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Std Chemistry |Volume-2| Chapter-8 |

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Data analysis is important from two points of view: first, it enables a large mass of information to be reduced to a reasonable compass, and second, it assists in the interpretation of experimental results against some framework of theory. The

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Freeman/Anderson

purpose of this text is to provide a practical introduction to numerical methods of data analysis which have application in the field of experimental chemical kinetics. Recognizing that kinetic data have many features in common with data derived from other sources, I have considered it appropriate to discuss a selection of general methods of data analysis in the early chapters of the text. It is the author's experience that an outline of these methods is not always easy to locate in summary form, and that their usefulness is often not sufficiently appreciated. Inclusion of these methods in the early chapters has been aimed at simplifying discussion in the later chapters which are more particularly concerned with kinetic systems. By the provision of a number of worked examples and problems, it is hoped that the reader will develop a feeling for the range of methods

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available and for their relative merits.

Throughout the text, the mathematical treatment has been kept relatively simple, lengthy proofs being avoided. I have preferred to indicate the 'sense' and usefulness of the various methods rather than to justify them on strict mathematical grounds.

This corrected second edition contains new material which includes solvent effects, the treatment of singlet diradicals, and the fundamentals of computational chemistry. "Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics" is an invaluable tool for teaching and researchers alike. The book provides an overview of the field, explains the basic underlying theory at a meaningful level that is not beyond beginners, and it gives numerous

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Equipment Answers
comparisons of different methods with one another and with experiment. The following concepts are illustrated and their possibilities and limitations are given: - potential energy surfaces; - simple and extended Hueckel methods; - ab initio, AM1 and related semiempirical methods; - density functional theory (DFT). Topics are placed in a historical context, adding interest to them and removing much of their apparently arbitrary aspect. The large number of references, to all significant topics mentioned, should make this book useful not only to undergraduates but also to graduate students and academic and industrial researchers.

* The present work is designed to provide a practical introduction to aqueous equilibrium phenomena for both students

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and research workers in chemistry, biochemistry, geochemistry, and interdisciplinary environmental fields. The pedagogical strategy I have adopted makes heavy use of detailed examples of problem solving from real cases arising both in laboratory research and in the study of systems occurring in nature. The procedure starts with mathematically complete equations that will provide valid solutions of equilibrium problems, instead of the traditional approach through approximate concentrations and idealized, infinite-dilution assumptions. There is repeated emphasis on the use of corrected, conditional equilibrium constants and on the checking of numerical results by substitution in complete equations and/or against graphs of species distributions. Graphical methods of calculation and display are used extensively because of their value in clarifying equilibria and in

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leading one quickly to valid numerical approximations. The coverage of solution equilibrium phenomena is not, however, exhaustively comprehensive. Rather, I have chosen to offer fundamental and rigorous examinations of homogeneous step-equilibria and their interactions with solubility and redox equilibria. Many examples are worked out in detail to demonstrate the use of equilibrium calculations and diagrams in various fields of investigation.

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