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Carbohydrate Polymers 65 (2006) 218–219
Carbohydrate Polymers
www.elsevier.com/locate/carbpol

Book Reviews

C.J. Kramer, Essentials of Computational Chemistry: Theories and Models2nd ed., Wiley, Chichester, UK; 2005 (xxii + 596 pp., £34.95, ISBN 0-470-09182-7)

Computational chemistry, also referred to as theoretical chemistry and molecular modelling, has undergone rapid development over the last decade, which is directly coupled to rapid developments in digital computer technology and thus processing power. The need for some understanding of theory, computation and modelling is becoming less restricted to the domain of the computational chemist as the synergy between theory and experiment has vastly accelerated progress in many areas. Many chemists are not fond of advanced mathematics, however, it is impossible to describe computational chemistry without using a number of equations, which can be somewhat daunting without detailed knowledge of the particular field.

Essentials of Computational Chemistry provides an accessible introduction to this fast developing subject, and carefully guides the reader through key equations by providing intuitive explanation of equations and their terms were possible, and if not possible then at least some qualitative discussion and links to useful background information are provided. The book begins with a gentle approach by starting with a presentation of classical molecular mechanics models, before gradually moving on to increasingly more complex quantum mechanical and dynamical theories. Coverage and examples are drawn from inorganic, organic and biological chemistry. Many topics have been expanded upon since the first edition, particularly, the evolving topics of density functional theory, continuum solvation models, and computational thermochemistry. New material includes discussion of docking, principal components analysis, force field validation in dynamics simulations, first-order perturbation theory for relativistic effects, tight-binding density functional theory, electronegativity equalization charge models, standard-state equilibrium constants, computation of pK_a values and redox potentials, molecular dynamics with implicit solvents, and direct dynamics.

The quality of a theory is necessarily judged by its comparison to (accurate) physical measurements. Thus, specific attention is paid to offering comparisons between theory and experiments for a broad range of physical observables. Case studies at the end of chapters are provided to illustrate the use of models most recently presented, and this new edition is accompanied by a supplementary website with exercises, problems and updates. This book is invaluable to all students taking a first course in computational chemistry, molecular modelling, computational quantum chemistry or electronic structure theory. However, it will also be of interest to postgraduates, researchers and professionals needing an up-to-date, accessible introduction to this subject.

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Available online 18 April 2006

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doi:10.1016/j.carbpol.2006.01.002

M.J. Kirwan, editor. Paper and Paperboard Packaging Technology, Blackwell Publishing Ltd, Oxford, UK, 2005 (xxii + 429 pp., £119.50, ISBN 1-4051-2503-9)

Papers and paperboards are sheet materials comprising an intertwined network of cellulosic carbohydrate polymer fibres. They are printable and have physical properties, which enable them to be made into various types of flexible, semi-rigid and rigid packaging. The use of paper and paperboard packaging accelerated during the latter part of the 19th century to meet the developing needs of manufacturing industry. The manufacture of paper had progressed from a laborious manual operation to continuous high-speed production with wood pulp replacing rags as the main material. Packaging represents the largest usage of paper and paperboard and therefore both influences and is influenced by the worldwide paper industry. Today, examples of the use of paper and paperboard packaging are found in many places.

Paper and Paperboard Packaging Technology discusses all the major issues related to packaging based on paper and paperboard. The volume opens with a chapter on the raw materials, their processing and properties. The issues related to environmental and waste management are discussed in Chapter 2. The subsequent chapters provide information on paper-based flexible packaging, paper labels, paper bags and composite cans.

Fibre drums are used globally and offer a strong, cost-effective means for the packaging of wide range of products. They are widely used by the chemical, pharmaceutical, and food industries as well as special applications in other industries. A fibre drum is a cylindrical container with a

sidewall made of paper or paperboard having ends and components made of similar or other materials. Chapter 7 summarizes the information on different aspects of fibre drums. Other types of packaging such as multiwall paper sacks, rigid boxes, folding cartons, corrugated fibreboard packaging, solid fibreboard packaging, paperboard-based liquid packaging and moulded pulp packaging are discussed in individual chapters.

In conclusion, this volume describes the manufacture of 12 types of paper- and paperboard-based packaging, together with their end-use applications and packaging machinery involved. The importance of pack design is stressed, including opportunities for innovative design solutions. This book can be highly useful source of information to the students of packaging technology.

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Available online 20 February 2006

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doi:10.1016/j.carbpol.2005.12.005