Big Bang Theory

The Chemistry of Explosives. By *Jacqueline Akhavan.* Springer, New York 1998. xii + 173 pp., paperback $ 36.95.—ISBN 0-85404-563-5

Many of us, like me, were initially attracted to chemistry during our adolescent years through pyrotechnics and explosions. Indeed, the fascination with explosives and fireworks, as spectators if not as practitioners, seems almost universal among all cultures and all times. When my former students return to visit me, they invariably recall my lecture demonstrations, usually those involving explosions. Because new technical books on explosives are relatively rare, this succinct introductory paperback manual on the chemistry, physics, and functioning of explosives is most welcome.

Jacqueline Akhavan, Senior Lecturer in the Department of Environmental and Ordnance Systems, Cranfield University, Royal Military College of Science, Swindon, England, carries out research on explosives and pyrotechnics and is interested in polymer-bonded explosives. Her eminently readable book outlines the basic principles and theories required to understand the chemical mechanisms of explosions.

Chapter 1, "Introduction to Explosives" (17 pp.), briefly reviews the development from 220 B.C. to A.D. 1978 of a number of explosives: black powder (a mixture of potassium nitrate, sulfur, and charcoal), the first known explosive; nitroglycerine; mercury fulminate; nitrocellulose; dynamite; ammonium nitrate; commercial explosives (ANFO and slurry explosives); and military explosives (picric acid, tetryl, TNT, nitroguanidine, PETN, RDX, HMX, polymer-bonded and heat-resistant explosives). In Chapter 2, "Classification of Explosive Materials" (26 pp.), extensive chemical data on explosives are presented, divided into three classes according to performance and uses: 1) primary explosives—those that undergo a very rapid transition from burning to detonation when subjected to heat or shock, and serve to transmit the detonation to less sensitive (secondary) explosives; 2) secondary or high explosives—those that cannot be detonated by heat or shock and are generally more powerful than primary explosives; and 3) propellants—combustible materials containing within themselves all the oxygen needed for their combustion, but which only burn and do not explode.

Chapter 3, "Combustion, Deflagration and Detonation" (14 pp.), considers the effects of various factors on these three processes: combustion is a chemical reaction between a substance and oxygen; deflagration means faster and more violent burning than in ordinary combustion; detonation is decomposition by the passage of a shock wave rather than a thermal mechanism. The latest theories on the formation of "hot-spots" are also discussed. Chapter 4, "Ignition, Initiation and Thermal Decomposition" (11 pp., the shortest chapter), deals with the successive stages in explosive reactions.

Chapter 5, "Thermochemistry of Explosives" (28 pp.), provides information on the types of chemical reactions, the energy changes, and the mechanisms and kinetics involved when a material undergoes an explosion. Detailed theoretical thermochemical calculations are carried out for oxygen balance, decomposition reactions, heats of formation and explosion, volume of gaseous products, explosive power and power index, mixed explosive compositions, and energized explosives (addition of beryllium, aluminum, and other elements), with the caveat that the results of such calculations will not always agree with those obtained experimentally because experimental results will vary according to the conditions. Although the Kistiakowsky–Wilson and Springall–Roberts rules give approximate estimates for decomposition products, which are independent of the explosion temperature, the formulas and calculations for determining the heat of explosion used in this chapter assume that the explosive reactions go to completion. In practice, explosive reactions do not go to completion but result in an equilibrium between reactants and products. Therefore, in Chapter 6, "Equilibria and Kinetics of Explosive Reactions" (15 pp.), Akhavan considers this situation, along with activation energy, rates, and measurement of kinetic parameters by differential thermal analysis (DTA), thermogravimetric analysis (TGA), and differential scanning calorimetry (DSC).

Chapter 7, "Manufacture of Explosives" (31 pp., the longest chapter), deals with the three types of nitration, classified according to the atom on which the nitro group is attached: C-nitration (picric acid, tetryl, TNT, TATB, and HNS); O-nitration (nitroglycerin, nitrocellulose, and PETN); and N-nitration (RDX, HMX, nitroguanidine, and ammonium nitrate). The chapter also discusses the very hazardous manufacture of primary explosives (lead azide, mercury fulminate, and tetrazene) as well as the manufacture of commercial explosive compounds (dynamite and ammonium nitrate and its slurries) and military explosive compositions, which are cast, pressed, or extruded into their final form.

Chapter 8, "Introduction to Propellants and Pyrotechnics" (16 pp.), discusses propellants (explosive materials that undergo rapid and predictable combustion without detonation, resulting in large volumes of hot gases) and pyro-

technics (explosive materials that, unlike explosives or propellants, react at visibly observable rates with the formation of solid residues). The chapter deals with performance and composition for gun propellants (those designed to provide large quantities of gas, which is used to propel projectiles with high kinetic energies) and rocket propellants (those designed to burn uniformly and smoothly without detonation but burning less rapidly than gun propellants). Among the pyrotechnics dealt with are heat-producing, smoke-generating, light-generating, and noise-generating varieties.

Akhavan's book contains a few errors, but these are mostly in the spelling of names (e.g., Berthold Schwarz (not Schwartz), Johann Kunckel (not Kunkel). It includes 35 figures, 64 tables, and 95 numbered items (mathematical or chemical equations and structural formulas or reaction schemes—many consisting of multiple formulas or schemes). A two-page bibliography of 30 articles and books dating from 1958 to 1996 and a 13-page (two columns per page) subject index conclude the volume.

The book is intended primarily for students at the British A-level (equivalent to advanced placement in U.S. high schools) and undergraduate or graduate students, all with no previous knowledge of explosive materials. As a volume in the RSC Paperbacks series, it is an "inexpensive text suitable for teachers and students and … a clear, readable introduction to selected topics in chemistry." It should also be useful for experienced chemists in the explosives industry or for anyone looking for concise information on the subject.

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Protein Structure Prediction. Methods and Protocols (Methods in Molecular Biology, volume 143). Edited by *David M. Webster.* Humana Press, Totowa 2000. 422 pp., hardcover $ 89.50.—ISBN 0-89603-637-5

The avalanche of genomic DNA sequences received by the genetic databanks will constitute comprehensible biological information only when proper links between genome sequence and protein (and possibly RNA) structure and function are established. This book, edited by David Webster, is concerned with the limiting step in the solution of this biological puzzle; namely, discovering (though not necessarily understanding) the connection between protein sequence and structure. To date, the joint SWISS-PROT-TrEMBL non-redundant database contains over 560 000 protein sequences. By contrast, only 7050 protein structures (with a maximum sequence homology of 95%) have been deposited in the Protein Data Bank (PDB). Whole genome sequencing of a number of organisms, including a working draft of the human genome (announced in June 2000), and subsequent efforts on genome annotation will yield an even larger gap between the number of known protein sequences and the number of solved three-dimensional structures. In the absence of an unprecedented revolution in experimental structure determination, theoretical methods are hoped to help fill this gap.

Protein Structure Prediction: Methods and Protocols covers the major topics in computational protein-structure prediction, with eighteen chapters contributed by experts in the field. The book is organised following a natural sequence in the process of structure prediction, from sequence analysis, through secondary and tertiary structure prediction, to molecular docking. In Chapter 1, D. G. Higgins and W. R. Taylor give a detailed introduction and practical guide with examples to their respective multiple sequence alignment programs. Unfortunately, the two programs presented are based on the same general type of alignment algorithm, a progressive global alignment, and no overview on other types of algorithms is provided, limiting the chapter's utility. W. R. Taylor has also written a chapter on protein-structure alignment, where he gives a brief outline of different methods and describes in some detail his own algorithm and program. In Chapter 3, I. Jonassen provides a nice introduction to sequence-pattern recognition, with special emphasis on pattern discovery from unaligned protein sequences. He surveys different algorithms and describes his own program in some more detail. The chapter by C. P. Ponting and E. Birney addresses the identification of structural domains from the analysis of the protein's sequence. For this purpose they propose a protocol which combines a number of programs from different authors. The chapter on secondary-structure prediction has been contributed by B. Rost and C. Sander. They have written an excellent retrospective review, with practical discussions and extensive bibliography. In addition, some special attention is devoted to their own secondary-structure prediction program. With Chapter 6 the book enters the frontiers of protein-structure prediction: comparative modeling, fold recognition, and ab initio prediction. R. Sánchez and A. Šali introduce the reader to comparative modeling, and provide a number of practical examples using their own methods and program. D. Jones has written a concise, instructive introduction to protein-structure prediction, including a practical guide with examples aimed at exploiting the possibilities of different programs at each stage of the prediction process. B. A. Reva, A. V. Finkelstein, and J. Skolnick sign a chapter on the derivation and testing of effective energy functions for use in fold recognition, illustrated with the authors' own functions. Ab initio prediction is treated by S. Schulze-Kremer, who has written a rather detailed introduction to the use of genetic algorithms in protein-structure prediction, and by E. S. Huang, R. Samudrala, and B. H. Park who give a survey of effective energy functions in the context of different ab initio structure-prediction methods. In Chapter 11, R. E. Bruccoleri presents his program for ab initio loop modeling, illustrating its functioning with an example. Again, one misses some discussion on alternative algorithms. Next, M. De Maeyer, J. Desmet, and I. Lasters describe the dead-end elimination theorem and their implementation to the modeling of side-chains on a fixed main-chain template. In Chapter 13, R. B. Russell gives an introduction to the classification of protein folds, with a brief description of different classification approaches and their related databases. M. S. P. Sansom and L. Davison treat the difficult yet biomedically important problem of structure prediction of membrane proteins. They describe an approach to

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