When Topology Meets Chemistry

The applications of topological techniques for understanding molecular structures have become increasingly important over the past thirty years. In this topology text, the reader will learn about knot theory, three-dimensional manifolds, and the topology of embedded graphs, while learning the role these play in understanding molecular structures. Most of the results that are described in the text are motivated by questions asked by chemists or molecular biologists, though the results themselves often go beyond answering the original question asked. There is no specific mathematical or chemical prerequisite; all the relevant background is provided. The text is enhanced by nearly 200 illustrations and more than 100 exercises.

Reading this fascinating book, undergraduate mathematics students can escape the world of pure abstract theory and enter that of real molecules, whereas chemists and biologists will find simple and clear but rigorous definitions of mathematical concepts they handle intuitively in their work.

Erica Flapan received her PhD from University of Wisconsin in 1983 in the field of knot theory. She held positions at Rice University and the University of California at Santa Barbara before joining the faculty at Pomona College, where she is currently a professor. She became interested in the applications of topology to chemistry in 1984, after learning about Jon Simon's proof that molecular Möbius ladders were topologically chiral. In addition to her many publications on three-dimensional manifolds and knot theory, she has published numerous papers in mathematics and chemistry journals about graphs embedded in space and their applications to chemistry.

Outlooks

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Mathematical content is not confined to mathematics. Eugene Wigner noted the unreasonable effectiveness of mathematics in the physical sciences. Deep mathematical structures also exist in areas as diverse as genetics and art, finance, and music. The discovery of these mathematical structures has in turn inspired new questions within pure mathematics.

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A Topological Look at Molecular Chirality

Erica Flapan

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To Francis and Laure

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Preface

The fields of topology, chemistry, and molecular biology have each made tremendous advances in the past thirty years, and as a result, there are more and more potential ways that topological techniques can be used to understand molecular structures. In particular, there have recently been a number of conferences and special issues of journals devoted to research that is at the intersection of topology, chemistry, and molecular biology. Although this work is all quite exciting, it is often technically difficult to wade through for those outside of these specific interdisciplinary areas. With some effort, mathematicians are able to bring together various sources and make sense of these results. In my experience teaching undergraduates, I have found that topology students are frequently eager to learn about results in topology that can be applied to science; however, they have quite a bit of difficulty understanding the existing literature. Many chemists and molecular biologists would also like to learn about topological techniques that they could use. However, scientists generally do not have the topological background necessary to read these results carefully. In addition to research articles, expository versions of some of these topics have been published with the details omitted. Although this has enabled many people to get a sense of the types of results that have been obtained, there has been no topology text that is written at an appropriate level for mathematics students and scientists who want to learn the topology that is necessary to understand the details of the interdisciplinary work.

This book is an attempt to provide such a text. It is a topology book written in the context of how topology can be applied to chemistry and molecular biology. The reader will learn a good deal of low dimensional topology, knot theory, and the topology of embedded graphs, while learning how these concepts can play a role in understanding molecular structures. Many of the topological results that I will describe were originally motivated by questions asked by chemists or molecular biologists, though the topological results themselves often go beyond answering the specific question asked. In fact, in some cases, questions arising in the scientific community have led to topological results that are of interest in their own right. Although not all of this work will be tied directly to chemistry or biology, I believe that all of it has at least potential applications to these fields.

This book is an expanded version of a series of lectures that I gave at the Centre Emile Borel while participating in a special semester on low dimensional topology in the spring of 1996. The audience for those lectures was primarily mathematics graduate students. However, my lectures were presented at a level that was accessible to advanced undergraduates without much background in topology. In writing up the notes as a manuscript, I have tried to make much of the material accessible to chemists and molecular biologists as well as to students of mathematics. The text assumes that the reader has a basic understanding of continuous functions of Euclidean space, but it has no other specific prerequisites in mathematics or chemistry. I have provided definitions for virtually all topological terms and tried to keep the book as nontechnical as possible. Students with some background in geometric topology should have no trouble understanding the book in complete detail. Those without such a background might have some difficulty with the proofs of Theorems 6.1 and 7.1, which make use of some deep results in topology. These two proofs are sketched rather than presented in complete detail, and those who are uncomfortable with the material should feel free to skip or skim these proofs. I include these two proofs in order to expose the reader to the power of current topological machinery, with the hope that this will give the reader some motivation to continue studying topology. The proofs of all of the results other than Theorems 6.1 and 7.1 can be understood based on the material developed in the text. Those readers who wish to read the concepts and examples without delving into many of the proofs should note that the end of each proof is denoted by a box □, so they can easily skip over whichever proofs they choose.

There are exercises at the end of each chapter that are meant to reinforce the definitions and proofs provided in the text. Many of the exercises can be done either intuitively or more rigorously, depending on the mathematical background of the reader.

All of the topological spaces considered in this book are actually subsets of Euclidean n-dimensional space. So, in order to avoid unnecessary abstraction, I never actually use the terms *topological space* or even *metric space*. Rather, I work exclusively with the usual Euclidean metric. In addition, I have not specified when I am working in the piecewise linear category and when I am working in the differentiable category. This should not concern most readers. However, those readers concerned about such things should assume that any homeomorphism is either piecewise linear or is a diffeomorphism according to whichever one is more appropriate in the given context.

I thank the Centre Emile Borel for inviting me to participate in the special semester on low dimensional topology and giving me the opportunity to present these lectures. I thank my former students Brian Forcum, Helgi Bloom, and Elizabeth John for creating many of the drawings. Thanks also go to Corinne Cerf for reading an early version of the manuscript and making suggestions on how it could be improved. I also thank Asuman Aksoy for suggesting the title of the book. Finally, I thank Kurt Mislow, whose papers on Chemistry and Topology have stimulated my interest and many of my ideas.