

Index

- Alkyl
 - normal long chain 21, 43, 103
- Alkenes 45, 104
- Amino group NH 22
- Anisotropic shielding effect 5
- APCI (atmosphere pressure ionization) 119
- Artifact 54
- Assignment 28
- Binomial 89
- Carbonyl compound (group) 21, 47, 131
- Characteristic absorption frequency 132
- ChemDraw (software) 6, 28-9
- Chemical equivalence 13
- Chemical shift 1, 3, 39, 41
- CI (chemical ionization) 117
- Complex cleavage 100
- Conjugation effect 6, 46-7, 131
- Correlated peak 54, 68
- COSY 54, 149
 - COSYLR (COSY optimized for long-range couplings) 67
 - H, C-COSY 68
 - DQF-COSY (double-quantum filtered COSY) 66
 - F, F-COSY 61-4
 - phase sensitive COSY 64
- Coupled splitting pattern 27
- Coupling constant 1, 7
- Cross peak see correlated peak
- Cycloalkanes 45, 103
- Daughter ion 88
- DEPT 47, 51, 149
- Deshielding effect 3
- Deuterium exchange 22
- Diagonal peak 54
- Dihedral angle 9
- EI [electron (impact) ionization] 88
- Electron density 3, 6
- Electron effect 131
- Electronegativity
 - of substituent 5, 10, 43, 134
- ESI (electrospray ionization) 115
- Even-electron ion 89
- FAB (fast atom bombardment) 118
- Fingerprint region 130, 135
- First-order spectrum (in ^1H NMR spectra) 18
- Fragment ion 88
- Functional group region 130, 133
- Fundamental frequency
- γ -Gauche effect 45-6
- Geminal coupling 8
- Heavy atom effect 45
- Heteroaromatic ring 21, 106
- Heteronuclear shift correlation spectroscopy (spectrum) 68
- High resolution MS spectrum 123
- HMBC [$(^1\text{H}\text{-detected})$ heteronuclear multiple bond coherence] 75, 149
- HMQC [$(^1\text{H}\text{-detected})$ heteronuclear multiple-quantum coherence] 69, 149
- HSQC [$(^1\text{H}\text{-detected})$ heteronuclear single-quantum coherence] 69, 149
- Hybridization 4
- Hydrogen bond effect 6, 132
- Hydroxyl group OH 22, 132

- Impurity peak 24, 49
 Induction effect 5, 131
 Integral value 2
 Interchange reaction, with reactive hydrogen atom 22
 Inverse mode 54, 69
 Isotopic ion 89
 Isotopic abundance 90
- J* coupling
 by F 23, 244
 by P 23, 179
- LC-MS 115
 Loss of neutral fragments 91
 Long-rang coupling 11, 75, 149
 Long-rang coupling heteronuclear shift correlation spectroscopy (spectrum) 68
- Magnetic equivalence 17
 MALDI (matrix-assisted laser desorption-ionization) 119
 Mass effect 132
 Mass-to-charge ratio 87
 McLafferty rearrangement 94
 Medium effect 6
 Mesomeric effect 131
 Metastable ion 89, 109
 Molecular ion 88
 Multiply-charged ion 89
- $n + 1$ rule 7, 26
 Nitrogen rule 92
 NOE (nuclear Overhauser effect) 79
 NOESY (nuclear Overhauser effect spectroscopy) 79
- Odd-electron ion 89
 Overhauser effect 79
- p- π Conjugation 6
 Parent ion 88
 Pair of equally spaced peaks 27
 Phenyl ring 6, 46, 105
- Quadrupole moment relaxation 22
 Quasi-molecular ion
- RDA (Retro-Diels –Alder reaction) 99
 Reactive hydrogen atom 22
 Rearrangement ion 88, 98, 102
 Reduced mass 130
 Related absorption band 139
 Resonance effect 131
 Retrieve standard spectra from the web 29, 51, 110, 140
 Ring current effect 5
- Saturated ring tension 45, 132
 Second-order spectrum (in ^1H NMR spectra) 19
 Shielding effect 3
 Simple cleavage 93
 rule of, 94
 Soft ionization 88, 115
 Solvent peak 24, 49
 Spin quantum number 7
 Standard spectrum 29, 51, 140
 Steric effect 5, 43, 132
 Substituted heteroaromatic ring 21, 106
 Substituted phenyl ring 46, 105, 138
 meta- substituted phenyl ring 21, 46
 mono-substituted phenyl ring 19
 ortho-substituted phenyl ring 20, 46
 para-substituted phenyl ring 20, 46
- Substitution
 electronegative functional group 5, 10, 43, 134
- Symmetric plan rule 14
- Tandem MS 126, 408
 in space 126
 in time 126
- Three type of substituents 6
 TOCSY (total correlation spectroscopy) 84, 404
- Two-dimensional NMR, introduction to 53
- Unsaturation number 24
- Vicinal coupling 9
- Water peak 24