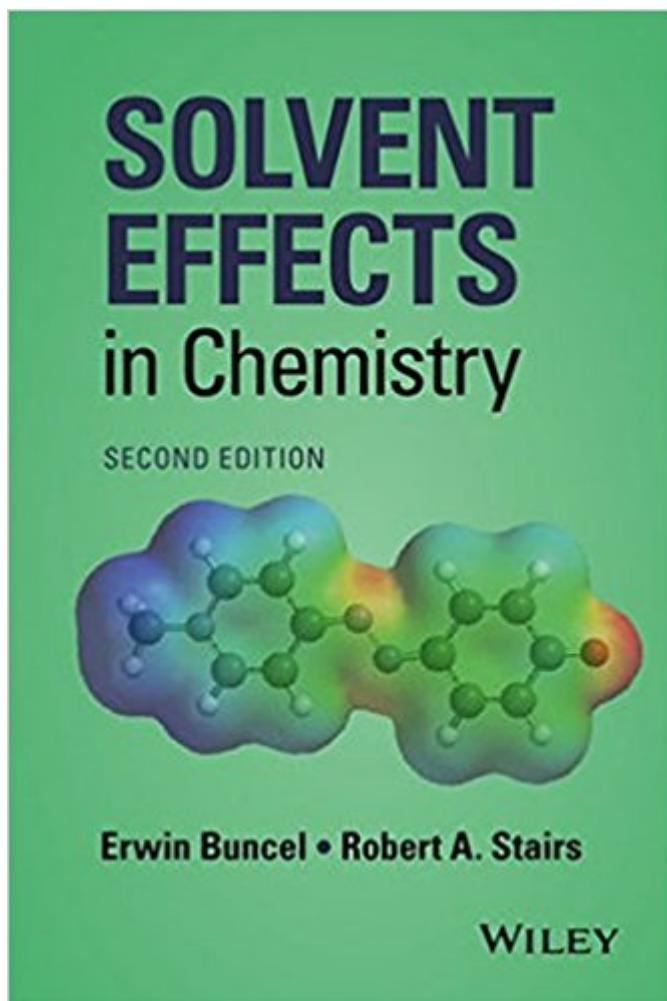


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# Solvent Effects In Chemistry



## Synopsis

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 utilization and disposal of chemical waste or by-products in an environmentally safe way is as important as achieving the desired end products by all chemists nowadays. The treatment progresses from elementary to advanced material in straightforward fashion. The more advanced topics are not developed in an overly rigorous way so that upper-level undergraduates, graduates, and newcomers to the field can grasp the concepts easily.

## Book Information

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Solvents are integral to everyday research activities. Choosing the appropriate solvent allows thermodynamic and kinetic control of a chemical reaction. Building on this foundation to cultivate a deeper understanding of the topic can better aid and result in the determination of reaction mechanisms and syntheses planning. Solvent Effects in Chemistry provides the introduction to the concepts, theory and experimental knowledge concerning solvent effects on the rate and equilibrium of chemical reactions. It begins with basic thermodynamics and kinetics, with consideration given to theoretical calculations (quantum chemistry, molecular dynamics, etc.), to

statistical methods (chemometrics), and to modern-day concerns such as  $\text{a} \text{oe} \text{green} \text{a} \cdot$  chemistry. Furthermore, this monograph:  $\text{a} \text{oe} \text{A}$  Employs a semi quantitative approach, avoiding unnecessary detail or rigor so that the discussions are accessible to students and professionals alike  $\text{a} \text{oe} \text{A}$  Is suitable for undergraduates, graduate students, and newcomers from related fields in chemistry and chemical engineering where an understanding of solvent effects is desired  $\text{a} \text{oe} \text{A}$  Provides examples from inorganic and organic chemistry As this book is aimed at upper-level undergraduates, graduates, and newcomers to the field, the more advanced topics in the book are presented in a succinct and clear way so that concepts can be easily grasped. It is also intended as a supplementary text for all kinds of chemists, namely, academic researchers, chemical engineers, environmental scientists, government and industrial workers in chemistry who will find the text a reliable source for their research.  $\text{a} \text{oe}$ The molecule represented on the front cover is 4-[(4 $\text{a} \text{TM}$ -hydroxyphenyl)azo-N-methylpyridine, called  $\text{a} \text{oe}$ Buncel $\text{a} \text{TM}$ s dye $\text{a} \cdot$  by Rauhut, Clark and Steinke (1993). The solvatochromism of this and a small number of related dyes forms the basis of the polarity parameter  $\text{I}^* \text{azo} \cdot$

Robert A. Stairs, Ph.D, FCIC, is Professor Emeritus in the Department of Chemistry at Trent University at Peterborough, Ontario, having joined at its opening in 1964, after teaching at Cornell and at Queen's University in Kingston. During his 25 years at Trent, he served as chair of the Department twice. Since retiring, Prof. Stairs keeps up a close relationship with Trent, returning regularly for seminars and special events, and maintaining a modest research program. Erwin Buncel, PhD, FRCS, is Professor Emeritus in the Physical Organic Chemistry department at Queen's University. He received his Ph.D. in Organic Chemistry in 1957 and his D.Sc. in Physical Organic Chemistry in 1970, both at the University of London. He has won several awards and honors, including the R.U. Lemieux Award in Organic Chemistry - Canadian Society for Chemistry in 1999 and he was a Fellow, World Innovation Foundation (2001). He has recently been elected a fellow of the Royal Society of Canada.

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