnetic resonance, infrared spectroscopy, ultraviolet–visible spectroscopy, and computer-based mass spectrometry reveal interactions and highlights the importance of such approaches through comparison and spectral simulations. The finalized section demonstrates the need for a variety of perspectives and overall

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explanations for promoting the synthesis of complex organic compounds. The field looks forward to significant progress with further real-time perspectives and education on reliable machine learning using spectroscopy.

INTRODUCTION

Returning to the question of the importance of studying reaction mechanisms, it is worth mentioning that understanding reaction mechanisms in organic chemistry is key to determining the basic processes that underlie chemical transformations (Anderson-Wile et al., 2024). This knowledge enables the determination of how structurally identical reactants can eventually turn into products, and already using this knowledge, chemists will be able to predict reactivity and selectivity trends to synthesize new pharmaceuticals, agrochemicals, and materials sciences (Koothradan et al., 2024). In addition, knowledge of the mechanisms of drug formation and the optimal reaction conditions will eliminate unwanted byproducts and only increase the yield of desired products (Bromfield Lee & Nelson, 2024). Moreover, the study of reaction mechanisms will further develop chemical theory and facilitate learning for future chemists, providing a thought focus to logically approach chemical problems (Venetos et al., 2024).

Among the most powerful modern tools for researching organic reaction mechanisms are spectroscopic methods. With their help, one can observe the dynamics and structure of molecules and their environments in real time under various conditions. The mainstream spectroscopy methods are as follows:

- Nuclear magnetic resonance (NMR) spectroscopy: This type of spectroscopy provides information about the molecule's backbone and is used to determine the atom's connectivity and molecular geometry (Anderson-Wile et al., 2024). NMR spectroscopy enables real-time monitoring of chemical reactions by tracking changes in the chemical shifts and peak intensities of reactants, intermediates, and products. This technique offers valuable insights into reaction kinetics and mechanisms.