

## Preface

Different people have different attitudes toward *Mathematica*. Some very gifted people find its step-by-step pace to be an impediment to scientific thought. If you are one of those talented people, this book is not for you. It is written by a person who understands theory only when it leads to calculation, with every logical step under full public scrutiny. That is what *Mathematica* excels at.

But *Mathematica* also permits a playful attitude toward theory, making possible little experiments and explorations that are usually left in a scientist's private notebook. These curiosity-driven excursions are an essential part of the creative process, which perhaps now, with *Mathematica* and with private websites, and in books like this one, can become a part of the public record of science.

This book was originally intended as a concise compendium of group theoretic data and algorithms. The concise statements are indeed there, in the two *Mathematica* packages that are loaded at the top of every chapter. A true theoretician, versed in the *Mathematica* language, would need nothing else. But humans are not computers, and the development and exposition of the package materials takes time and space, and one thing led to another. I have tried to break the materials into lectures of fifty minutes length (if multiple examples are omitted).

I remember with great loss those from whom I learned group theory. First, Prof. Andreas C. Albrecht taught it to his spectroscopic research students at Cornell. Afterwards, I was a post-doc with Prof. Cristopher Longuet-Higgins, Cambridge University, who pioneered the use of permutation groups in flexible molecule spectroscopy. And especially I remember Prof. Leo Falicov, Physics Department, University of California, Berkeley, who helped me with my first by-hand application of projection operators many years ago.

And of course, this book owes its very existence to the monumental achievement of Stephen Wolfram in creating and developing *Mathematica* over the last twenty years. He created a genuinely “new kind of science”, even before applying *Mathematica* to complexity theory.

The Wolfram customer support group was helpful on many occasions; I would especially like to thank developers Adam Strzemboski, Andre Kuzniarek, and Buddie Richie, who pulled me out of several deep holes.

I am grateful to several colleagues for help with mathematics and chemical theory: Prof. Kay Magaard, Math Department, Wayne State; H. Bernard Schlegel and Vladimir Chernyak, Chemistry Department, Wayne State; and Robert A. Harris, Chemistry Department, University of California, Berkeley.

I thank Tom von Foerster, formerly of Springer Verlag, for agreeing to this wild new way of publishing a book directly from *Mathematica* notebooks. The style sheet vonFoerster is named after him. Many special thanks to Jeanine Burke for making Tom's agreement come true, in spite of vicissitudes too numerous to mention.

My wife, Carol Bluestone McClain, was my enabler through years of computer addiction. She is now helping me to dry out in the February summer of South America.

I thank the students of Chem 8490, Winter 2007, Wayne State University, who helped with such intelligent attention, suggestions, and corrections: Michael Cato, Armando Estillore, Hao Li, Dr. Barbara Munk, Brian Psciuk, Sushant Sahu, Fadel Shalhout, Jason Sonk, Dr. Jason Sonnenberg, Huali Wang, and Jia Zhou. The book consists of all the materials that could be presented to this class in one semester.

Wm. Martin McClain

Professor, Chemistry, Wayne State University, Detroit, Michigan

wmm@chem.wayne.edu

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