Mathematics for Chemists

MATHEMATICS FOR CHEMISTS

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Preface

A sound knowledge of the elementary aspects of many areas of mathematics is indispensable to the study of the quantitative aspects of chemistry. This book presents the mathematics required for the study of chemistry to honours degree level in British universities and polytechnics. The material presented should also be suitable for chemistry majors and first-year graduate students in North American universities. It has evolved from a course of lectures given over the past ten years to first-year students in Molecular and Biological Sciences at the University of Warwick.

Students of chemistry have, in general, a more limited mathematical background than physics or engineering students. This book does not assume that the student has followed an A-level or other post-O-level course in mathematics. Therefore the calculus is developed from first principles. The approach is descriptive rather than formal in that the emphasis is on the application of mathematical techniques rather than on the proving of theorems. Some results are quoted without proof where the derivation is more confusing than illuminating.

Wherever possible, mathematical techniques and ideas have been illustrated with chemical examples. It has often been necessary to present applications without explaining the underlying theory; for a full explanation the reader should consult texts on physical or quantum chemistry such as those included in the bibliography.

The material presented here should prepare the student for the study of quantum mechanics and group theory. A chapter on group theory has not been included because it was felt that the topic could not be adequately covered in one chapter and because many excellent texts on group theory in chemistry are available.

Numerical and statistical methods are becoming increasingly important in the analysis of experimental data. Introductory chapters on these topics have been included to give the student some background before he consults more complete treatments of these subjects.

Several problems, indicated by '(U.W.)', have appeared in University of Warwick examinations. The copyright for these problems is vested in the University of Warwick and the author is grateful for permission to reproduce them here.

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