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CHEM-756: Nuclear Magnetic Resonance Spectroscopy Principles and applications: Spectroscopy. Solid-state (NMR): Masterrements of liquids in solutions; (1H, 13C) spectras and nuclei; phase shift experiments (imaging); relaxation, spin echo and carbon spin echo and carbon spin echo and carbon spin echos and subulions; hydrogen's nuclei (including protons, deuterium, (15)N). Solutions and subulions; hydrogen's nuclei (including protons, deuterium, (15)N). Solutions and subulions; hydrogen's nuclei (including protons, deuterium, (15)N). Solutions and subulions; hydrogen's nuclei; (including protons, deuterium, (15)N). Solutions and subulions; hydrogen's nuclei; (including protons, deuterium, (15)N). Solutions and subulions; hydrogen's nuclei; (including protons, deuterium, (15)N). Solutions and subulions; hydrogen's nuclei; (including protons, deuterium, (15)N). Solutions; hydrogen's nuclei; (including protons, deuterium, (15)N). So

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CHEM-848: Soft-Core Coulombic Interactions: Theoretical Techniques and Investigations Soft-core Coulombic interactions: Theoretical background; basic theory of the covalent binding energy; "soft-core" potential; approximate theory of covalent binding energies; extended system; approximate theory of covalent binding energies using extended systems; "hard-core" potential and its approximation. Experimental methods for the determination of the soft-core potential: Calibration of the experiments and the relationship with the covalent binding energies. Absorption spectroscopy: Theoretical background; absorption spectroscopy. Calculated spectra of complex molecules: Approximate theory and experimental results. CHEM-849: Computational Chemisty: Experimental Methods Computational chemistry: Nature of electronic wave functions; general formalism; density functional theory (DFT) and its application; second-order DFT, GIAO, and B3LYP; density perturbation theory (PT2), second-order reaction field (SE), and post-SCF and Spin-Density Matrix (SDM) methods, Molecular Geometries; Simple Molecular Structure and Molecular Bonding; Electronic properties (LUMO and HOMO; Electrostatic potential); Applications to chemical and biological systems, the Nature of Transition States; the Nature of Bonding in Molecules; Interaction of ions with clusters. Experimental Methods: Experimental techniques, Instrumentation and calibration, Data Processing. Recommended Books: 5ec8ef588b

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