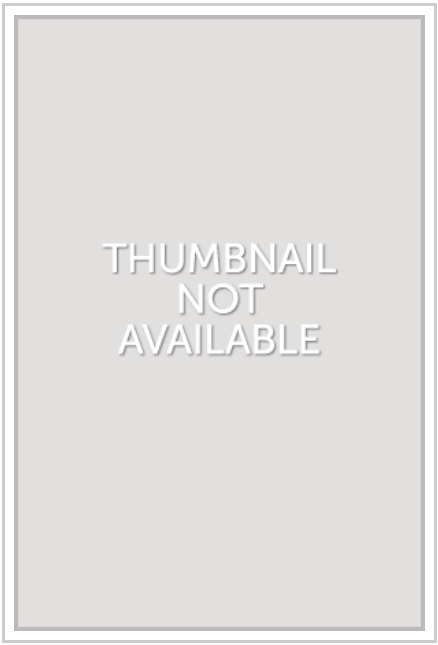

Theoretical analysis of structure and vibrational spectra

By Sapna Pathak

LAP Lambert Academic Publishing Jan 2012, 2012. Taschenbuch. Book Condition: Neu. 220x150x14 mm. This item is printed on demand - Print on Demand Neuware - Computational chemistry is used in a number of different ways. One particularly important way is to model a molecular system prior to synthesizing that molecule in the laboratory. A second use of computational chemistry is in understanding a problem more completely. There are some properties of a molecule that can be obtained computationally more easily than by experimental means. There are also insights into molecular bonding, which can be obtained from the results of computations that cannot be obtained from any experimental method. Present work highlights complete normal mode analysis, Phonon dispersion, potential energy distribution(PED) of some substituted polyacetylenes.Considering their potential applications in harmonic generation, amplitude and phase modulation, switching and other optical signal processing devices, nonlinear materials are chosen for study of geometry optimization,electrostatic potential, band gap, interpretation IR and Raman activity, natural bond orbital analysis (NBO) and HOMO-LUMO using density functional theory. 236 pp. Englisch.

Reviews

An extremely wonderful book with perfect and lucid information. This can be for all those who statte there had not been a really worth reading through. Its been written in an exceptionally easy way and it is only after i finished reading this ebook in which actually modified me, alter the way i really believe.

-- ***Kaelyn Reichel***

A really great publication with perfect and lucid explanations. Of course, it is play, continue to an amazing and interesting literature. I discovered this book from my i and dad suggested this publication to find out.

-- ***Dr. Augustine Borer***