

1. Record Nr.	UNINA9910139364503321
Autore	Laurence Christian
Titolo	Lewis basicity and affinity scales [[electronic resource]] : data and measurement // Christian Laurence, Jean-Francois Gal
Pubbl/distr/stampa	Chichester, : Wiley, 2010
ISBN	1-282-68724-7 9786612687242 0-470-68190-X 0-470-68189-6
Descrizione fisica	1 online resource (490 p.)
Altri autori (Persone)	GalJean-Francois
Disciplina	541.39 541.395 546.24
Soggetti	Lewis acids Chemistry Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di contenuto	Lewis Basicity and Affinity Scales; Contents; Preface; 1 Lewis Basicity and Affinity Measurement: Definitions and Context; 1.1 The Br onsted Definition of Acids and Bases; 1.2 Scales of Br onsted Basicity and Affinity in Solution; 1.3 Scales of Br onsted Basicity and Affinity in the Gas Phase; 1.4 The Lewis Definition of Acids and Bases; 1.5 Quantum Chemical Descriptions of Lewis Acid/Base Complexes; 1.5.1 Valence-Bond Model; 1.5.2 Perturbation Molecular Orbital Theory; 1.5.3 Variational Supermolecular Method and Energy Decomposition Schemes; 1.5.4 Natural Bond Orbital Theory 1.5.5 Quantum Theory of Atoms in Molecules1.6 Measurement of Lewis Basicity; 1.6.1 Gas-phase Reactions; 1.6.2 Solution Reactions; 1.6.3 Standard State Transformations; 1.6.4 Choice of Solvent; 1.7 Measurement of Lewis Affinity; 1.8 The Role of the Solvent; 1.9 Spectroscopic Scales of Basicity (Affinity); 1.10 Polybasic Compounds; 1.11 Attempts at a Quantitative Formulation of the Lewis Definition of Acids and Bases; 1.11.1 Hard and Soft Acids and Bases; 1.11.2 The ECW

and ECT Models; 1.11.3 The Beta and Xi Equation; 1.11.4 A Chemometric Approach
1.11.5 Quantum Chemical Descriptors for Basicity Scales
1.12 Concluding Remarks and Content of Chapters 2-7; References; 2 The Donor Number or SbCl₅ Affinity Scale; 2.1 Structure of SbCl₅ Complexes; 2.2 Definition of the Donor Number Scale; 2.3 Experimental Determination of the Donor Number; 2.4 The Donor Number Scale: Data; 2.5 Critical Discussion; References; 3 The BF₃ Affinity Scale; 3.1 Structure of BF₃ Complexes; 3.2 Definition of the BF₃ Affinity Scale; 3.3 Experimental Determination of the BF₃ Affinity Scale; 3.4 The BF₃ Affinity Scale: Data; 3.5 Discussion; 3.5.1 Medium Effects 3.5.2 Hardness of BF₃ 3.5.3 Comparison of the BF₃ and SbCl₅ Affinity Scales; 3.5.4 Computation of the BF₃ Affinity; 3.6 Conclusion; References; 4 Thermodynamic and Spectroscopic Scales of Hydrogen-Bond Basicity and Affinity; 4.1 Structure of Hydrogen-Bonded Complexes; 4.2 Hydrogen-Bond Basicity Scales: Early Works; 4.3 The 4-Fluorophenol Hydrogen-Bond Basicity Scale; 4.3.1 Definition; 4.3.2 Method of Determination; 4.3.3 Polyfunctional Hydrogen-Bond Acceptors; 4.3.4 Data; 4.3.5 Range of Validity of the Scale; 4.4 Hydrogen-Bond Affinity Scales: Early Studies
4.5 The 4-Fluorophenol Affinity Scale
4.6 Comparison of 4-Fluorophenol Affinity and Basicity Scales; 4.7 Spectroscopic Scales; 4.7.1 Infrared Shift of Methanol; 4.7.2 Solvatochromic Shifts of 4-Nitrophenol and 4-Nitroaniline; 4.8 Conclusion; References; 5 Thermodynamic and Spectroscopic Scales of Halogen-Bond Basicity and Affinity; 5.1 Structure of Halogen-Bonded Complexes; 5.2 The Diiodine Basicity Scale; 5.2.1 Definition of the Scale; 5.2.2 Methods for the Determination of Diiodine Complexation Constants; 5.2.3 Temperature Correction; 5.2.4 Solvent Effects; 5.2.5 Data
5.3 Is the Diiodine Basicity Scale a General Halogen-Bond Basicity Scale?

Sommario/riassunto

The Lewis concept of acids and bases is discussed in every general, organic and inorganic chemistry textbook. This is usually just a descriptive treatment, as it is not possible to devise a single numerical scale suitable for all occasions. However quantitative Lewis acid-base chemistry can be developed by compiling reaction-specific basicity scales which can be used in specific branches of chemistry and biochemistry. Lewis Basicity and Affinity Scales: Data and Measurement brings together for the first time a comprehensive range of Lewis basicity/affinity data in one volume. More t
