Computational Spectroscopy Tools for Molecular Structure Analysis

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Streszczenie

An overview of the theoretical background and computational requirements needed for molecular structure analysis by means of spectroscopic techniques is provided. Different types of spectroscopy are considered: the account spans across rotational motion to electronic transitions. Particular emphasis is given to the interplay of experiment and theory, and illustrative examples have been chosen.

Słowa kluczowe

Computational spectroscopy, Conformers, ECD, Equilibrium structure, ESR, IR, Raman, Rotational spectroscopy, Semi-experimental structure, Tautomers, UV-Vis, VCD, Vibronic spectra

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