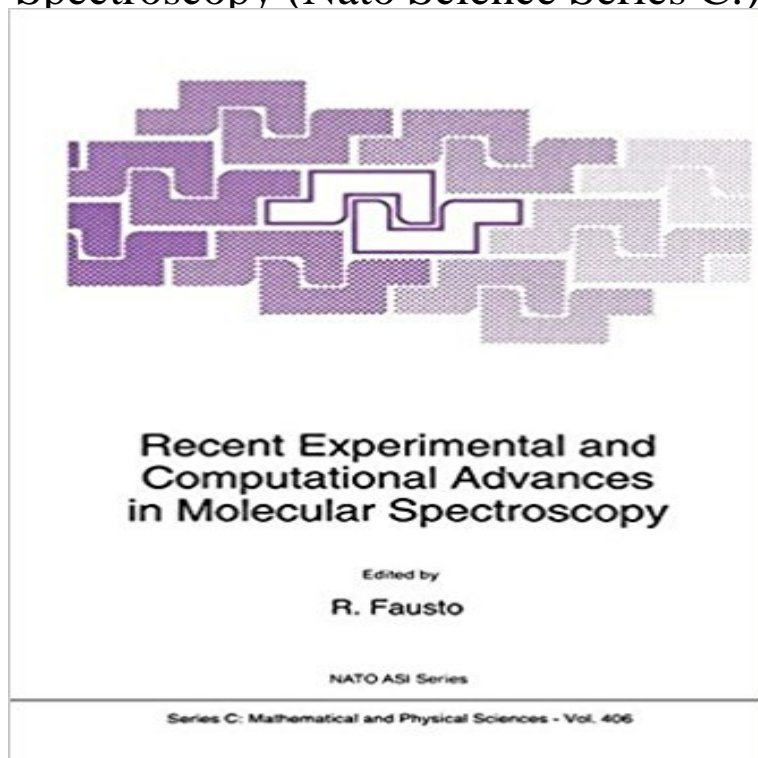


Recent Experimental and Computational Advances in Molecular Spectroscopy (Nato Science Series C:)



Both molecular spectroscopy and computational chemistry have witnessed rapid significant progresses in recent years. On the one hand, it is nowadays possible to compute, to quite a reasonable degree of accuracy, almost all fundamental spectroscopic properties for small molecular systems. The theoretical approach is now properly considered to be of fundamental importance in attaining a high degree of understanding of spectroscopic information. Moreover, it may be also a great help in designing and planning experiments. On the other hand, new and very powerful experimental techniques have been developed. This book combines an advanced teaching standpoint with an emphasis on the interplay between theoretical and experimental molecular spectroscopy. It covers a wide range of topics (such as molecular dynamics and reactivity, conformational analysis, hydrogen bonding and solvent effects, spectroscopy of excited states, complex spectra interpretation and simulation, software development and biochemical applications of molecular spectroscopy) and considers a large variety of molecular spectroscopic techniques, either from an experimental or from a theoretical perspective. (short text)

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