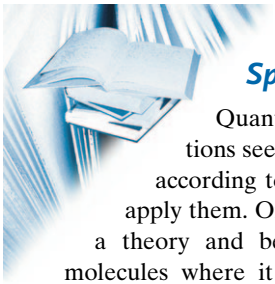


Computational Spectroscopy

Quantum-chemical computations seem to fall into two classes according to the aims of those who apply them. One is the development of a theory and benchmarking on simple molecules where it is guaranteed to work well. The other side is populated by people who are using the apparatus, programs, and computers to interpret their data and shed light on molecular properties. Although there is no sharp divide between them, it clearly helps to bring the two communities together, as proved by the book *Computational Spectroscopy* that came out at the end of 2010.

There is yet another reason for reading the book, as the editor emphasizes at the beginning, namely the fast rate of development of both theory and experiment. The Schrödinger equation appeared in 1926, but it was not until the 1970s that computers were capable of calculating what chemists could use, and in the 1990s the results of computations finally started to match experimental data. The process is far from being simple, and many spectroscopically interesting molecular properties are still difficult to implement in computer codes and to calculate reliably. Nevertheless, there has been an explosion of computational chemistry applications; we can now calculate not only the orbitals and energy states of a molecule, but also its color, magnetic response, or how it reacts with a solvent.

I would add that theory has also been feeding back into advances in spectroscopic experiments. Progress with some new techniques (even on a commercial basis) is at least partially due to the reliable computational support of measured data, for example in vibrational optical activity spectroscopy. In some other areas, such as nuclear magnetic resonance, the quantum-chemical computations are not critically necessary; yet even the NMR fraternity realized that a parallel theoretical modeling of observed chemical shifts and spin–spin coupling constants could be helpful in interpreting spectra to determine molecular structure.

The book, a compilation of 13 chapters authored by the most distinguished scientists in the field, covers the most frequently used spectroscopic methods. Inevitably, some techniques and procedures are missing due to space constraints. Nevertheless, even considering just mainstream science, one might have expected some parts of the subject to be covered more deeply or extensively. The encyclopedic nature of the book could make it difficult for a beginner in the field to advance smoothly from the basic principles of quantum mechanics (as reviewed briefly in the first chapter) to the specific applications.

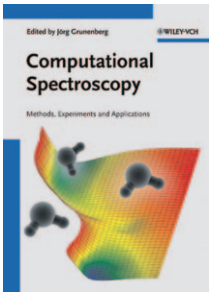
However, the book does provide a well-balanced insight into modern computational spectroscopy. I was indeed pleased to see that the first general chapter (by J. F. Ogilvie) does not present quantum chemistry as something "fallen from the heavens", but rather discusses its conceptual limits and leaves some open questions. This is important in helping readers new to the field to realize that a number coming from the computer is always prone to errors due to inherent simplifications and approximations.

In the second chapter, I. Alkorta and J. Elguero provide both a practical guide for computation of NMR parameters of organic compounds and a useful review of the recent literature (2004–2009). The general trend to involve the environmental/solvent effects in the computations is apparent here, and even more so in the following theoretically orientated chapter on EPR spectroscopy by P. Cimino, F. Neese, and V. Barone.

The chapter on UV/Vis spectroscopy by B. Mennucci nicely introduces the available theoretical methodology. H. Rhee, S. Yang, and M. Cho cover vibrational circular dichroism, focusing on the extension to time-dependent experiments, which have so far been very rare. The chapter by L. Di Bari and G. Pescitelli on electronic circular dichroism employs a more classical approach, explaining more aspects of spectroscopy, including a simplified methodology for spectral simulations. Probably the most complex modeling is that required in dielectric spectroscopy, as presented by C. Schröder and O. Steinhauser, and I myself was rather surprised by the many applications that this technique has already found in structural studies of biomolecules.

In addition to the chapters mentioned above, some more specialized ones deserve particular attention here, as the "mainstream" has been changing ever so quickly. Thus, E. Kraka, J. A. Larsson, and D. Cremer present their concept of adiabatic vibrational modes. A vibrational topic is also chosen by L. Andrews, demonstrating how a precise computation can help to identify molecules released during laser ablation. I was impressed by the complexity of calculations of molecular dipole moments related to many theoretical aspects, as described by F. M. Fernandez and J. Echave. The search for a parity violation in molecules is discussed by P. Schwerdtfeger; unfortunately it is still difficult to verify that it occurs. J. D. Kubicki and K. T. Mueller review interesting applications of computation in environmental chemistry; the only drawback is that the theory is rather simplified.

If the final chapter by T. W. Schmidt was meant to elevate our minds again, it clearly succeeded for me, as I learned something new about the history of



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spectroscopy and how it is intertwined with astronomy. So this book is not a mere textbook, but is highly relevant for scientists active in the field, and full of pleasant surprises. I am glad to own a copy.

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