CaF_2, growth front structure in the crystallization of $CBr_4 + C_2Cl_6$, and methods for determining the compositions of congruently melting three-component solid solutions. This last paper is typical of the impressive advances in phase diagram theory and applications of the phase rule which have appeared over the last 30 years or so in the *Russian Journal of Physical Chemistry*.

Volume 20 is appropriate reading for crystal growth specialists and those interested in keeping up with Russian and Ukrainian advances in the field. Unfortunately, readers will have to write the editors directly for more information, since nowhere do the addresses of the individual authors appear. The publishers, however, have promised to include both conventional addresses and e-mail addresses in the next volume. In keeping with Russian practice, Volume 20 does not contain an index, although since the longest paper extends over only 16 pages, this omission is of little consequence.

James K. Baird, *University of Alabama at Huntsville*

JA965670C

S0002-7863(96)05670-3

Solvent Effects and Chemical Reactivity. Edited by O. Tapia (University of Uppsala, Sweden) and J. Bertrán (Universitat Autònoma de Barcelona). Kluwer Academic Publishers: Dordrecht, The Netherlands. 1996. X + 377 pp. ISBN O-7923-3995-9.

This book contains seven review chapters dealing with various aspects of the theoretical treatments of solvent effects with a special emphasis on chemical reactivity.

The first chapter by Cramer and Truhlar, entitled Continuum Solvation Models, is an excellent introduction to the various quantum chemical methods in which the solvent is treated as a dielectric continuum. It starts with a clear theoretical introduction in which the electrostatic bases of the models and their introduction into the quantum chemical treatments are reviewed. The role of nonelectrostatic contributions to the solvation free energy is then analyzed. The various implementations of these models in computer codes is then thoroughly reviewed, with a remarkable modest presentation of the authors' increasingly popular SMx approaches. The treatment of equilibrium properties in solution takes a large place in this chapter. The problem of computing solvation free energies is first addressed, and then several illustrative examples are reviewed. They are focused on intra- and intermolecular proton transfers, tautomeric equilibria, and lactolization. The chapter ends with a short review of dynamic effects in chemical kinetics and spectroscopy. An extensive bibliography (385 references) makes this contribution a basic text to anyone who intends to enter the very active field of solvent effects by means of the simple and very effective continuum models.

The second chapter by Contreras, Pérez, and Aizman deals with the use of density functional theory. It is a rather technical chapter in which the authors mainly develop their own approach which is based on a reaction field (i.e., continuum) model.

The use of Monte Carlo techniques to compute the thermodynamic quantities which enter the transition state theory of chemical reactivity when the solvent molecules are considered explicitly is developed in the third chapter by González-Lafont, Lluch, and Bertrán. A large part of the text is devoted to the methodologies derived from the Monte Carlo method, with some illustrative reference examples.

The next chapter, entitled Computer simulations for chemical systems: from vacuum to solution, by Corongiu, Estrin, and Paglieri mainly deals with aqueous solutions studied at different levels of theory. The chapter starts with a methodological review of density functional theory and its use in molecular dynamics simulations and of the self-consistent reaction field models. A series of illustrative examples is analyzed, starting with the ammonia−hydrochloric acid reaction. The solvation of Li^+, the structure of water clusters, and finally the stability and vibrational spectra of DNA base pairs are the other examples considered in the review.

The basic aspects of chemical reaction dynamics in solution are analyzed in a short (27 pages) but very clear chapter by Hynes entitled Crossing the transition state in solution. The author develops the so-called "stochastic" theoretical approach of the reaction rates in solution and the molecular dynamics simulations designed to test the theoretical conclusions. The paper is based on the Grote−Hynes theory of reaction rate constants which is developed first. The author then considers the case of charge transfer reactions involving a quantum particle. The part devoted to simulation studies briefly relates some simulation results on S_N2 and S_N1 reactions and ion pair combinations in aqueous solutions and some examples of nonadiabatic solvation effects. In the second half of this part, transfer reactions of light particles (proton, electron) are analyzed, mainly from a theoretical point of view.

Bianco and Hynes develop, in the sixth chapter, a combination of valence bond treatment of the solute with a dielectric continuum description of the solvent. The nonequilibrium solvation effects are approached by considering the time dependent molecular reorientation contribution to the electric polarization of the solvent. The method is applied to the authors' favorite reactions ($I_2^- \rightarrow I + I^-$; S_N1 and S_N2).

The last chapter, by Tapia, Andres, and Stamato, entitled Quantum Theory of Solvent Effects and Chemical Reactions, develops some rather formal views on the various phenomena expected to influence chemical reactions in solution, and their theoretical consequences. The chemically interesting examples are just mentioned without great detail. Nevertheless, a long and useful bibliography (more than 300 references) makes the chapter interesting to consider.

In conclusion, this book contains some very useful reviews on various aspects of solvent effects, and although it appears as a simple collection of contributions, without any visible editorial effort, it is highly recommendable to all the theoretical or computational chemists having some concern with solution chemistry.

Jean-Louis Rivail, *Université Henri Poincaré Nancy I*

JA965788T

S0002-7863(96)05788-5

Annual Review of Physical Chemistry, Vol. 48. Edited by Herbert L. Strauss (University of California—Berkeley), Gerald T. Babcock (Michigan State University), and Stephen R. Leone (University of Colorado). Annual Reviews, Inc.: Palo Alto, CA. 1997. x + 875 pp. $64.00. ISBN 0-8243-1048-9.

The field of physical chemistry continues to progress in many surprising directions. The applications reviewed in this volume involve systems that range from new views of traditional physical chemistry problems (e.g., hydrogen bonding) to new techniques that have just started to contribute to physical chemistry (e.g., subfemtosecond kinetics, single-molecule spectroscopy). There is an author index, subject index, cumulative index of contributing authors, Volumes 44−48, and cumulative index of chapter titles, Volumes 44−48.

JA9756883

S0002-7863(97)05688-6

Kirk-Othmer Encyclopedia of Chemical Technology, Volume 23, Sugar to Thin Films. Edited by Jacqueline I. Kroschwitz and Mary Howe-Grant. Wiley/VCH: New York. 1997. xxviii + 1118 pp. $325.00. ISBN 0-471-52692-4.

This is the 23rd volume of a 25-volume encyclopedia set, four volumes being published each year. The fourth edition is similar in format to the earlier editions with updates to the entries as necessary and the addition of several new subjects. This volume contains 36 entries ranging from Sugar to Thin Films. This volume does not contain an index; however, paperback indexes are published every four volumes, and the supplement and index volumes are scheduled for publication in 1998.

JA975689V

S0002-7863(97)05689-8