



Advances in Molten Salt Chemistry: Volume 3 (Paperback)

By J. Braunstein, Gleb Mamantov, G. P. Smith

Springer-Verlag New York Inc., United States, 2012. Paperback. Book Condition: New. 229 x 152 mm. Language: English . Brand New Book ***** Print on Demand *****. The first chapter of this volume deals with computer simulation of molten salt behavior by molecular dynamics calculations. The next four chapters are reviews of experimental work: Chapter 2 deals with the solubility of nonre- active gases in molten salts, Chapter 3 with various types of organic reactions in molten tetrachloroaluminates, Chapter 4 with techniques for the study of molten fluorides, and Chapter 5 with the physical and chemical properties of thiocyanate melts. The last chapter is a collection of phase diagrams for binary and ternary fluoride systems. J. B., G. M., G. P. S. v CONTENTS Chapter 1 MOLECULAR DYNAMICS CALCULATIONS ON MOLTEN IONIC SALTS L. V. Woodcock 1. Introduction. . 42. Intermolecular Forces in Molten Salts 42.1. True and Effective Pair Potentials 2.2. Semiempirical Models 6 3. Computational Techniques 13 3.1. Molecular Dynamics Simulation 13 3.2. The Monte Carlo Method 15 3.3. Electrostatic Summations . . 18 4. Calculation of Physical Properties 23 4.1. Equilibrium Properties . 23 4.2. Transport Coefficients 27 4.3. Spectroscopic Properties 32 5. Applications.35 5.1. Studies of...



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