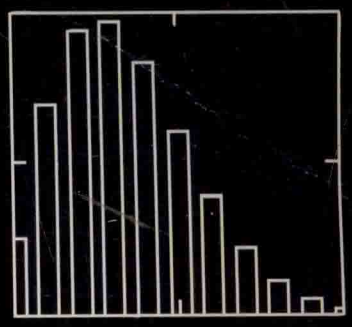
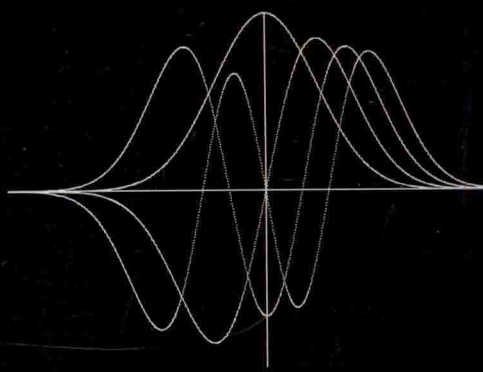
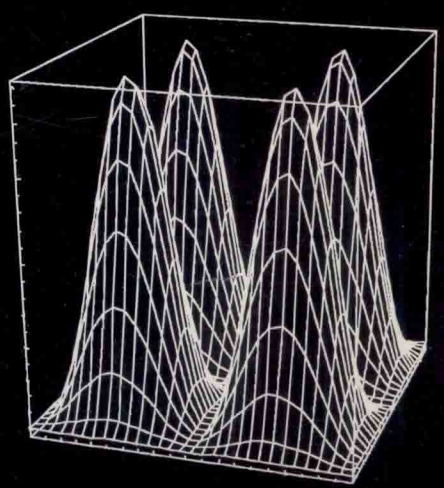
Physical Chemistry Calculations

with

Excel
Visual Basic
Visual Basic for Applications
Mathcad
Mathematica







Rodney J. Sime

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Excel
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Mathmatica

RODNEY J. SIME

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For my wife, Ruth

Preface

Who This Book Is For

This book is written for you, the scientists, engineers, and students who do numerical and graphical calculations. It is written for those of you who are open to exploring alternative approaches and widening your computer background. You should already know the basics of computer hardware and software, such as word processors, and a little about Microsoft Windows. You probably have already enjoyed using some kind of spreadsheet.

In any case, this book covers the fundamentals from the beginning. Little previous experience is expected for Part I on spreadsheets, and no previous knowledge is required for the remainder of the book. For example, you probably remember from your elementary chemistry courses that an *s* orbital looks like a circle, a *p* orbital resembles a dumbbell, and a *d* orbital is similar to a flower; in this book you will review the chemistry, physics, and mathematics underlying the particular geometries of these orbitals and learn to calculate their graphs.

How This Book Is Organized

Part I, Spreadsheets, consists of eight chapters that provide examples for doing numerical calculations and graphs with Microsoft Excel, by far the most widely used spreadsheet. These chapters cover thermodynamics, quantum mechanics, statistical thermodynamics, gases, kinetics, statistics, and three-dimensional plots. Part I includes nearly all the physics and physical chemistry used for the application examples in the remainder of the book. The final chapter in Part 1 provides a brief introduction to Lotus 1-2-3 and Quattro Pro.

Part II, Visual Basic, is a complete primer for the Microsoft Visual Basic (VB) language. Its purpose in this book is twofold; the first purpose is to provide a source book and index for the VB language used in Microsoft Visual Basic for Applications (VBA), the subject of Part III of this book. The second purpose is to provide a stand-alone introduction to the VB language, with an emphasis on numerical calculations, something ignored by most books on the VB language. Part II uses the physical chemistry presented in Part I but is otherwise completely independent of other parts of the book. It's not necessary to master VB to use VBA, but it sure is fun.

Part III, Visual Basic for Applications, is an introduction to VBA. Chapter 17 and Chapter 18 introduce VBA for Microsoft Word and VBA for Microsoft Excel, respectively. You might not realize it, but VBA is included in many Microsoft applications you may already use and still more in non-Microsoft applications that you may also be using. VBA is the language of *macros*, those underused utilities that can greatly multiply your application's power and versatility. With few exceptions, Part III uses the physical chemistry background presented in Part I. Part III also uses the VB developed in Part II as a source book and index.

Part IV, Mathcad and Mathematica, covers these applications in Chapters 19 and 20, respectively. Both chapters use the physical chemistry presented in Part I but are otherwise independent of other parts of the book. Mathcad and Mathematica are powerful applications not only for numerical calculating and graphing but also for symbolic calculations.

Rodney J. Sime
Sacramento, California
November, 2004

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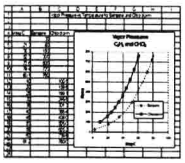

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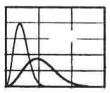

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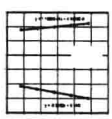

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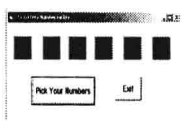

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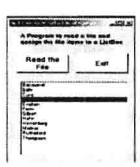

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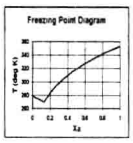

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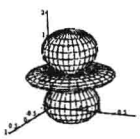

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