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Computational Strategies Spect

Computational spectroscopy is a rapidly evolving field that is becoming a versatile and widespread tool for the assignment of experimental spectra and their interpretation as related to chemical physical effects. This book is devoted to the most significant methodological contributions in the field, and to the computation of IR, UV-VIS, NMR and EPR spectral parameters with reference to the underlying vibronic and environmental effects. Each section starts with a chapter written by an experimental spectroscopist dealing with present challenges in the different fields; comprehensive coverage of conventional and advanced spectroscopic techniques is provided by means of dedicated chapters written by experts. Computational chemists, analytical chemists and spectroscopists, physicists, materials scientists, and graduate students will benefit from this thorough resource.

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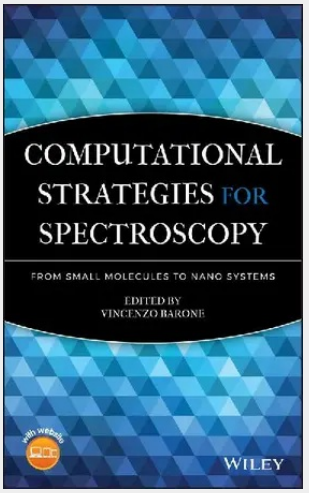

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