

Comprehensive Chiroptical Spectroscopy

When asked about a good introduction to chiroptical methods, I usually recommend an illuminating chapter in the “Bible” of organic stereochemistry by E. L. Eliel and S. H. Wilen.^[1] If you wish to learn more, then a comprehensive volume on circular dichroism (CD) and its applications, edited by N. Berova, K. Nakanishi, and R. W. Woody more than a decade ago, is still a must in the field.^[2] Now, however, these three editors, together with Prasad L. Polavarapu, have produced a nearly encyclopedic treatment of chiroptical spectroscopies in a two-volume set, which should be the indispensable reference source not only for scientists who plan to work on chiral molecules and asymmetric processes in the near future, but also for other scientists who wish to develop a deeper understanding of chiroptical properties.

Volume 1 is largely devoted to methods and instrumentation, and consequently it contains a significant amount of theoretical background, occasionally illustrated by examples. An introductory chapter guides the reader well through the interaction of light with matter and the origin of chiroptical phenomena. However, this treatment and the rest of the theory presented do not entirely replace other extensive works such as Barron’s book on optical activity and light scattering,^[3] even though every chapter provides a well-selected list of literature for further reading.

Part II of this volume (18 chapters) focuses on the different CD spectroscopies, with some emphasis on vibrational optical activity, which has evolved dynamically in recent years, from an academic curiosity to a very informative technique with new instrumentation for measuring both vibrational CD and Raman optical activity. This middle part also covers areas that are new to most practitioners of chiroptical methods and fall outside the scope of other books; to name a few: solid-state CD, chiroptical imaging of crystals, magnetochiral dichroism, optical activity in the X-ray region, and nonlinear spectroscopies. The chapters also provide practical information about the experimental measurement techniques and how to avoid misinterpretations and pitfalls. The authors of the chapters are leading experts who have contributed much of the existing literature in their fields.

The third part of Volume 1 (7 chapters) deals with theoretical simulations of chiroptical spectra and properties. This section also reminds us that we might go wrong when chiroptical spectroscopy is used as the only tool for determining absolute configurations and molecular conformations. In

principle, an experimentally observed spectrum of a given stereoisomer should be satisfactorily predicted by quantum-chemical calculations. However, it is true that the latter might be a daunting task, as one must consider a number of electronic transitions, all possible conformations, and solvent effects, even without taking into account that the results will also depend on the level of theory employed.

Volume 2 begins with a historical perspective on the discovery of the Cotton effect and the subsequent development of methods to generate CD and ORD (optical rotatory dispersion) curves. This is an interesting and stimulating chapter, although in my opinion it could have been moved to Volume 1, thereby providing a complete historical and conceptual background of chiroptical spectroscopy.

The rest of the volume, Chapters 2–25, constitutes a superb and authoritative collection of information that illustrates the power and usefulness of chiroptical methods in structure elucidation and investigation of the dynamic aspects of molecular interactions. The topics include organic compounds with extended conjugation, supramolecular aggregates, and natural products. The description of the chiroptical spectroscopy of inorganic and metal-coordination compounds is somewhat distracting, as Volume 2 contains two separate chapters (7 and 13) on these topics, and also Chapter 9 of Volume 1 deals with lanthanide complexes. The last chapter, on drug–receptor interactions, serves as an appropriate epilogue and unveils the potential of chiroptical methods in biomedical studies. In general, the treatments are exhaustive and well referenced, and some chapters compare experimental data with the corresponding theoretical calculations.

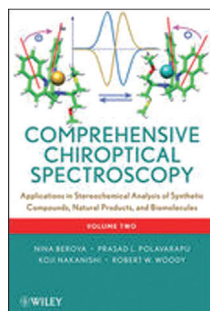
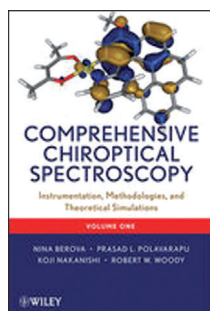
Is there anything else that should have been covered? In such an ambitious work the answer is probably yes. For example, I would have liked to see a bit more on magnetic circular dichroism (as distinct from magnetochiral dichroism and birefringence), which provides complementary information about electronic states and molecular orbitals, especially in paramagnetic systems, and can be applied to achiral molecules when a magnetic field is applied along the direction of light propagation.^[4]

Despite the above remarks and minor criticisms, I strongly recommend *Comprehensive Chiroptical Spectroscopy*. Well-trained scientists and postgraduate students will benefit a lot from using it. The set should survive for years to come, because it is unlikely that the scientific community will see anything like it for a while.

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- [2] N. Berova, K. Nakanishi, R. W. Woody, *Circular Dichroism: Principles and Applications*, 2nd ed., John Wiley & Sons, New York, **2000**.
- [3] L. Barron, *Molecular Light Scattering and Optical Activity*, 2nd ed., Cambridge University Press, Cambridge, **2004**.
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