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Nota di contenuto	Modelling 1H NMR Spectra of Organic Compounds; Contents; Preface; 1 Introduction to 1H NMRChemical Shifts; 1.1 Historical Background; 1.2 Basic Theory of NMR; 1.3 The 1H Chemical Shift; 1.3.1 Nuclear Shielding and Reference Compounds; 1.4 1H Substituent Chemical Shift (SCS); 1.4.1 Two-bond (H.C.X) Effects; 1.4.2 Three-bond (H.C.C.X) Effects; 1.4.3 1H SCSs in Olefins and Aromatics; 1.5 Long-range Effects on 1H Chemical Shifts; 1.5.1 Steric (van der Waals) Effects; 1.5.2 Electric Field Effects; 1.5.3 -Electron Effects; 1.5.4 Hydrogen Bonding Shifts 1.6 Tables of 1H Chemical Shifts of Common Unsaturated and Saturated Cyclic SystemsReferences; 2 Interpretation of 1H NMR Coupling Patterns; 2.1 Fine Structure due to HH Coupling; 2.2 The Analysis of NMR Spectra; 2.2.1 Nomenclature of the Spin System, Chemical and Magnetic Equivalence; 2.2.2 Two Interacting Nuclei, the AB Spectrum; 2.2.3 Three Interacting Nuclei, the ABX Spectrum; 2.2.4 Four Interacting Nuclei; 2.2.5 Iterative Computer Analysis; 2.2.6 Automatic Iteration of Complex Spectra; 2.3 The Mechanism of Spin-

Spin Coupling; 2.3.1 Geminal HH Couplings (2JHH)
2.3.2 Vicinal HH Couplings (3JHH)2.3.3 Ab initio Calculated Couplings; 2.3.4 Long-range HH Couplings; 2.4 HF Couplings; 2.4.1 Geminal HF Couplings (2JHF); 2.4.2 Vicinal HF Couplings; 2.4.3 Long-range HF Couplings; References; 3 Chemical Shift Calculations and Molecular Structure; 3.1 Introduction; 3.2 Quantum Mechanical Calculations of 1H Chemical Shifts; 3.3 The Database Approach; 3.4 Semi-empirical Calculations; 3.5 Theory of the CHARGE Program; 3.5.1 Through Bond Effects; 3.5.2 1H Chemical Shifts of Substituted Methanes and Ethanes; 3.5.3 Through Space Effects
3.5.4 Hydrogen Bonding Shifts3.5.5 Aromatic Compounds; References; 4 Modelling 1H Chemical Shifts, Hydrocarbons; 4.1 Introduction; 4.2 Alkane Chemical Shifts; 4.2.1 H..H and C..H Steric Interactions; 4.2.2 The Methyl Effect; 4.2.3 CC Bond Anisotropy; 4.2.4 Observed versus Calculated Shifts; 4.3 Alkene Chemical Shifts; 4.3.1 Introduction; 4.3.2 CC Bond Anisotropy and Shielding; 4.3.3 Observed versus Calculated Shifts; 4.4 Alkyne Chemical Shifts; 4.4.1 Introduction; 4.4.2 CC Bond Anisotropy and Shielding; 4.4.3 Observed versus Calculated Shifts
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6.2 Fluorine Substituent Chemical Shifts

Sommario/riassunto

Provides a theoretical introduction to graduate scientists and industrial researchers towards the understanding of the assignment of 1H NMR spectraDiscusses, and includes on enclosed CD, one of the best, the fastest and most applicable pieces of NMR prediction software availableAllows students of organic chemistry to solve problems on 1H NMR with access to over 500 assigned spectra