International Journal of Spectroscopy

Hindawi

Special Issue on

Quantum Chemical Calculations and Vibrational Spectroscopy of Chemical and Biological Systems

CALL FOR PAPERS

Vibrational spectroscopy (midinfrared, near-infrared, and Raman scattering) is primarily sensitive to the short-range structure of molecular solids. Both Raman and infrared spectroscopies provide information on the structure, configuration, and conformation in the solid state by probing the vibrations of atoms. In order to fully discern the vibrational modes of a molecule, one needs to examine both IR and Raman spectra. There are some similarities between the information provided by both techniques, but a fundamental difference is that the selection rules for IR and Raman spectroscopy are not identical. Vibrational spectroscopy is of utmost importance in many areas of chemical research and the application of electronic structure methods, such as quantum chemical methods, for the calculation of frequencies has been of great value for the interpretation of complex experimental spectra.

Computational chemistry might be broadly defined as the attempt to model chemical and biochemical phenomena (structure, properties, reactivity, etc.) via computer implementation of the theoretical principles of classical and quantum mechanical physics. Quantum chemical calculations have nowadays become an indispensable tool for analyzing the experimental data and for planning new experiments. Application of quantum chemical techniques to real chemical systems represents the essence of computational chemistry. These techniques such as molecular orbital theory (MO) and Density Functional Theory (DFT) are used to study molecular spectra such as vibrational and electronic. DFT finds increasing use in applications related to biological systems.

The purpose of this special issue is to publish high quality research papers as well as review articles addressing recent advances in quantum chemical calculations and vibrational spectroscopy of chemical and biological systems. Original, high quality contributions that are not yet published or that are not currently under review by other journals or peer-reviewed conferences are sought.

Potential topics include, but are not limited to:

- IR and Raman spectroscopy: recent advancements and techniques
- Electronic, vibrational, or rotational spectra of molecules
- Molecular modelling: chemical reactions and mechanism elucidations
- Density Functional Theory of chemical and biological molecules
- Cheminformatics and computational chemistry
- Nonconventional hydrogen bonds

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