

Preface

This book has been written in an attempt to provide students with the mathematical basis of chemistry and physics. Many of the subjects chosen are those that I wish that I had known when I was a student. It was just at that time that the no-mans-land between these two domains – chemistry and physics – was established by the “Harvard School”, certainly attributable to E. Bright Wilson, Jr., J. H. van Vleck and the others of that epoch. I was most honored to have been a product, at least indirectly, of that group as a graduate student of J. C. Decius. Later, in my post-doc years, I profited from the Harvard–MIT seminars. During this experience I listened to, and tried to understand, the presentations by those most prestigious persons, who played a very important role in my development in chemistry and physics. The essential books at that time were most certainly the many publications by John C. Slater and the “Bible” on mathematical methods, by Margeneau and Murphy. They were my inspirations.

The expression “Chemical Physics” appears to have been coined by Slater. I should like to quote from the preface to his book, “*Introduction to Chemical Physics*” (McGraw-Hill, New York, 1939).

It is probably unfortunate that physics and chemistry ever were separated. Chemistry is the science of atoms and of the way in which they combine. Physics deals with the interatomic forces and with the large-scale properties of matter resulting from those forces. So long as chemistry was largely empirical and nonmathematical, and physics had not learned how to treat small-scale atomic forces, the two sciences seemed widely separated. But with statistical mechanics and the kinetic theory on the one hand and physical chemistry on the other, the two sciences began to come together. Now [1939!] that statistical mechanics has led to quantum theory and wave mechanics, with its explanations of atomic interactions, there is really nothing separating them any more

A wide range of study is common to both subjects. The sooner we realize this the better. For want of a better name, as Physical Chemistry is already preempted, we may call this common field Chemical Physics. It is an overlapping field in which both physicists and chemists should

be trained. There seems no valid reason why their training in it should differ . . .

In the opinion of the present author, nobody could say it better.

That chemistry and physics are brought together by mathematics is the “raison d’être” of the present volume. The first three chapters are essentially a review of elementary calculus. After that there are three chapters devoted to differential equations and vector analysis. The remainder of the book is at a somewhat higher level. It is a presentation of group theory and some applications, approximation methods in quantum chemistry, integral transforms and numerical methods.

This is not a fundamental mathematics book, nor is it intended to serve a textbook for a specific course, but rather as a reference for students in chemistry and physics at all university levels. Although it is not computer-based, I have made many references to current applications – in particular to try to convince students that they should know more about what goes on behind the screen when they do one of their computer experiments. As an example, most students in the sciences now use a program for the fast Fourier transform. How many of them have any knowledge of the basic mathematics involved?

The lecture notes that I have written over many years in several countries have provided a basis for this book. More recently, I have distributed an early version to students at the third and fourth years at the University of Lille. It has been well received and found to be very useful. I hope that in its present form the book will be equally of value to students throughout their university studies.

The help of Professor Daniel Couturier, the ASA (Association de Solidarité des Anciens de l’Université des Sciences et Technologies de Lille) and the CRI (Centre de Ressources Informatiques) in the preparation of this work is gratefully acknowledged. The many useful discussions of this project with Dr A. Idrissi, Dr F. Sokolić, Dr R. Withnall, Prof. M. Walters, Prof. D. W. Robinson and Prof. L. A. Veguillia-Berdicía are much appreciated.

My wife, Irène, and I have nicknamed this book “Mathieu”. Throughout its preparation Irène has always provided encouragement – and patience when Mathieu was a bit trying or “Miss Mac” was in her more stubborn moods.

George Turrell
Lille, May 1, 2001