



PROGRAMS AND BIBLIOGRAPHY

Subject	
Code	Name
QO424	Fundamental concepts in Nuclear Magnetic Resonance Spectroscopy

Vector

OF:S-5 T:002 P:000 L:000 O:000 D:000 HS:002 SL:002 C:002 AV:N EX:S FM:75%

Pre requirement

QO321

Summary

Fundamental concepts in NMR, structural determination and spectral assignments

Program

1 – Fundamental concepts
angular momentum, magnetic moment, active nuclei in homogeneous magnetic field, population of spin states, resonance phenomenon;
2 - Nuclear Magnetic Resonance Spectroscopy (NMR)
Basic NMR components (inner coil and probes), signal detection, Fourier transform, sample preparation, deuterated solvents (lock)
3 – Measured NMR parameters
Chemical shift (δ)
Shielding constant and chemical shift, diamagnetic and paramagnetic shielding, reference compound, chemical shift range in ^1H NMR spectra, signal intensity/area (integrals)
Scalar Coupling constant (J)
Origin for the scalar spin-spin coupling constant (J), $2nI + 1$ rule, signal patterns, Pascal triangle, homonuclear and heteronuclear couplings
4- $^1J_{\text{HH}}$ coupling constants
Vicinal $^3J_{\text{HH}}$ couplings (Karplus equation), Geminal $^2J_{\text{HH}}$ couplings (positive and negative couplings), long range coupling (allyl groups), coupling in rigid and flexible molecules (conformation), keto-enol tautomerism; diastereotopic hydrogens, chemical and magnetic equivalence (first and second order spin system)
5- ^{13}C NMR spectra
 ^{13}C nucleus, ^1H -coupled and ^1H -decoupled ^{13}C NMR spectra, ^{13}C NMR chemical shift range
6-Spectral assignments
Assignment of ^1H and ^{13}C NMR signals and structural determination for saturated and unsaturated organic compounds, aromatic and heteroaromatic compounds.
7 - NMR for other nuclei
 ^1H and ^{13}C NMR spectra for ^{19}F and/or ^{31}P containing compounds, quadrupolar nuclei (^2H and ^{14}N) and its effects on ^1H and ^{13}C NMR spectra, ^1H NMR spectra for ^{15}N containing molecules - comparison with ^{14}N containing molecules.
8- Advanced NMR experiments
 ^{13}C DEPT edited; 2D homonuclear (COSY, TOCSY and NOESY) contour plots, heteronuclear HSQC and HMBC contour plots.

Bibliography

1. Silverstain, Bassler, Morril, Identificação Espectrométrica de Compostos Orgânicos.
2. Friebolin, basic One-and-Two-Dimensional NMR Spectroscopy, 2 ed, 1993.
3. Pavia, Lampman, Kriz, Introduction to Spectroscopy, 2 ed, 1996.

Evaluation criteria

For grading policy, see: Regimento Geral de Graduação, Seção I – Normas Gerais, Capítulo V – Da Avaliação do Aluno na Disciplina. Students are required to attend 75 % of the lectures. For further details, see: Regimento Geral de Graduação, capítulo VI, seção X, artigo 72.