



Computational Spectroscopy: Methods, Experiments and Applications

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Unique in its comprehensive coverage of not only theoretical methods but also applications in computational spectroscopy, this ready reference and handbook compiles the developments made over the last few years, from single molecule studies to the simulation of clusters and the solid state, from organic molecules to complex inorganic systems and from basic research to commercial applications in the area of environment relevance.

In so doing, it covers a multitude of apparatus-driven technologies, starting with the common and traditional spectroscopic methods, more recent developments (THz), as well as rather unusual methodologies and systems, such as the prediction of parity violation, rare gas HI complexes or theoretical spectroscopy of the transition state.

With its summarized results of so many different disciplines, this timely book will be of interest to newcomers to this hot topic while equally informing experts about developments in neighboring fields.

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Editorial Review

Review

From the Back Cover

Accurate prediction of spectroscopic properties of single molecules, molecular clusters or the solid state in combination with detailed information from apparatus-based experiments are currently paving the way to a promising revolution in the borderland between theory and experiment, namely computational spectroscopy. Though, at first sight, the term seems to contradict itself, the rapid developments in this field are opening up the study of increasingly large and chemically complex systems. At the same time, experimental molecular spectroscopy is an extremely active and fast-developing area that is heading towards the possibility of performing precise measurements on single molecules.

Unique in its comprehensive coverage of not only theoretical methods but also applications in computational spectroscopy, this ready reference and handbook compiles the developments made over the last few years.

This book is a must-have for Spectroscopists, Theoretical Chemists, Libraries, and Physical Chemists wanting to catch up with the state-of-the-art in Computational Spectroscopy.

About the Author

Jorg Grunenberg studied chemistry at the University Erlangen-Nurnberg.

After his doctorate he moved to the Technische Universitat Braunschweig and is now head of the scientific computing section at the Institute of Organic Chemistry. His interests are the *in silico* prediction of molecular spectroscopic properties, the quantification of covalent and non-covalent interactions, and molecular recognition in general. He is author and co-author of more than 80 original papers and book chapters on computational chemistry.

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