Shinsaku Fujita

Diagrammatical Approach to Molecular Symmetry and Enumeration of Stereoisomers

Mathematical Chemistry Monographs

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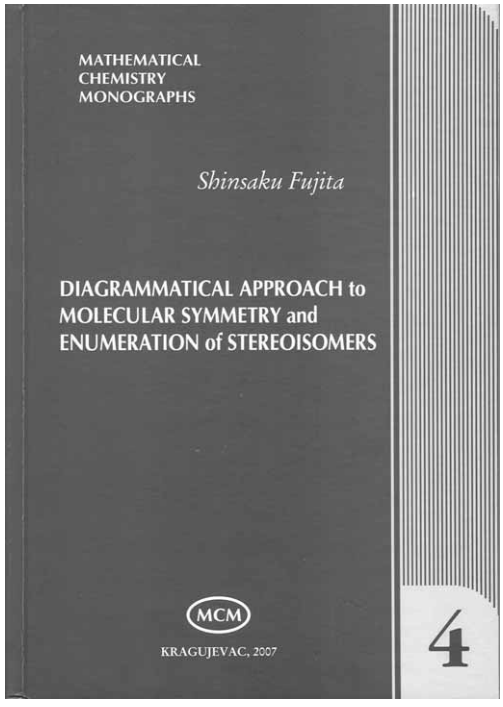

This is the fourth monograph in the series *Mathematical Chemistry Monographs*, diligently edited by Professor Ivan Gutman (Faculty of Science, University of Kragujevac, Kragujevac, Serbia) and published by the University of Kragujevac. The previous three monographs were *Mathematical Aspects of Randić-type Molecular Structure Descriptors* by X. Li and I. Gutman (published in 2006 and reviewed in *Croat. Chem. Acta* **79** (2006) A31–A32), *Numbers Zero, One, Two, and Three in Science and Humanities* by L. Pogliani (published in 2006 and reviewed in *Croat. Chem. Acta* **80** (2007) A25–A26) and *Graph Theoretical Matrices in Chemistry* by D. Janežič, A. Miličević, S. Nikolić, and N. Trinajstić (published in 2007, and reviewed in the *Journal of Chemical Information and Modeling* **47** (2007) 1996).

The author, Shinshaku Fujita, is a well-known researcher in mathematical stereochemistry and a member of the International Academy of Mathematical Chemistry.

The present monograph consists of: Preface, Introduction, seven chapters and Index. Chapters contain updated and revised versions of Fujita's papers that have appeared over the years in several journals. Each chapter is followed by a list of references.

In the *Preface* (pp. VII–IX), the author presents the scope and aims of the monograph. His ambition was to develop fundamentals of mathematical stereochemistry. The author's biography is given at the end of the *Preface*.

In the *Introduction*, also marked as Chapter 1 (pp. 1–9), the author briefly discusses the concepts on which the monograph is based, that is, stereochemistry, stereoisomers, chemical group theory, graph theory, chemical combinatorics and mathematical stereochemistry. *Introduction* is supported by 80 references.

Chapter 2 (pp. 11–36), entitled *Molecular Symmetries and Point Groups*, is based on the article that Fujita published in 1986 (*J. Chem. Educ*. **63** (1986) 744–746). In this chapter, the author presents symmetry elements, symmetry operations and a flow chart approach for classifying the symmetry of an organic molecule into the appropriate point group. He then presents point groups based on the methane skeleton and adamantane skeleton. The chapter ends with a discussion on cosets. This chapter is followed by 18 references.

Chapter 3 (pp. 37–46), entitled *Symmetries in Molecules and Sphericity Indices*, is rather brief and is based on Fujita's article in *Chem. Educ. J*. (2005), Registration No. 8–8. It contains a discussion on desymmetrization of the tetrahedron, orbits as equivalence classes, concurrent desymmetrization of orbits and sphericity indices. There are 11 references supporting this chapter.

Chapter 4 (pp. 47–58), entitled *Local Symmetries and Sphericities*, is also short and is based on Fujita's ar-

ticle in *Chem. Educ. J*. (2005), Registration No. 8–9. In it, the author discusses proligands and ligands, orbits and coset representations, desymmetrization of molecules, sphericity of orbits and sphericity indices, and symmetry fittingness for matched and mismatched molecules. The chapter is followed by 15 references.

Chapter 5 (pp. 59–72), entitled *Sphericities vs. Topicities*, is based on Fujita's article in *J. Comput. Chem. Jpn.* **3** (2004) 113–120. In this chapter, the author presents relationships *vs.* equivalence classes (orbits), conventional stereochemical terminology, new stereochemical terminology and its application to methane and adamantane derivatives. There are 18 references at the end of the chapter.

Chapter 6 (pp. 73–122), entitled *Intramolecular Stereochemistry*, is based on Fujita's article that appeared in *MATCH Commun. Math. Comput. Chem*. **54** (2005) 251–300. In this rather lengthy chapter, the author discusses symmetries and point groups of allenes (these structures are selected as examples), orbits and sphericities (where the method from Chapter 3 is applied to allene derivatives), right and left coset representations, exhaustive diagrammatic derivation of coset representations, novel mathematical models for chemical structures, subductive derivations, *etc.* The 23 references supporting this chapter are all, but four, Fujita's. It appears that Fujita is single-handedly developing a novel approach to intramolecular stereochemistry.

Chapter 7 (pp. 123–160), entitled *Intermolecular Stereochemistry*, is based on Fujita's article that appeared in *MATCH Commun. Math. Comput. Chem*. **55** (2006) 25–38. Here, Fujita presents the correspondence between right and left cosets, his approach to stereoisomerism, subductions of orbits assemblies, mandalas as nested regular bodies, common theoretical framework for both intramolecular and intermolecular stereochemistry, mandalas, assembled mandalas and reduced mandalas. This chapter is supported only by 11 references, all by the author.

The last chapter, chapter 8 (pp. 161–196), entitled *Enumeration of Stereoisomers*, is based on Fujita's article in *MATCH Commun. Math. Comput. Chem*. **55** (2006) 237–270. It consists of a discussion on the integration of intramolecular and intermolecular stereochemistry, fixed-point vectors as ordered sets of marks, combinatorial enumeration and perspectives. This chapter is followed by 23 references, again predominantly by Fujita. The monograph ends with an *Index* (pp. 196–206), which contains terms used in the text.

The monograph *Diagrammatical Approach to Molecular Symmetry and Enumeration of Stereoisomers* represents a fine summary of Fujita's research in mathematical stereochemistry. Beginners may find it difficult to read, but a persistent reader will learn a lot about the new trends in organic stereochemistry. This monograph is a worthy addition to the series *Mathematical Chemistry Monographs*. Information about the three published monographs and the forthcoming monographs can be found at the address http//www.pmfkg.ac.yu/match/.

Nenad Trinajstić