
Preface

This book contains chapters on thermodynamics, chemical kinetics, quantum chemistry, molecular symmetry, molecular structure, crystals, and water, and is intended for second-year master's students in chemistry. It presents the subject through real examples, discussing the results of molecular orbital calculations performed by *Gaussian* on small molecules, exploring and running *Mathematica* codes presented at the end of each chapter that enable the student to plot functions, normalize functions, fit data, solve equations, and test physical models; they are accompanied by detailed explanations that provide insight and a suitable environment for active learning. Each chapter contains a glossary of important scientific and technical terms, and the book includes detailed and complete answers to all exercises. Since the molecular orbital calculations presented are standard, packages other than *Gaussian* can alternatively be used to provide the necessary data. Students who are unfamiliar with *Mathematica* should watch the set of short videos provided by this software to learn to write and run small programs and follow the explanations to the selected codes at the end of each chapter. Those who are familiar with other computational tools can alternatively use them.

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