
Fuzzy logic has been viewed as a system of concepts, principles, and methods for dealing with modes of reasoning and computing that are approximate rather than exact. The basis of fuzzy logic is fuzzy set theory which was introduced by Professor Lofti A. Zadeh in 1965. During the last two decades, a very strong growth of theoretical development and engineering applications has been witnessed. This book is the first one addressing the notion of fuzzy logic and exploring application opportunities in the science of chemistry. The book is edited on the basis of the Sixth International Conference on Mathematical Chemistry which was held in Pitlochry, Scotland, on July 10–14, 1995.

The book is organized in nine chapters which are the contributions from the individual presenters in the conference. The first chapter is an exposition of the philosophy for fuzzy logic in the treatment of uncertainty in sciences in general. Chapter 2 presents the basic notions of fuzzy sets and fuzzy logic with a focus on uncertainty. These two very readable chapters discuss the uncertainty issue from various aspects in chemistry. The discussion concludes that fuzzy logic is an attractive paradigm deserving study. The chapters greatly help readers understand the rationale of using fuzzy logic in chemistry research. The main portion of the book is the presentation of different applications in several subfields of chemistry. These include chirality study, quantum system analysis, and molecular structural classification and recognition. It is evident that the available information for these studies is almost always incomplete, redundant, ambiguous, impure, and in different forms. Thus, classical mathematical methods may be feeble in applications. In contrast, fuzzy logic is a viable alternative technique for seeking a much more acceptable solution. Chapter 3 is concerned with the concept of chirality. It concludes that chirality in a real system is a primitive fuzzy concept. Chapter 4 discusses a quantum-theoretical concept. It is intended to investigate some particular pure state, such as the ground state, of a molecular species, using fuzzy logic notions. Admittedly, it is a very difficult task. As the author points out, a precise connection of the study on quantum mechanics to fuzzy sets theory is still lacking. However, this explores the opportunities of using fuzzy logic to understand the fuzziness of chemical structures, and to reduce the fuzziness with an increasing number of spins in a magnet or increasing nuclear molecular masses. Chapters 5–8 focus on molecular recognition and classification by using fuzzy linguistic variables, fuzzy clustering techniques, and fuzzy graph theory. While these applications have shown an initial success, all demonstrate that fuzzy logic theory should be highly recommended for further study. They believe that fuzzy logic techniques may make a great impact on molecular recognition and classification. Different from other chapters, the last chapter focuses more specifically on hierarchical fuzzy clustering techniques as applied to a broad area of analytical chemistry. These include the selectivity control in acrylonitrile electrodereaction, the provenance of archaeological artifacts, the optimal choice of solvent systems, and the classifications of mineral waters, Roman pottery, and therapeutic muds. It seems that the advent of fuzzy logic concepts and models can give a new flavor to classification techniques in analytical chemistry. Reading these interesting chapters, we can predict that fuzzy logic will play an important role in developing more systematic and promising new techniques in mathematical chemistry research.

What is missed in this book is a clear discussion about what Professor Lofti A. Zadeh called computing with words. Note that the uniqueness and the strength of fuzzy logic is to compute with words in which a variety of uncertainties exist. This is in certain sense a focal point to distinguish fuzzy logic from classical mathematical methods. It is expected chemists may find values of computing with words by fuzzy logic and approximate reasoning in their fields in the near future. Chemistry is probably the discipline in sciences least affected by the emergence of fuzzy logic. However, the situation may change in the following decade or so that chemists may more extensively use fuzzy logic, or fuzzy mathematics in large, to cope with uncertainty and complexity encountered in their study. Needless to say, this book will greatly benefit researchers, students, and practitioners in the chemistry community who are looking for nonconventional mathematical approaches in their research.

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This book has evolved from the basic reference Handbook of Physical Properties of Liquids and Gases that was published between 1963 and 1975 in four editions. Since the last edition, both the scope of the experimental material and the methods of processing and compilation of data have undergone considerable changes. The experimentally studied regions of the reference parameters have been expanded to cover higher pressures as well as the regions of both high and very low temperatures, including the extreme states. The handbook gives the data in the form of both detailed tables and correlation equations demonstrating the temperature and pressure dependences of the properties. In some regions extrapolated values are given, which, as a rule, are indicated in the text.


This book is the result of the proceedings of the NATO Advances Research Workshop on Chemical, Structural and Electronic Analysis of Heterogeneous Surfaces on Nanometer Scale held in Trieste, Italy, April 24–26, 1995. Some of the chapter headings are Surface State Electrons: Transport Through Dangling Bonds on Silicon, and Scattering and Confinement on Metals; SPPM and SNOM of Heterogeneous Materials; Synchrotron Radiation Spectromicroscopy: Opportunities, Limitations and Data Analysis Strategies; and Scanning Spectromicroscopy with 250 to 900 eV X-rays.