

## Organic Spectroscopy

**Reading:** Harwood and Claridge. *Introduction to Organic Spectroscopy*, OCP 43  
Clayden, Greeves, Warren and Wothers, *Organic Chemistry* Chap 3, 11 and 15  
Williams and Fleming, *Spectroscopic Methods in Organic Chemistry*

### Topics for notes:

*NMR is the most important spectroscopic technique in chemistry. Your notes should concentrate on the interpretation of spectra and the use of NMR in determining structures.*

*NMR Spectroscopy:* Observable Nuclei.

Spin, sensitivity, abundance, high and low field.

<sup>1</sup>H NMR: Shift range, (de)shielding, effect of hybridization, first order coupling patterns, "roofing" in AB quartets, coupling constants, Karplus curve, integration.

<sup>13</sup>C NMR: Shift range, effect of hybridization, integration, coupling patterns, decoupling, isotope effects.

Solvents, slow and fast exchange (and why this is useful) in hydrogen bonding and conformational equilibria.

Homotopic, diastereotopic and enantiotopic, ring currents and aromaticity, magnetic and chemical equivalence.

Modern techniques: the basics of nOe-spectra, DEPT, 2-D spectra (COSY).

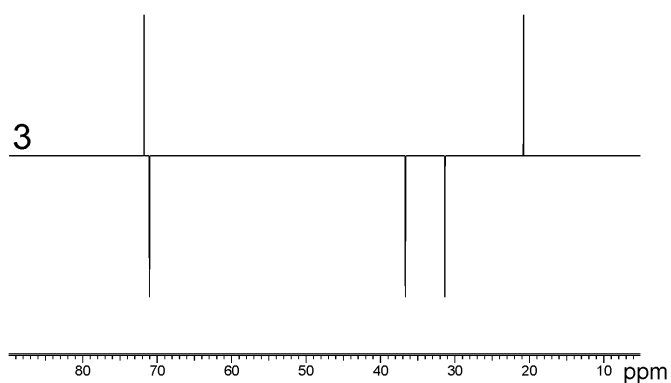
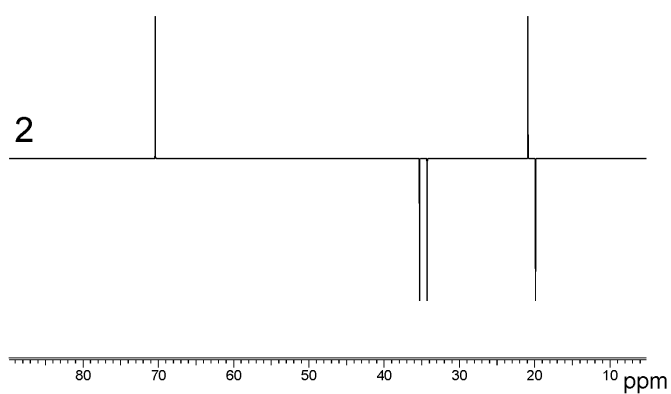
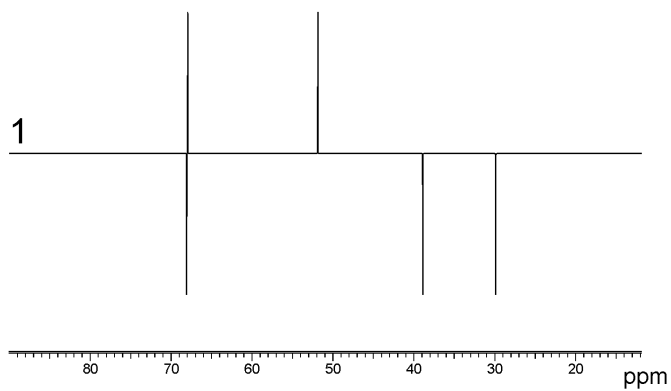
*IR Spectroscopy:* Physical basis of vibrational spectroscopy, absorptions of major functional groups, carbonyl groups and the effects of conjugation / strain, etc.

*Mass spectroscopy:* Isotope patterns, fragmentation patterns, odd number nitrogen rule

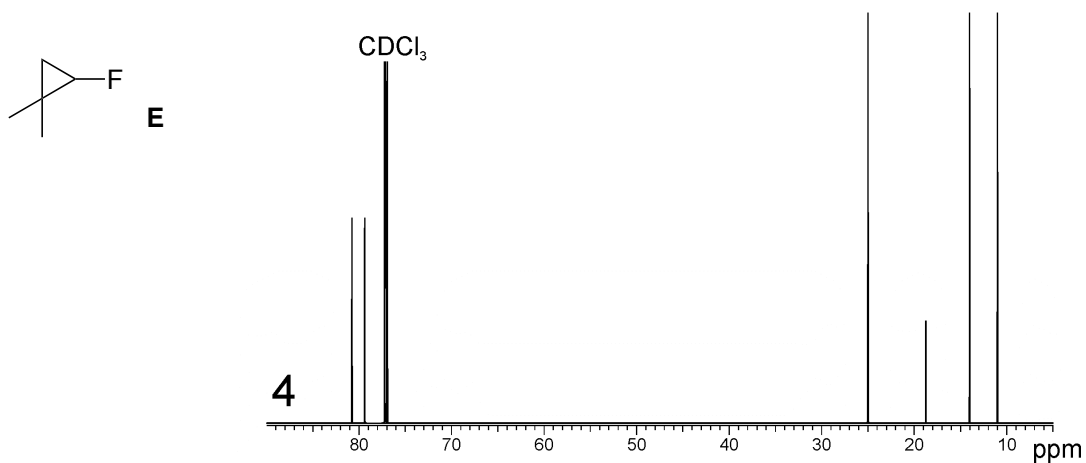
*UV Spectroscopy:* The very basics of energy transitions and chromophores

*Polarimetry:* The very basics of optical rotation

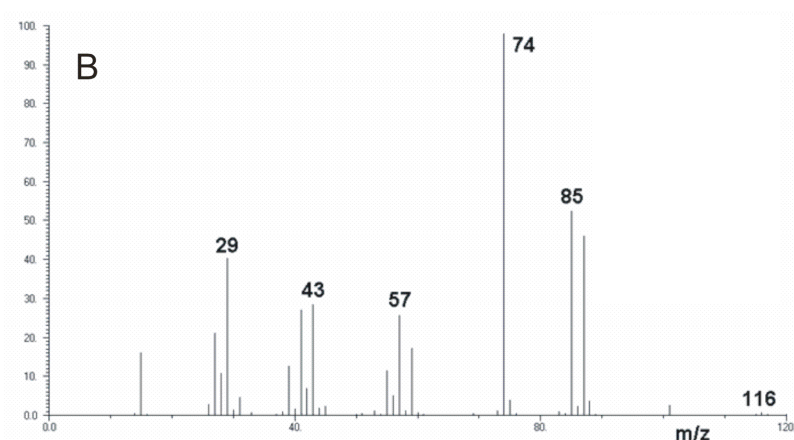
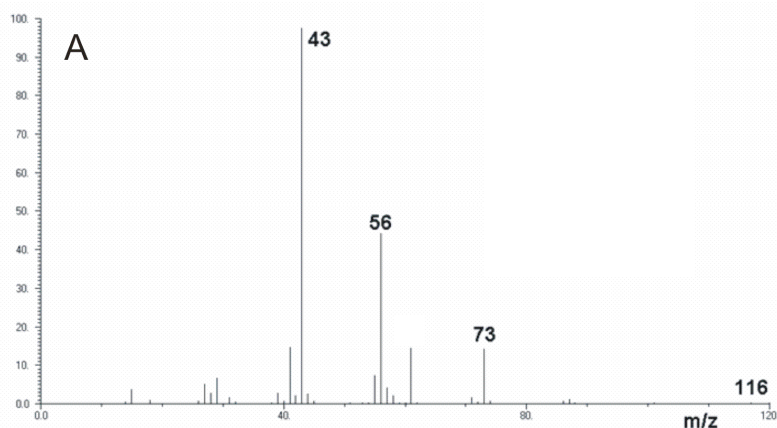




7. Account for the observed proton decoupled one dimensional  $^{13}\text{C}$  spectrum 4 of compound **E**.



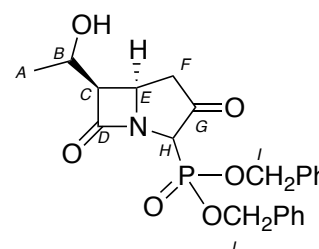
8. Two compounds **F** and **G** with the same molecular formula ( $C_6H_{12}O_2$ ) and same IR signal ( $1740\text{ cm}^{-1}$ ) gave mass spectra **5** and **6** below. Deduce the structures of **F** and **G**.



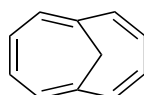
9. Give complete assignments for the non-aromatic carbons (A-J) of this compound. The multiplicities refer only to one-bond C-H splitting. Explain your assignments.

[In this question the multiplicities of the  $^{13}C$  resonances indicate  $^{13}C$ - $^1H$  coupling, so for example “d” means the carbon couples directly to one proton. “ $J_{CP}$ ” is a carbon-phosphorous coupling constant.

$\delta_c$ (ppm)	multiplicity from proton coupling	$^{31}P$ coupling	comments
21.9	q	-	
41.3	dd	-	
51.8	d	-	
61.0	d	$J_{CP} = 161\text{ Hz}$	
65.8	d	-	coupled to proton at $\delta_H = 4.19$ (dq, $J_{HH} = 6.5, 6.2\text{ Hz}$ )
68.5	d	-	coupled to proton at $\delta_H = 4.01$ (ddd, $J_{HH} = 2.0, 7.1, 6.9\text{ Hz}$ )
69.0	t	$J_{CP} = 7\text{ Hz}$	
69.3	t	$J_{CP} = 7\text{ Hz}$	
173.2	s	-	
207.3	s	-	



10. The  $^1H$  NMR spectrum of this compound has a 2 H singlet at  $-0.5\text{ ppm}$ . What does this imply about its electronic structure.



11. Identify the unknowns, **A**, **B**, **C** and **D** using the listed data.

