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Collana	QSAR in Environmental and Health Sciences QSAR in environmental and health sciences ; ; 4
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Nota di contenuto	Front Cover; Contents; Series Introduction; Foreword; Acknowledgments; About the Authors; Preface; Chapter 1: Introduction; Chapter 2: Absolute pKa Calculations; Chapter 3: Relative pKa Calculations; Chapter 4: Quantitative Structure-Acidity Methods; Chapter 5: Oxyacids and Related Compounds; Chapter 6: Nitrogen Acids; Chapter 7: Additional Types of Acids; Chapter 8: Acidities in Nonaqueous Solvents; Chapter 9: Additional Factors Influencing Acidity and Basicity; Chapter 10: Conclusions; References; Back Cover
Sommario/riassunto	The book describes how one can calculate the acidities and basicities of chemicals (pKa is the dissociation constant). Many drugs, industrial chemicals, biochemicals and pollutants dissociate to form new species under different conditions. The nature of the species present has a profound effect on how the species act, and it is important to be able to estimate which species will be present under different conditions. No other book summarizes how one can estimate the natures of the species present using modern theoretical methods. This book fills that need--

