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Spin Resonance Spectroscopy: Principles and applications

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¹H and ¹³C nuclear magnetic resonance spectroscopy (Book Chapter)

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Abstract

This chapter focuses on interpretation, assignment of chemical shifts including factors affecting it, additive rule for its calculation, spin-spin coupling, and comparison of ¹Hand ¹³C nuclear magnetic resonance (NMR) spectroscopy. It also highlights symmetry in NMR systems and the effect of chirality on NMR. Spin decoupling and nuclear double resonance spectroscopy including single frequency off-resonance decoupling (SFORD), distortionless enhancement by polarization transfer (DEPT), insensitive nuclei enhanced by polarization transfer (INEPT), and chemically induced dynamic nuclear polarization for sensitivity enhancement (CIDNP) and spectral simplification are discussed. Nuclear Overhauser effect (NOE) enhances the signal intensity through space effect, and its mechanism and types are discussed. Multidimensional NMR viz., 2D and 3D for structure elucidation are also presented. The principles and advantages of 2D techniques viz., homonuclear (¹H¹H viz., correlations spectroscopy, total correlation spectroscopy (TOCSY), nuclear Overhauser effect spectroscopy (NOESY), rotating frame nuclear Overhauser effect spectroscopy, exchange spectroscopy, ¹³C¹³C: incredible natural-abundance double-quantum transfer experiment) and heteronuclear (¹H¹³C viz., heteronuclear multiple quantum correlation, heteronuclear single quantum coherence (HSQC), heteronuclear multibond connectivity are illustrated using examples. 3DNMR experiments constructed by combining the two 2D experiments viz., NOESY-HSQC, TOCSY-HSQC and triple resonance experiments using ¹H, ¹³C, ¹⁵N nuclei are also discussed. © 2018 Elsevier Inc. All rights reserved.

Author keywords

(2D and 3D NMR) $(^{13}C \text{ and } ^{1}H \text{ NMR assignment})$ (INEPT) (NOE) (Organic NMR) (Symmetry in NMR)

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