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SOLVENTS; 3.4 BRØNSTED-LOWRY ACIDS AND BASES; 3.5 ACIDITY FUNCTIONS; 3.6 ACIDS AND BASES IN KINETICS; 3.7 LEWIS ACIDS AND BASES; 3.8 HARD AND SOFT ACIDS AND BASES (HSAB) 3.9 SCALES OF HARDNESS OR SOFTNESS 3.10 ACIDS AND BASES IN REACTIVE APROTIC SOLVENTS; 3.11 EXTREMES OF ACIDITY AND BASICITY; 3.12 OXIDATION AND REDUCTION; 3.13 ACIDITY/REDOX DIAGRAMS; 3.14 UNIFICATION OF ACID-BASE AND REDOX CONCEPTS; PROBLEMS; 4 CHEMOMETRICS: SOLVENT EFFECTS AND STATISTICS; 4.1 LINEAR FREE ENERGY RELATIONSHIPS; 4.2 CORRELATIONS BETWEEN EMPIRICAL PARAMETERS AND OTHER MEASURABLE SOLVENT PROPERTIES; 4.3 REPRESENTATION OF CORRELATION DATA ON THE HEMISPHERE; 4.4 SOME PARTICULAR CASES; 4.5 ACIDITY AND BASICITY PARAMETERS; 4.6 BASE SOFTNESS PARAMETERS; 4.7 CONCLUSION 5 THEORIES OF SOLVENT EFFECTS 5.1 INTRODUCTION: MODELING; 5.2 QUANTUM-MECHANICAL METHODS; 5.3 STATISTICAL-MECHANICAL METHODS; 5.4 INTEGRAL EQUATION THEORIES; 5.5 SOLVATION CALCULATIONS; 5.6 SOME RESULTS; PROBLEMS; 6 DIPOLAR APROTIC SOLVENTS; 6.1 INTRODUCTION; 6.2 ACIDITIES IN DMSO AND THE H-SCALE IN DMSO-H₂O MIXTURES; 6.3 USE OF THERMODYNAMIC TRANSFER FUNCTIONS; 6.4 CLASSIFICATION OF RATE PROFILE-MEDIUM EFFECT REACTION TYPES; 6.5 BIMOLECULAR NUCLEOPHILIC SUBSTITUTION; 6.6 PROTON TRANSFER; 6.7 D₂-HO EXCHANGE; PROBLEMS; 7 EXAMPLES OF OTHER SOLVENT CLASSES; 7.1 INTRODUCTION; 7.2 ACIDIC SOLVENTS 7.3 BASIC SOLVENTS 7.4 CHIRAL SOLVENTS; 8 NEW SOLVENTS AND GREEN CHEMISTRY; 8.1 NEOTERIC SOLVENTS; 8.2 SUPERCRITICAL FLUIDS; 8.3 IONIC LIQUIDS; 8.4 LOW-TRANSITION-TEMPERATURE MIXTURES; 8.5 BIO-BASED SOLVENTS; 8.6 FLUOROUS SOLVENTS; 8.7 SWITCHABLE SOLVENTS; 8.8 GREEN SOLVENT CHEMISTRY; 9 CONCLUDING OBSERVATIONS; 9.1 CHOOSING A SOLVENT; 9.2 ENVOI; APPENDIX; ANSWERS; CHAPTER 1; CHAPTER 2; CHAPTER 3; CHAPTER 6; REFERENCES; INDEX; END USER LICENSE AGREEMENT

Sommario/riassunto

This book introduces the concepts, theory and experimental knowledge concerning solvent effects on the rate and equilibrium of chemical reactions of all kinds. It begins with basic thermodynamics and kinetics, building on this foundation to demonstrate how a more detailed understanding of these effects may be used to aid in determination of reaction mechanisms, and to aid in planning syntheses. Consideration is given to theoretical calculations (quantum chemistry, molecular dynamics, etc.), to statistical methods (chemometrics), and to modern day concerns such as "green" chemistry, where ut

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