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Theory and Methods of Computational Vibronic Spectroscopy

By Sergey A. Astakhov, Victor I. Baranov, Lev Aleksandrovich Gribov

Nova Science Publishers Inc. Paperback. Book Condition: new. BRAND NEW, Theory and Methods of Computational Vibronic Spectroscopy, Sergey A. Astakhov, Victor I. Baranov, Lev Aleksandrovich Gribov, This book discusses semi-empirical approaches and parametric methods developed for modelling molecular vibronic spectra. These methods, together with databases of molecular fragments, have proved efficient and flexible for solving various problems ranging from detailed interpretation of conventional vibronic spectra and calculation of radiative transition probabilities to direct simulations of dynamical (time-resolved) spectra and spectrochemical analysis of individual substances and mixtures. A number of specific examples and applications presented in this book show the potential of the semiempirical approach for predictive calculations of spectra and solution of inverse spectral problems. It is noteworthy that these advances provide computational insights into developing theories of photoinduced isomer transformations and non-radiative transitions in polyatomic molecules and molecular ensembles, theory of new methods for standardless quantitative spectral analysis.



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