

**20572 STRUCTURAL DETERMINATION
PROGRAMME**

Year 2007-2008
Second Semester

- 1.- **Electronic Spectroscopy (UV, VIS).** The experimental method. Definitions: chromophores, effects. Characteristic absorptions. Dienes and enones: Woodward-Fieser rules. Solvent effects. Other chromophores.
- 2.- **Vibrational spectroscopy (IR, Raman).** The experimental method. General distribution of the absorptions. Organic functional groups (hydrocarbons, carbonyl compounds, hydroxyl compounds, hydrogen bonds, nitrogen derivatives...). Vibrational frequencies in inorganic compounds and complexes. Interpretation of spectra.
- 3.- **Mass spectrometry.** Spectral resolution. Isotope analysis. Fragmentation processes: homolytic and heterolytic bond fissions.
- 4.- **MS fragmentations.** Fragmentations associated to functional groups. Examples.
- 5.- **NMR: the experimental method.** The spectrometer. Sample preparation: solvents. General look at the spectra: chemical shifts, coupling constants, scales and references.
- 6.- **¹H NMR: the chemical shift.** Shielding mechanisms. Topical relationships and molecular symmetry. Factors influencing the shift δ : magnetic anisotropy, solvent effects. Correlations: hydrogens linked to carbon, hydrogens linked to other nuclei. Examples.
- 7.- **¹H NMR: spin-spin coupling.** Coupling constants. The Karplus equation. Spin systems: the $\Delta\nu/J$ ratio, first and second order spectra. Examples.
- 8.- **¹H NMR: analysis of the spectra.** Time-dependent phenomena. Methods of analysis. Simplification of spectra: changing the magnetic field, spin decoupling, shift reagents. The nuclear Overhauser effect (nOe), examples.
- 9.- **¹³C NMR.** Overview. Recording methods (broad band, off resonance, DEPT). Chemical shifts: additivity. Spin-spin couplings. Analysis of the spectra.
- 10.- **NMR in Inorganic Chemistry.** ¹H NMR in inorganic compounds and complexes: organometallics, phosphines, hydrides. ³¹P NMR: phosphates, phosphines and derivatives. Metal complexes. ¹³C NMR: organometallics, metal carbonyls. Multinuclear NMR: ¹⁴N, ¹⁵N, ¹⁹F, ²⁷Al, ²⁹Si, ⁵⁹Co, ¹⁰³Rh, ¹⁹⁵Pt, ¹¹³Cd, ¹⁹⁹Hg.
- 11.- **Electron spin resonance.** Overview. Examples.
- 12.- **Structural determination.** Combined application of the spectroscopic techniques. Examples.

BIBLIOGRAPHY

TEXT BOOKS

- D.H. Williams, I. Fleming, *Spectroscopic methods in organic chemistry*, McGraw-Hill, London, 1995. ISBN 0-07-709147-7.
- R. Silverstein, G.C. Bassler, T.C. Morrill, *Spectrometric identification of organic compounds*, Wiley, New York, 1991. ISBN 0-471-63404-2.
- R. V. Parish, *NMR, NQR, EPR, and Mössbauer spectroscopy in inorganic chemistry*, Ellis Horwood, New York, 1990. ISBN 0-13-625518-3.
- R.J. Abraham, J. Fisher, P. Loftus, *Introduction to NMR spectroscopy*, Wiley, Chichester, 1988. ISBN 0-471-91894-6.
- R.S. Drago, *Physical methods for chemists (2nd Ed.)*, Saunders, Ft. Worth, 1992. ISBN 0-03-075176-4.

FURTHER READING

- E.A.V. Ebsworth, D.W.H. Rankin, S.Cradock, *Structural methods in inorganic chemistry*, Blackwell, Oxford, 1991. ISBN 0-632-02963-3.
- K. Nakamoto, *Infrared and Raman spectra of inorganic and coordination compounds (5th Ed.)*, Wiley, New York, 1997. ISBN 0-471-16394-5 (Part A) i 0-471-16392-9 (Part B).

PROBLEMS

- L.D. Field, S. Sternhell, J.R. Kalman, *Organic structures from spectra (2nd. Ed.)*, Wiley, Chichester, 1995. ISBN 0-471-95631-7.
- R. Davis, C.H.J. Wells, *Spectral problems in organic chemistry*, International Textbook, Glasgow, 1984. ISBN 0-7002-0288-9.
- P.L. Fuchs, C.A. Bunnell, *Carbon-13 NMR based organic spectral problems*, Wiley, New York, 1979. ISBN 0-471-04907-7.

TABLES

- E. Pretsch, T. Clerc, J. Seibl, W. Simon, *Tablas para la elucidación estructural de compuestos orgánicos por métodos espectroscópicos*, Alhambra, Madrid, 1980. ISBN 84-205-0762-8.
- E. Pretsch, T. Clerc, J. Seibl, W. Simon, *Tablas para la determinación estructural por métodos espectroscópicos*, Springer, Barcelona, 1998. ISBN 84-07-00501-0.
- **E. Pretsch, P. Bühlmann, C. Affolter, A. Herrera, R. Martínez, *Determinación estructural de compuestos orgánicos*, Springer, Barcelona, 2001. ISBN 84-07-00526-6.**

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