Computational Spectroscopy: Methods, Experiments and Applications
Jörg Grunenberg (Editor)

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DESCRIPTION

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.

ABOUT THE AUTHOR

Jörg Grunenberg studied chemistry at the University Erlangen-Nürnberg.

After his doctorate he moved to the Technische Universität 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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