

agrochemicals. It is also useful for scientists in related areas such as design and mode of action of pharmaceuticals.

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Organic Coatings: Science and Technology

2nd ed.; Z.W. Wicks, Jr., F.N. Jones, S.P. Pappas; Wiley, New York, 1999, 630 pages, ISBN 0-471-24507-0, £80.95

Coatings are everywhere: in the home, they are on walls, furniture, white goods and on printed circuit boards in many electrical appliances, while outside the home they are on houses and cars. The functional and aesthetic requirements of coatings are extremely broad, reflected in the diverse science and technology which supports their development, production and use. Coating technology evolved empirically, but recent decades have seen a marked increase in the scientific understanding of the underlying principles. The modern need to develop, maintain and improve coating performance still demands the understanding of complexities present in the formulation process, which are often overlooked. The quality of literature in the coatings field is very variable, so that there was a need for an authoritative 'one-stop' publication that would help scientists, engineers and coatings formulators understand the principles underlying the technology, and to utilise them effectively.

Organic Coatings: Science and Technology, Second Edition: provides a structured and systematic, up-to-date account of the technology and principles underlying the production and use of organic coatings. Completely updated and rewritten in a single volume since the *First Edition*, this book introduces readers to the subject with seven chapters on key properties of coatings. Subsequent chapters describe raw materials, physical concepts, formulations, applications and properties. Coatings industry terminology is carefully defined to help newcomers to the field understand esoteric coatings jargon. Practical troubleshooting advice for scientists and technologists in all branches of the industry is prominently featured. There are comprehensive sets of references in each chapter, as well as an appendix listing useful information sources including electronic ones such as the Internet, WWW and proprietary databases.

The book provides an up-to-date, clearly written and presented compendium, equally of value as a textbook or as an essential reference tool. It is highly recommended for scientists in all branches of the coatings industry, but much

of the material will be of value to workers in related areas of adhesives, plastics and printing ink industries.

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Molecular Modeling on the PC

M.F. Schlecht; Wiley, Chichester, 1998, xviii + 763 pp., £80.95. ISBN 0-471-18567-1

A dramatic increase in the use of PC's in the home and for teaching in schools, colleges and universities has led to the development of numerous readily available software packages that allow users to perform sophisticated mathematical data manipulations. Inexpensive PC's equipped with a satisfactory software package allow individuals with basic PC literacy to perform molecular modelling and carry out molecular structure calculations. The number of molecular modelling techniques is ever increasing, however they all fall into three categories, namely ab initio methods, semiempirical methods, and empirical force field methods.

This volume deals exclusively with empirical force field methodologies and is aimed at individuals with little or no experience in the field. In-depth coverage of the key terms, hardware and software, and basic modelling strategies utilised in the field are provided. Using a problem-solving approach and using the popular PCMODEL[®] program, readers are guided through an array of powerful techniques. Tested examples and skill-building exercises are provided throughout, along with numerous illustrations and figures that clarify important points. Detailed appendices and a comprehensive list of references are also provided, along with a diskette that contains a structure input file library with structure files for the PCMODEL[®] experiments, template files for rapid structure building, and a hypertext directory of molecular modelling web sites and resources.

Exercises presented cover several key areas. Simple model building exercises are aimed at generating 3-D structures that approximate the shape and relative geometries of particular molecules. Discovering the lowest energy conformation, or group of conformations, for a flexible molecule, with a quantitative energy ranking is also presented. Results

of such determinations can be used to predict or correlate properties, with the added dimension of considering a molecule not as a single structure but as a weighted average of several structures. Docking experiments examine the optimisation of intermolecular association, driven by specific interactions such as hydrogen bonding, dipole or charge attractions, metal atom coordination, or van der Waals attractions. Such information can be used to study solvation, the structure of aggregates, or specific binding interactions. Comparison between conformations of portions of different molecules aids in mapping structure-property relationships, whilst comparison of conformations of reactive intermediates and transition states aids in the analysis of reaction pathways. *Molecular Modeling on the PC* is an excellent introduction to the field for students and

professionals with interests in the structure of simple and complex molecules.

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