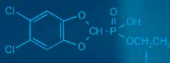


Terence N. Mitchell
Burkhard Costisella

NMR – From Spectra to Structures

An Experimental Approach

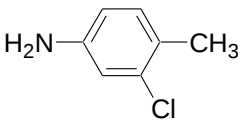
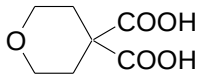
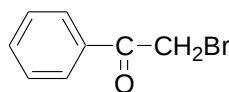
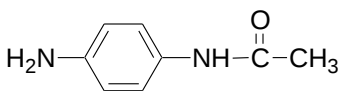
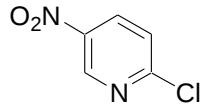
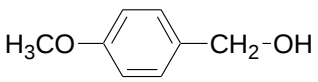
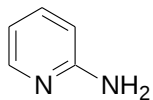
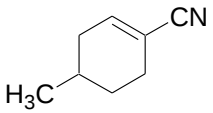
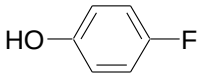
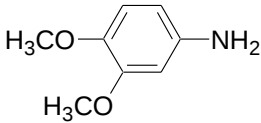
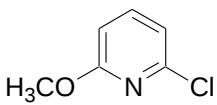
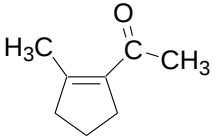
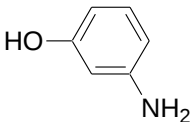
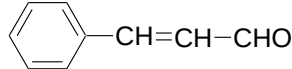
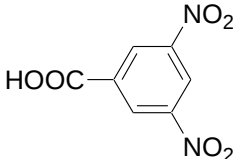
2nd Edition



Solutions Manual

 Springer

NMR - From the Spectra to the Structure

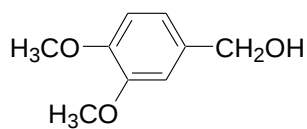
Problem number	Formula	Problem number	Formula
1	$\text{Cl}(\text{CH}_2)_3\text{CN}$	11	
2	$\text{H}_3\text{C}-\text{CH}=\text{CH}-\text{CHO}$	12	
3	$\text{H}_3\text{C}-\overset{\text{O}}{\parallel}{\text{C}}-\text{COOCH}_3$	13	
4	$\text{H}_3\text{C}-\text{CH}_2-\underset{\text{NH}_2}{\text{CH}}-\text{CH}_2\text{OH}$	14	
5		15	
6		16	
7		17	
8		18	
9		19	
10			

NMR - From the Spectra to the Structure

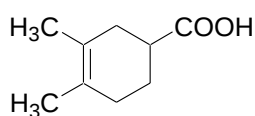
Problem
number

Formula

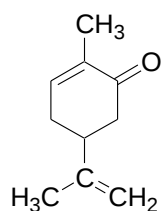
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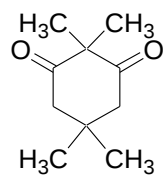
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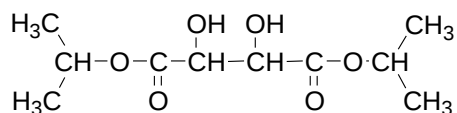
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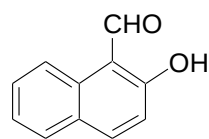
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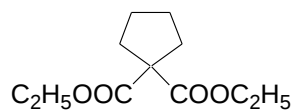
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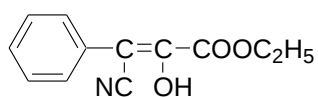
25



26



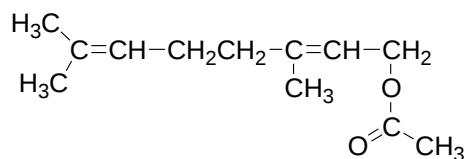
27



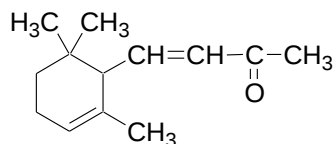
Problem
number

Formula

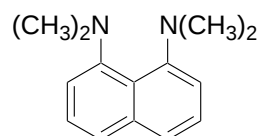
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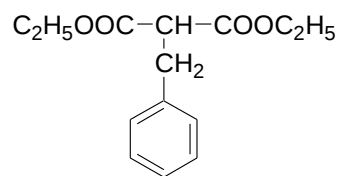
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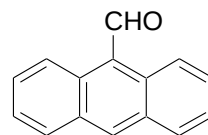
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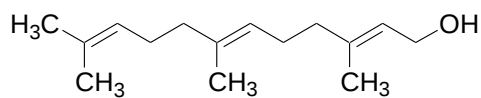
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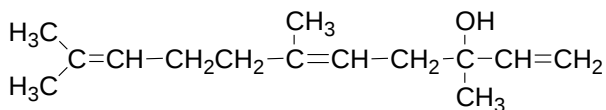
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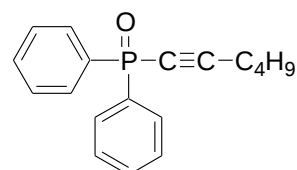
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34



35

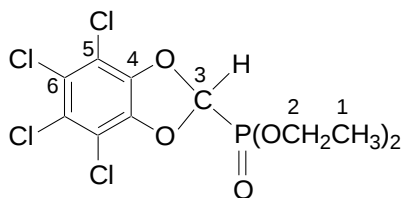


Problems 36-50 (2nd Edition)

**Problem
number**

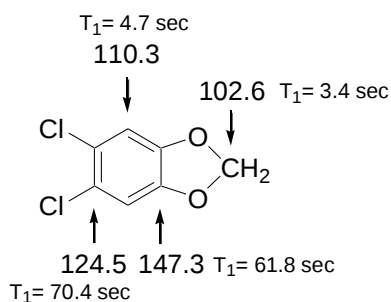
Formula and data

36

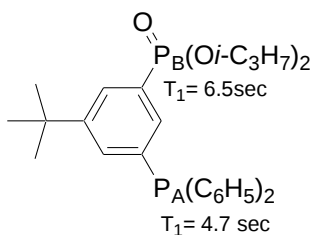


C atom	δ [ppm]	$J(^{31}\text{P}-^{13}\text{C})$ [Hz]	$J(^{13}\text{C}-^1\text{H})$ [Hz]
1	16.77	5.2	$^1J_{\text{CH}} = 127.5$; $^2J_{\text{CH}} = 2.5$
2	64.98	6.8	$^1J_{\text{CH}} = 149.9$; $^2J_{\text{CH}} = 4.3$
3	107.75	196.7	$^1J_{\text{CH}} = 176.6$
4	144.33	2.3	$^3J_{\text{CH}} = 2.3$
5	113.40	-	-
6	126.10	-	-

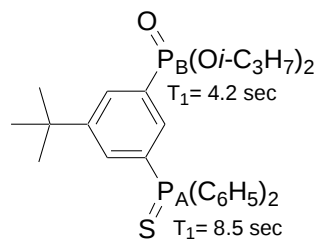
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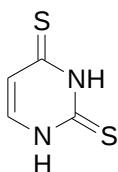
38a



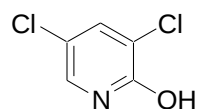
38b



39



40

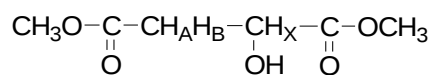


**Problem
number**

Formula and data

41

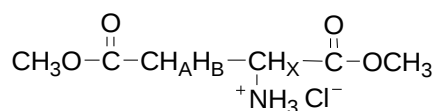
protons of the CH₂ group not equivalent :
(AB system)



$$\begin{aligned}\delta(\text{H}_\text{A}) &= 2.78 \text{ ppm} & {}^2\text{J}(\text{H}_\text{A}\text{H}_\text{B}) &= 16.5 \text{ Hz} ; & {}^3\text{J}(\text{H}_\text{A}\text{H}_\text{X}) &= 4.4 \text{ Hz} \\ \delta(\text{H}_\text{B}) &= 2.71 \text{ ppm} & {}^2\text{J}(\text{H}_\text{A}\text{H}_\text{B}) &= 16.5 \text{ Hz} ; & {}^3\text{J}(\text{H}_\text{B}\text{H}_\text{X}) &= 6.2 \text{ Hz} \\ \delta(\text{H}_\text{X}) &= 4.44 \text{ ppm} & {}^3\text{J}(\text{H}_\text{A}\text{H}_\text{X}) &= 4.4 \text{ Hz} ; & {}^3\text{J}(\text{H}_\text{B}\text{H}_\text{X}) &= 6.2 \text{ Hz}\end{aligned}$$

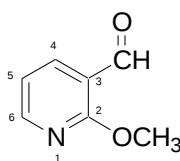
42

protons of the CH₂ group not equivalent :
(AB system)



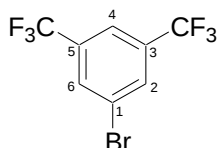
$$\begin{aligned}{}^2\text{J}(\text{H}_\text{A}\text{H}_\text{B}) &= 18.3 \text{ Hz} ; & {}^3\text{J}(\text{H}_\text{A}\text{H}_\text{X}) &= 5.1 \text{ Hz} ; \\ {}^3\text{J}(\text{H}_\text{B}\text{H}_\text{X}) &= 5.1 \text{ Hz} ; & {}^3\text{J}(\text{H}_\text{X}-\text{NH}) &= 5.3 \text{ Hz}\end{aligned}$$

43



$$\begin{aligned}\delta(\text{CHO}) &= 10.30 \text{ ppm d} \quad ({}^5\text{J}_{\text{HH}} = 0.83\text{Hz}) \\ \delta(\text{H4}) &= 8.08 \text{ ppm dd} \quad ({}^3\text{J}_{\text{HH}} = 7.3 \text{ Hz} ; {}^4\text{J}_{\text{HH}} = 2.08 \text{ Hz}) \\ \delta(\text{H5}) &= 6.98 \text{ ppm ddd} \quad ({}^3\text{J}_{\text{HH}} = 7.3 \text{ Hz} ; {}^3\text{J}_{\text{HH}} = 4.83 \text{ Hz} ; {}^5\text{J}_{\text{HH}} = 0.83\text{Hz}) \\ \delta(\text{H6}) &= 8.36 \text{ ppm dd} \quad ({}^3\text{J}_{\text{HH}} = 7.3 \text{ Hz} ; {}^4\text{J}_{\text{HH}} = 2.08 \text{ Hz}) \\ \delta(\text{OCH}_3) &= 4.08 \text{ ppm s}\end{aligned}$$

44



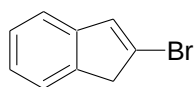
characteristic coupling constants :

$$\begin{aligned}\delta(\text{CF}_3) &= 122.6 \text{ ppm q} \quad ({}^1\text{J}(\text{FC}) = 273.0 \text{ Hz}) \\ \delta(\text{C3}) &= 133.5 \text{ ppm q} \quad ({}^2\text{J}(\text{FC}) = 34.2 \text{ Hz})\end{aligned}$$

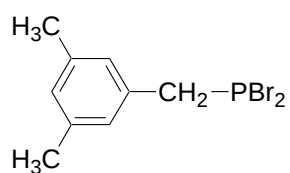
**Problem
number**

Formula and data

45

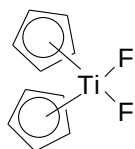


46



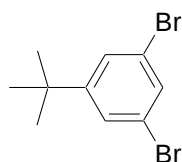
characteristic coupling constants :
 $^2J(\text{PH}) = 16.8 \text{ Hz}$; $^1J(\text{PC}) = 49.6 \text{ Hz}$

47

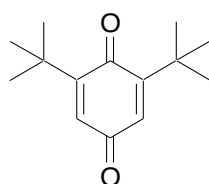


$^3J(\text{FH}) = 1.7 \text{ Hz}$; $^2J(\text{FC}) = 2.5 \text{ Hz}$

48



49



50

