

## BOOK REVIEW

### Mathematical Stereochemistry

by SHINSAKU FUJITA

Walter De Gruyter GmbH, Berlin/Boston, 2015, XVIII + 437 pp. ISBN 978-3-11-037197-0 (Hardback), e-ISBN (PDF) 978-3-11-036669-3 (eBook), e-ISBN (EPUB) 978-3-11-038637-0 (eBook)

“Mathematical Stereochemistry” is an interdisciplinary field which aims at investigating theoretical foundation of stereochemistry with mathematical formulations. The large portion of this new field stems from Fujita’s contributions during about 25 years. The essences of the state-of-the-art accomplishments of “Mathematical Stereochemistry” are summarized in this book.

This book consists of Preface, fifteen chapters:

1. Introduction, 2. Classification of Isomers, 3. Point-Group Symmetry, 4. Sphericities of Orbits and Prochirality, 5. Foundations of Enumeration Under Point Groups, 6. Symmetry-Itemized Enumeration Under Point Groups, 7. Gross Enumeration Under Point Groups, 8. Enumeration of Alkanes as 3D Structures, 9. Permutation-Group Symmetry, 10. Stereoisograms and *RS*-Stereoisomers, 11. Stereoisograms for Tetrahedral Derivatives, 12. Stereoisograms for Allene Derivatives, 13. Stereochemical Nomenclature, 14. Pro-*RS*-Stereogenicity Based on Orbits, and 15. Perspectives,

and Index, where each chapter is attached by a list of references. Most chapters contain several exercises which are related to the topics of the respective chapters. They also contain “Remarks” which critically demonstrate misleading foundations or terminology of conventional stereochemistry. The practices of his new methods are summarized as “Rules”.

Chapters 1–8 are concerned with geometric features of stereochemistry, where the descriptions mainly depend on point-group symmetry. In particular, Chapter 6 is a short introduction of Fujita’s unit-subduced-cycle-index (USCI) approach which has once been discussed in his book (S. Fujita, *Symmetry and Combinatorial Enumeration in Chemistry*, Springer, 1991); and Chapter 7 succinctly deals with Fujita’s proligand method which has once been discussed in his book (S. Fujita, *Combinatorial Enumeration of Graphs, Three-Dimensional Structures, and Chemical Compounds*, Kragujevac Univ., 2013). On the other hand, Chapter 9 is devoted to an introduction of stereoisomeric features of stereochemistry, where permutation-group symmetry is emphasized as a key of understanding.

Chapters 10–12 deal with the stereoisogram approach, which has been proposed by Fujita to integrate point-group symmetry and permutation-group symmetry. This integration results in the integration of chirality (for supporting enantiomers) and *RS*-stereogenicity (for supporting *RS*-diastereomers) so as to create *RS*-stereoisomerism (for supporting *RS*-stereoisomers). Stereoisograms are proposed as diagrammatic expressions of *RS*-stereoisomerism. Chapters 13 and 14 are concerned with the application of Fujita’s stereoisogram approach to stereochemical nomenclature, where the misleading terminology of the Cahn-Ingold-Prelog (CIP) system and that of Hanson’s *pro-R/pro-S* system are discussed.

As the author has pointed out at the end of Preface, Fujita’s stereoisogram approach has created the intermediate concept of *RS-stereoisomers*, which mediates between enantiomers and stereoisomers. This fact is parallel to the historical event that Avogadro’s theory has brought about the creation of the intermediate concept of *molecule*, which mediates between atoms and substances. As a result, Fujita’s stereoisogram approach has stopped the long-standing gap (during about 140 years) between van’t Hoff’s way (related implicitly to permutation-group symmetry) and Le Bel’s way (related implicitly to point-group symmetry) and has brought about *Aufheben* of the two ways.

The present reviewer strongly advises not only for fresh chemistry students but also for established researchers who are involved in stereochemistry to read and digest the essence of “Fujita’s paradise”. It is also useful for mathematicians and physicists who got interested in the mathematical features of chemistry but are looking for some logical introduction to the seemingly messy world of chemistry full of jargons.