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Intermolecular Forces Intermolecular and Surface Forces Chemistry 2e Intermolecular Forces The Theory of Intermolecular Forces Theory of Intermolecular Forces Order from Force Intermolecular Forces Intermolecular Forces Intermolecular Forces Intermolecular Interactions Intermolecular Forces and Clusters II Intermolecular Forces and Clusters The Forces Between Molecules The Theory of Intermolecular Forces Dielectrics, Intermolecular Forces, Optical Rotation Intermolecular Forces and Their Evaluation by Perturbation Theory Intermolecular Forces Intermolecular and Surface Forces Vibrational Linewidth Broadening Mechanisms in Liquids Revealed by the Separation of the Rapidly and Slowly Varying Intermolecular Forces Electronic Transitions and Intermolecular Forces Intermolecular Forces and Molecular Spectroscopy Intermolecular Forces and Clusters I Intra- and Intermolecular Forces Infrared Spectroscopy of Molecular Clusters Dielectrics - Intermolecular Forces - Optical Rotation Direct Measurements of Intermolecular Forces by Chemical Force Microscopy Lattice Dynamics and Intermolecular Forces Simultaneous Transitions and Intermolecular Forces Theory of Molecular Fluids Reaction Field Techniques and Their Applications to Intermolecular Forces Long-range Intermolecular Forces Studies in Intermolecular Forces The World of Quantum Chemistry Intermolecular Forces and Equation of State of Liquids Introduction to Applied Colloid and Surface Chemistry Theoretical Calculations of Surface Tension Gradients and Intermolecular Forces in Thin Wetting Films Studies in Intermolecular Forces London Dispersion Forces in Molecules, Solids and Nano-structures Intermolecular Interactions

Proceedings of the First International Congress of Quantum Chemistry, held at Menton, France, July 4-10, 1973 The study of intermolecular forces began over one hundred years ago in 1873 with the famous thesis of van der Waals. In recent decades, knowledge of this field has expanded due to intensive research into both its theoretical and the experimental aspects. This is particularly true for the type of very strong cohesive force stressed in 1920 by Latimer and Rodebush: the hydrogen bond, a phenomenon already outlined in 1912 by Moore and Winemill. Hydrogen bonds exert a profound influence on most of the physical and chemical properties of the materials in which they are formed. Not only do they govern viscosity and electrical conductivity, they also intervene in the chemical reaction path which determines the kinetics of

chemical processes. The properties of chemical substances depend to a large extent on intermolecular forces. In spite of this fundamental fact, too little attention is given to these properties both in research and in university teaching. For instance, in the field of pharmaceutical research, about 13000 compounds need to be studied in order to find a single new product that can be successfully marketed. The recognition of the need to optimize industrial research efficiency has led to a growing interest in promoting the study of inter molecular forces. Rising salary costs in industry have encou raged an interest in theoretical ideas which will lead to tailor made materials. Proceedings of the Second Structural Chemistry Indaba held in Kruger Park, South Africa, August 3-8, 1997 The aim of these notes is to offer a modern picture of the pertur bative approach to the calculation of intermolecular forces. The point of view taken is that a perturbative series truncated at a low order can provide a valuable way for ~valuating interaction energies, especial ly if one limits oneself to the case of intermediate- and long-range distances between the interacting partners. Although the situation corresponding to short distances is essen tially left out from our presentation, the problems which are within the range of the theory form a vast and important class: a large var iety of phenomena of matter, in fact, depends on the existence of in teractions among atoms or molecules, which over a substantial range of distances should be classified as weak in comparison to the interactions occurring inside atoms or molecules. We are aware of the omission of some topics, which in principle could have been included in our review. For instance, a very scarce at tention has been paid to the analysis of problems involving interacting partners in degenerate states, which is of particular relevance in the case of interactions between excited atoms (only a rather quick presen tation of the formal apparatus of degenerate perturbation theory is in cluded in Chap. III). Interactions involving the simultaneous presence of more than two atoms (or mOlecules) have not been considered, with the consequent non-necessity of considering nonadditive effects which characterize the general N-body problem. The mechanisms for vibrational linewidth broadening in liquids are investigated using the temperature dependence of coherent picosecond Stokes scattering. Both rapidly varying repulsive and slowly varying attractive intermolecular forces are determined to cause significant linewidth broadening. The liquid's local number density distribution width is shown to play an important role in inhomogeneous linewidth broadening. This is in agreement with both the model of George, Auweter and Harris and the recent theory by Schweizer and Chandler. Theory of Intermolecular Forces deals with the exposition of the principles and techniques of the theory of intermolecular forces. The text focuses on the basic theory and surveys other aspects, with particular attention to relevant experiments. The initial chapters introduce the reader to the history of intermolecular forces. Succeeding chapters present topics on short, intermediate, and long range atomic interactions; properties of Coulomb interactions; shape-dependent forces between molecules; and physical adsorption. The book will be of good use to experts and students of quantum mechanics and advanced physical chemistry. Chemistry 2e is designed to meet the scope and sequence requirements of the two-

semester general chemistry course. The textbook provides an important opportunity for students to learn the core concepts of chemistry and understand how those concepts apply to their lives and the world around them. The book also includes a number of innovative features, including interactive exercises and real-world applications, designed to enhance student learning. The second edition has been revised to incorporate clearer, more current, and more dynamic explanations, while maintaining the same organization as the first edition. Substantial improvements have been made in the figures, illustrations, and example exercises that support the text narrative. Changes made in Chemistry 2e are described in the preface to help instructors transition to the second edition. The theory of intermolecular forces has advanced very greatly in recent years. It has become possible to carry out accurate calculations of intermolecular forces for molecules of useful size, and to apply the results to important practical applications such as understanding protein structureand function, and predicting the structures of molecular crystals. The Theory of Intermolecular Forces sets out the mathematical techniques that are needed to describe and calculate intermolecular interactions and to handle the more elaborate mathematical models. It describes the methods that areused to calculate them, including recent developments in the use of density functional theory and symmetry-adapted perturbation theory. The use of higher-rank multipole moments to describe electrostatic interactions is explained in both Cartesian and spherical tensor formalism, and methods thatavoid the multipole expansion are also discussed. Modern ab initio perturbation theory methods for the calculation of intermolecular interactions are discussed in detail, and methods for calculating properties of molecular clusters and condensed matter for comparison with experiment aresurveyed. London dispersion interactions are responsible for numerous phenomena in physics, chemistry and biology. Recent years have seen the development of new, physically well-founded models, and dispersion-corrected density functional theory (DFT) is now a hot topic of research. This book is an overview of current understanding of the physical origin and modelling of London dispersion forces manifested at an atomic level. It covers a wide range of system, from small intermolecular complexes, to organic molecules and crystalline solids, through to biological macromolecules and nanostructures. In presenting a broad overview of the of the physical foundations of dispersion forces, the book provides theoretical, physical and synthetic chemists, as well as solid-state physicists, with a systematic understanding of the origins and consequences of these ubiquitous interactions. The presentation is designed to be accessible to anyone with intermediate undergraduate mathematics, physics and chemistry. The subject of this book—intermolecular interactions— is as important in physics as in chemistry and molecular biology. Intermolecular interactions are responsible for the existence of liquids and solids in nature. They determine the physical and chemical properties of gases, liquids, and crystals, the stability of chemical complexes and biological compounds. In the first two chapters of this book, the detailed qualitative description of different types of intermolecular forces at large, intermediate and short-range distances is presented. For the first time in the literature, the temperature dependence of the

dispersion forces is analyzed and it is shown that the famous Casimir-Polder formula for dispersion forces is incorrect at any finite temperature. The author has aimed to make the presentation understandable to a broad scope of readers without oversimplification. In Chapter 3, the methods of quantitative calculation of the intermolecular interactions are discussed and modern achievements are presented. This chapter should be helpful for scientists performing computer calculations of many-electron systems. The last two chapters are devoted to the many-body effects and model potentials. More than 50 model potentials exploited for processing experimental data and computer simulation in different fields of physics, chemistry and molecular biology are represented. The widely used optimization methods: simulated annealing, diffusion equation method, basin-hopping algorithm, and genetic algorithm are described in detail. Significant efforts have been made to present the book in a self-sufficient way for readers. All the necessary mathematical apparatus, including vector and tensor calculus and the elements of the group theory, as well as the main methods used for quantal calculation of many-electron systems are presented in the appendices. All those working on the theoretical and experimental studies of intermolecular interactions in chemistry, physics, biochemistry and molecular biology will find this text of interest and it will appeal to advanced undergraduates, graduates and researchers. Intermolecular and Surface Forces describes the role of various intermolecular and interparticle forces in determining the properties of simple systems such as gases, liquids and solids, with a special focus on more complex colloidal, polymeric and biological systems. The book provides a thorough foundation in theories and concepts of intermolecular forces, allowing researchers and students to recognize which forces are important in any particular system, as well as how to control these forces. This third edition is expanded into three sections and contains five new chapters over the previous edition. Starts from the basics and builds up to more complex systems Covers all aspects of intermolecular and interparticle forces both at the fundamental and applied levels Multidisciplinary approach: bringing together and unifying phenomena from different fields This new edition has an expanded Part III and new chapters on non-equilibrium (dynamic) interactions, and tribology (friction forces) Colloid and Surface Chemistry is a subject of immense importance and implications both to our everyday life and numerous industrial sectors, ranging from coatings and materials to medicine and biotechnology. How do detergents really clean? (Why can't we just use water?) Why is milk "milky"? Why do we use eggs so often for making sauces? Can we deliver drugs in better and controlled ways? Coating industries wish to manufacture improved coatings e.g. for providing corrosion resistance, which are also environmentally friendly i.e. less based on organic solvents and if possible exclusively on water. Food companies want to develop healthy, tasty but also long-lasting food products which appeal to the environmental authorities and the consumer. Detergent and enzyme companies are working to develop improved formulations which clean more persistent stains, at lower temperatures and amounts, to the benefit of both the environment and our pocket. Cosmetics is also big business! Creams, lotions

and other personal care products are really just complex emulsions. All of the above can be explained by the principles and methods of colloid and surface chemistry. A course on this topic is truly valuable to chemists, chemical engineers, biologists, material and food scientists and many more. Existing texts on the statistical mechanics of liquids treat only spherical molecules. However, nearly all fluids of practical interest are composed of non-spherical molecules that are often dipolar or exhibit other kinds of electrostatic forces. This book describes the statistical mechanical theory of fluids of non-spherical molecules and its application to the calculation of physical properties, and is a sequel to Theory of Molecular Fluids. Volume 1: Fundamentals by C.G. Gray and K.E. Gubbins. The emphasis is on the new phenomena that arise due to the non-spherical nature of the intermolecular forces, such as new phase transitions, structural features and dielectric effects. It contains chapters on the thermodynamic properties of pure and mixed fluids, surface properties, X-ray and neutron diffraction structure factors, dielectric properties and spectroscopic properties. The book is aimed at beginning graduate students and research workers in chemistry, physics, materials science and engineering. Improved experimental and computational methods mean that more detailed measurements are available in the study of intermolecular forces. This book describes the advanced mathematical techniques required to cope with this improvement. Describes at an introductory level the nature of intermolecular forces and their influence on the properties of solids, liquids, and gases. A more advanced treatment of the subject may be found in the same authors' 'Intermolecular Forces'. This book is intended to give an introduction to intermolecular forces from an experimental point of view. Within the last 10 years the interest has turned more and more into an understanding of the weak, but important, int- molecular forces. New experimental techniques have been developed which have helped to gain more insight into this interesting topic. This book is intended as an introduction for graduate students who are familiar with the main concepts of n~olecular spectroscopy. Special emphasis will be laid on the theoretical concepts. After a detailed description of experimental techniques, the results for two prototype systems which have been the subject of several studies in the literature within recent years will be presented. Ar-CO is becoming the most extensively studied van der Waals complex, theoretically and experimentally. Nevertheless, this example shows that even though the theory has greatly improved and has helped us to improve our knowledge of intermolecular forces, even for relatively simple cases the theory car1 still fall short of an accurate description. For a long time (NH3)2 was considered as a prototype for hydrogen bo-ing. However, subsequent experimental and theoretical studies have revealed the mysteries of the obtained spectra and proved that our previous concept of hydrogen bonds was just too naive. The present theme concerns the forces of nature, and what investigations of these forces can tell us about the world we see about us. The story of these forces is long and complex, and contains many episodes that are not atypical of the bulk of scientific research, which could have achieved greater acclaim 'if only...'. The intention of this book is to introduce ideas of how the visible world, and those

parts of it that we cannot observe, either because they are too small or too large for our scale of perception, can be understood by consideration of only a few fundamental forces. The subject in these pages will be the authority of the commonly termed, laws of physics, which arise from the forces of nature, and the corresponding constants of nature (for example, the speed of light, c, the charge of the electron, e, or the mass of the electron, me). Proceedings of the 14th Jerusalem Symposium on Quantum Chemistry and Biochemistry, Jerusalem, Israel, April 13-16, 1981