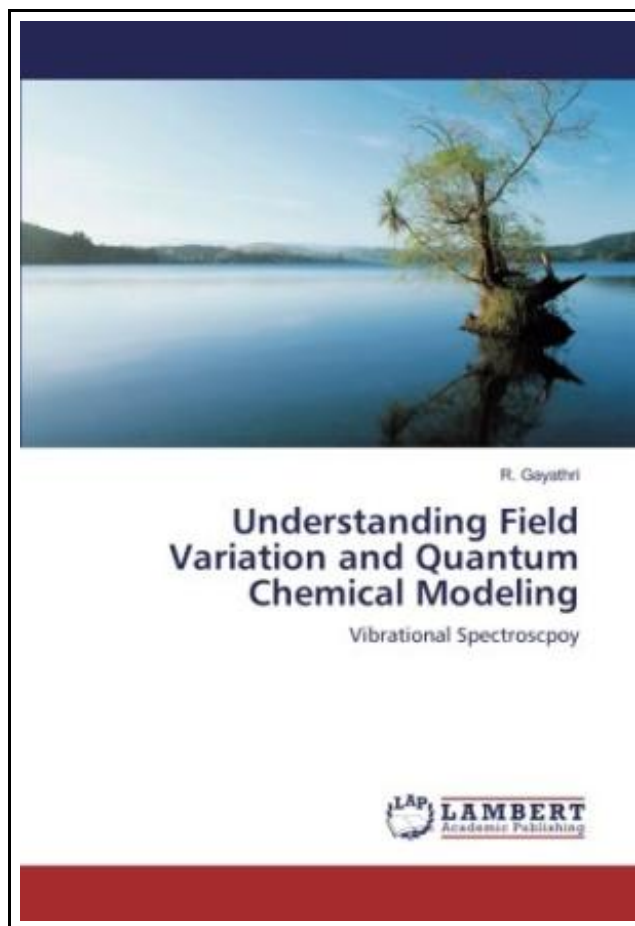# Understanding Field Variation and Quantum Chemical Modeling

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UNDERSTANDING FIELD VARIATION AND QUANTUM CHEMICAL MODELING

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Condition: New. Publisher/Verlag: LAP Lambert Academic Publishing | Vibrational Spectroscpoy | In this work, a joint experimental (FTIR and FT-Raman) and theoretical (DFT and ab-initio) study on the structure and the vibrations of Trans-3-(trans-4-imidazolyl) acrylic acid (TTIAA) are compared and analyzed. The assignment of each normal mode has been made using the observed and calculated frequencies. The optimized geometries, harmonic vibrational wavenumbers and intensities of vibrational bands of trans-3-(trans-4-imidazolyl) acrylic acid (TTIAA) have been carried out using the HF/B3LYP method using the standard 6-311++G(d,p) basis set calculations in this investigation. The result describes the variation in electrostatic and transport properties for zero and various external applied field. The variation in MPA charges are small due to the application of EFs: however, in most cases it is found to be systematic and almost uniform. When the field increases from 0.00 to 0.02 VÅ 1, the hybridization of molecular levels broadens the DOS and decreases the HLG from 3.6609 to 1.2325 eV; the decrease of band gap at the high field indicates that this molecule exhibit considerable electrical conductivity. Fukui indices to determine the local reactive site for the molecular systems. | Format: Paperback | Language/Sprache: english | 72 pp.

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