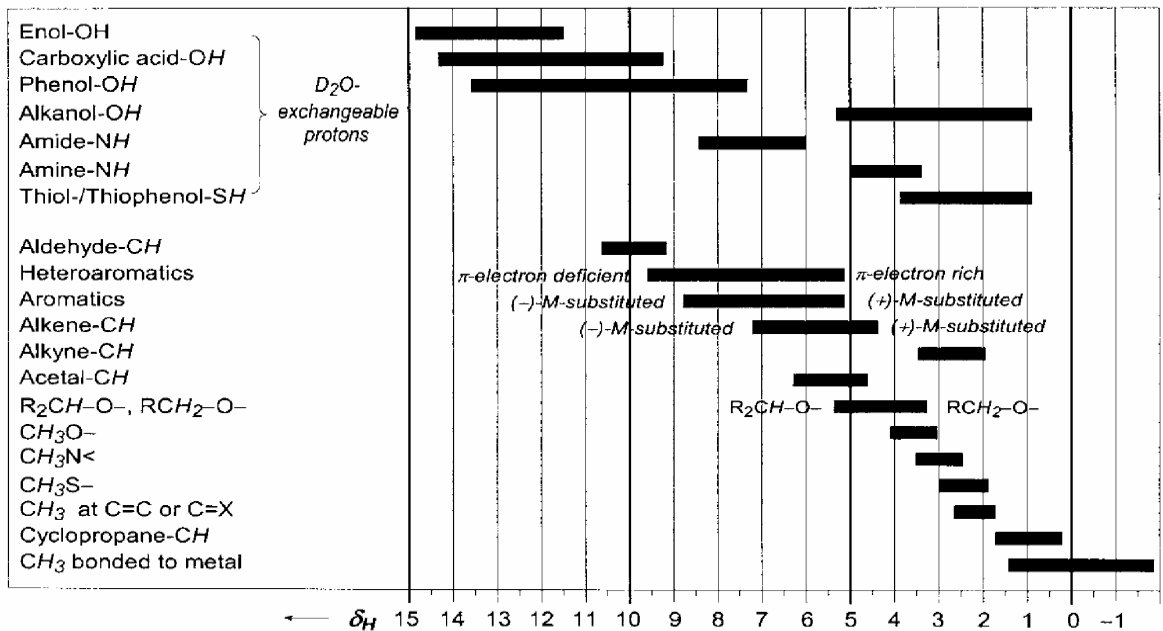


Reconocimiento de fragmentos:
Grupos funcionales:

Table 2.1. ^1H chemical shift ranges for organic compounds



Intercambio con Deuterio: Identificación de protones “activos”



Table 2.3. ^{15}N Chemical shift ranges for organonitrogen compounds

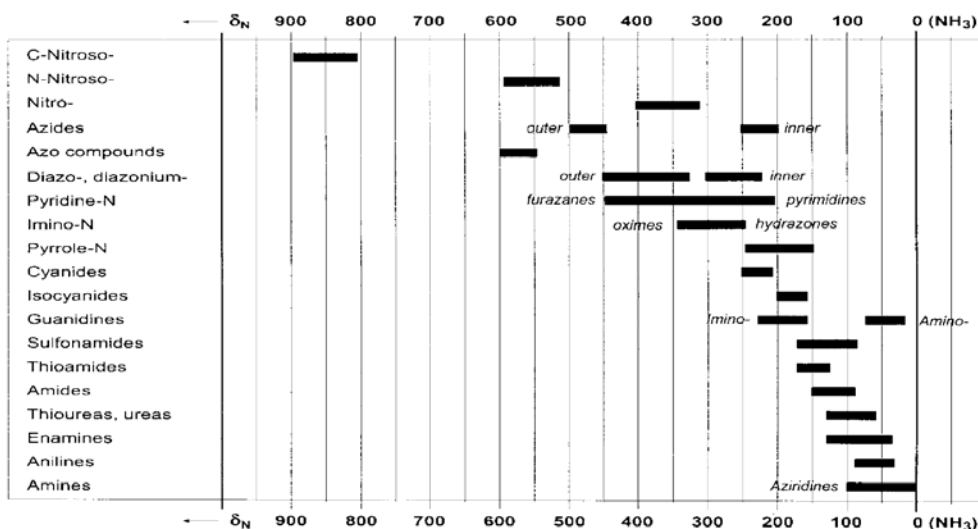
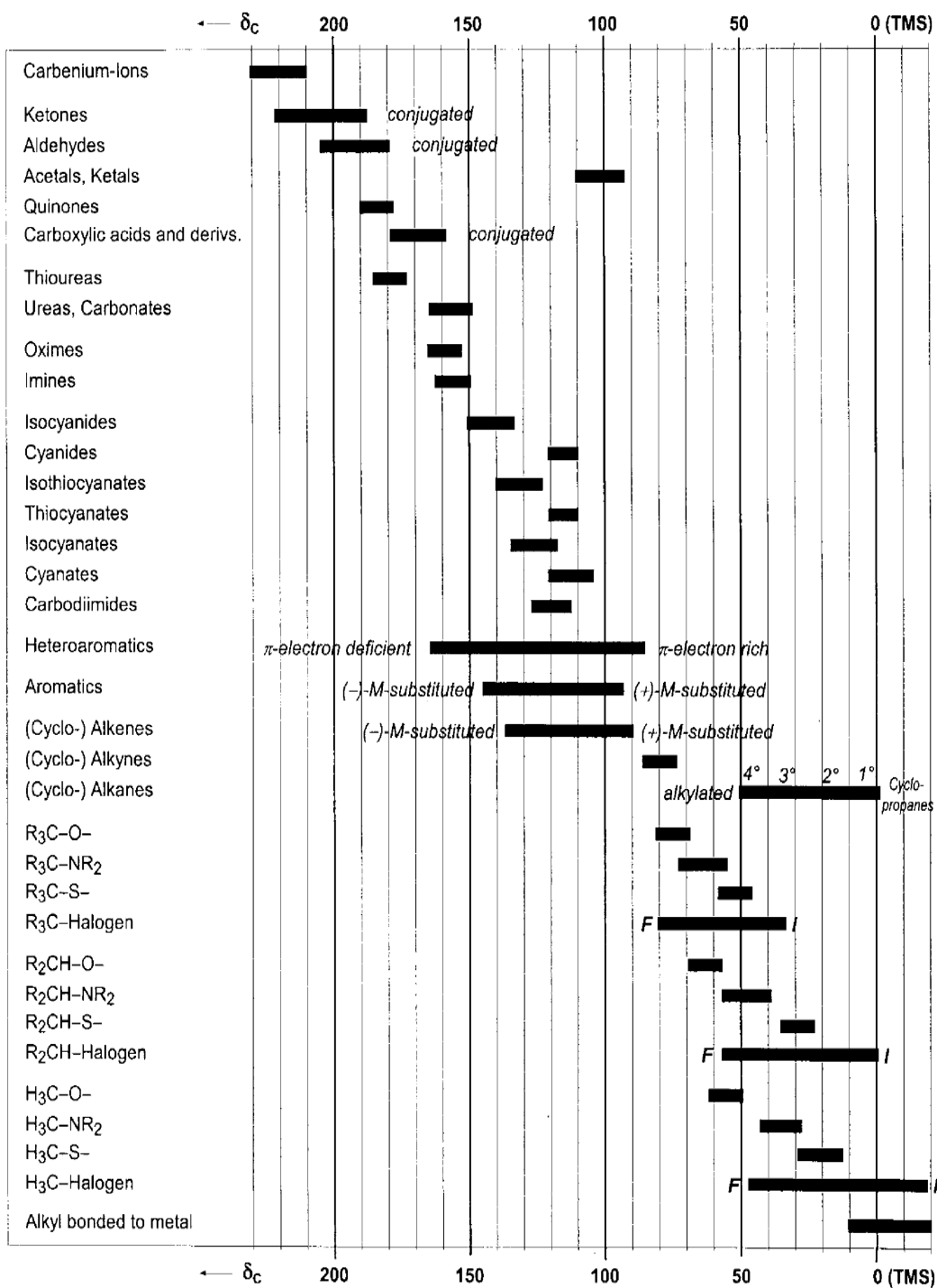


Table 2.2. ^{13}C chemical shift ranges for organic compounds



Acoplamiento escalares HH

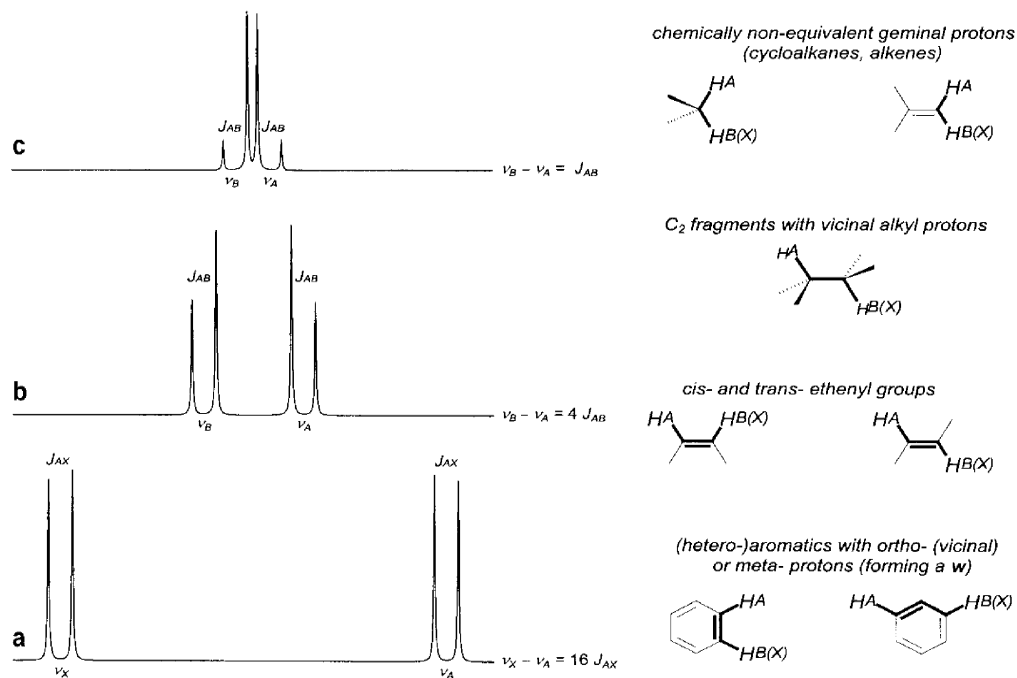


Figure 2.1. AX (AB) systems and typical molecular fragments

Table 2.4. Typical *HH* coupling constants (Hz) of some units in alicycles, alkenes and alkynes^{2,3}

${}^2J_{HH}$ geminal protons		${}^4J_{HH}$ protons with w-relationships		${}^5J_{HH}$
 -12.5	 -6.0	 -2.5		
 -4.5	 5.5	 -2.0		
 2.5	 16.5	 -3.0	 1.0	

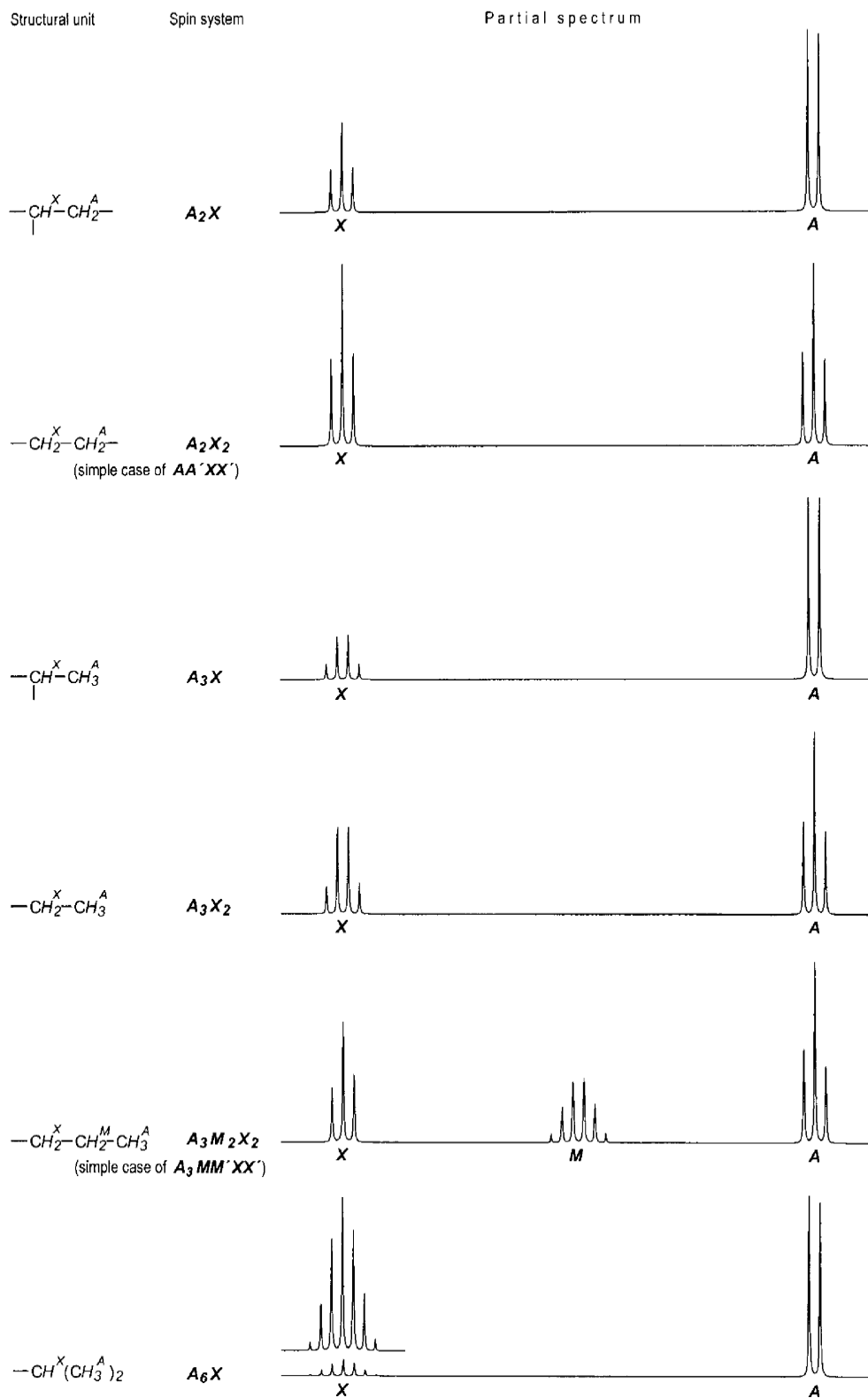


Figure 2.2. Easy to recognise A_mX_n systems and their typical molecular fragments

Table 2.5. Typical HH coupling constants (Hz) of aromatic and heteroaromatic compounds ^{2,3}

${}^3J_{HH}$		${}^4J_{HH}$		${}^5J_{HH}$	
	7.5		1.5		0.7
	8.3		1.3		0.7
	7.0		0.7		0.8
	5.5		1.9		0.4
	7.6		1.6		0.9
	1.8 2.6 4.8		3.4 3.5 3.5		0.9 1.3 1.0
			1.5 2.1 2.8		
				X = O	
				X = NH	
				X = S	

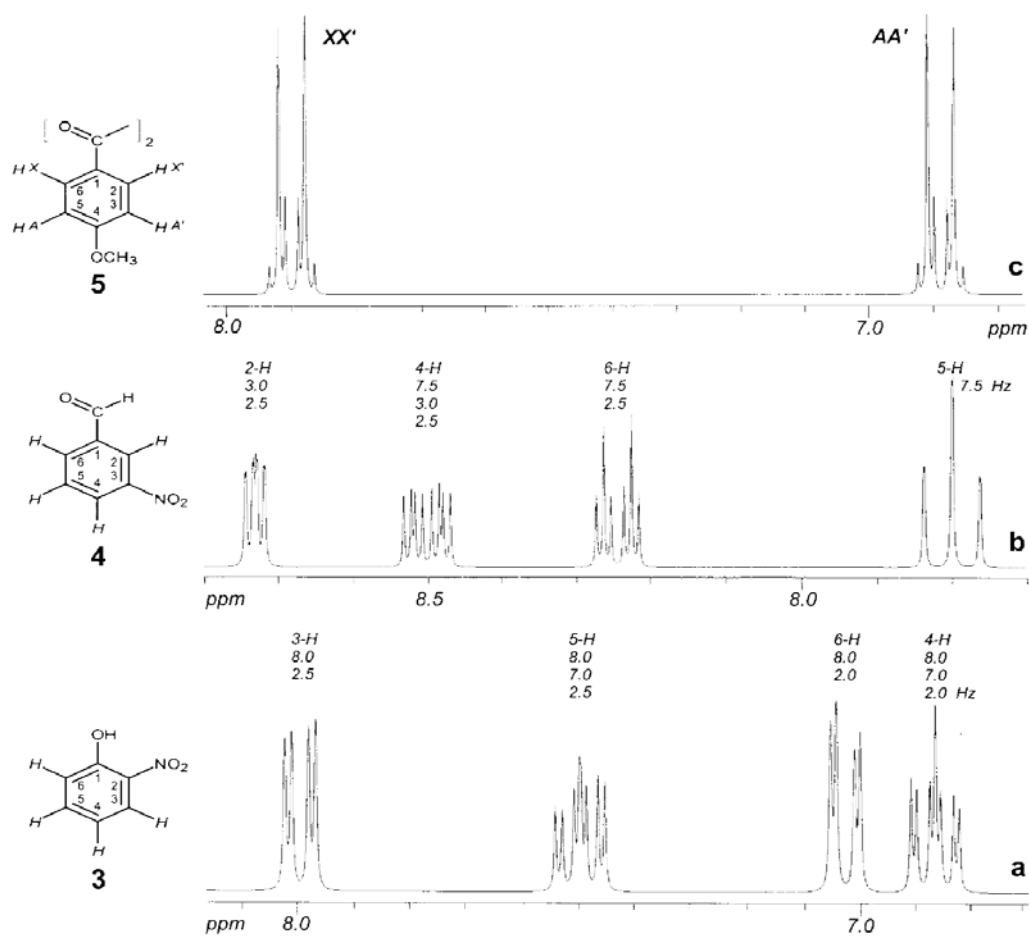


Figure 2.6. ^1H NMR spectra of disubstituted benzene rings [CDCl_3 , 25 $^\circ\text{C}$, 200 MHz]. (a) *o*-Nitrophenol (3); (b) *m*-nitrobenzaldehyde (4); (c) 4,4'-dimethoxybenzil (5)

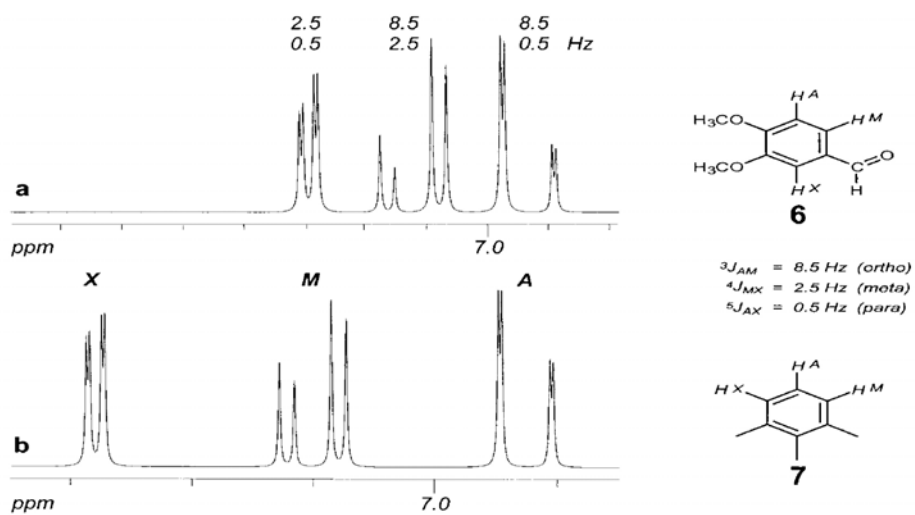


Figure 2.7. ^1H NMR spectrum of 3,4-dimethoxybenzaldehyde (6) [aromatic shift range, CDCl_3 , 25 $^\circ\text{C}$, (a) 100 MHz, (b) 200 MHz]

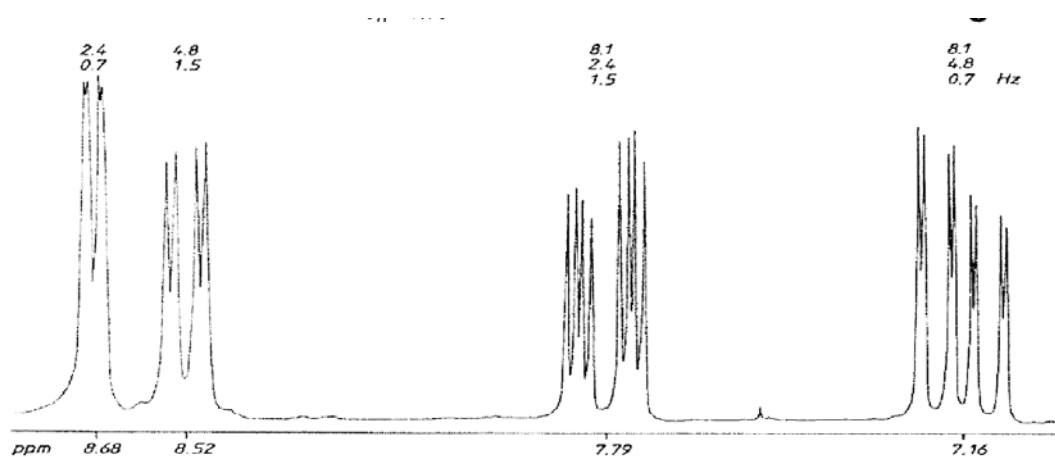
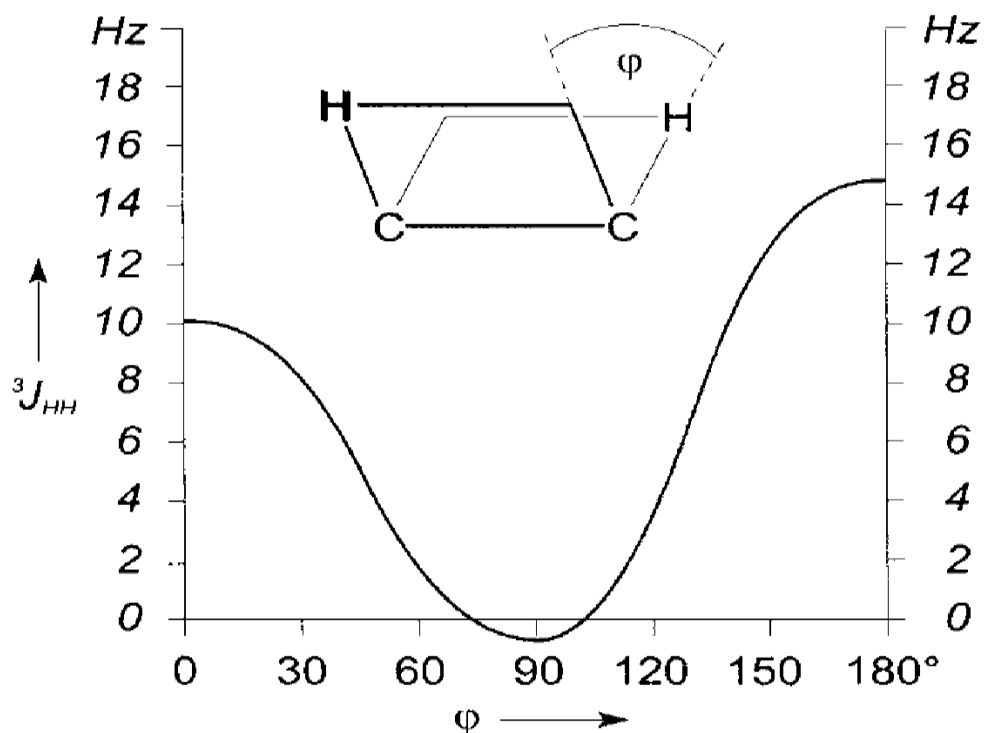


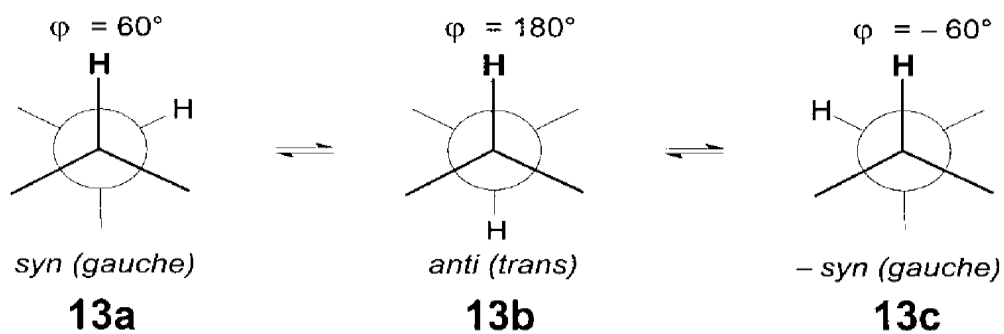
Figure 2.8. ^1H NMR spectrum of 3-bromopyridine (8) [CDCl_3 , 25°C , 90 MHz]

Acoplamiento HH: Relación entre J y ángulo dihedro, conformación y estereoquímica

Ecuación de Karplus-Conroy

$${}^3J_{\text{HH}} = a \cos^2 \varphi - 0.28 \quad (\text{up to } \varphi = 90^\circ: a \approx 10; \text{ above } \varphi = 90^\circ: a \approx 15)$$





$${}^3J_{(\text{average})} = ({}^2J_s + J_a) / 3 = 21/3 = 7 \text{ Hz}$$

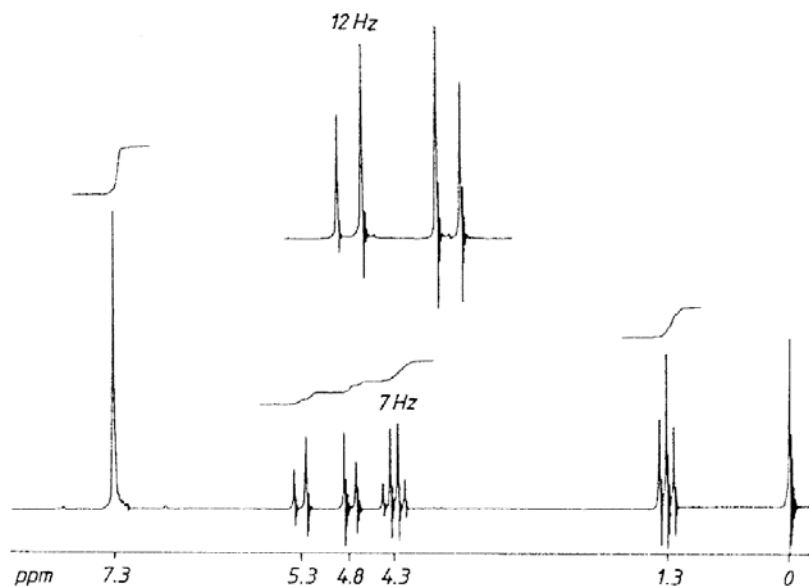
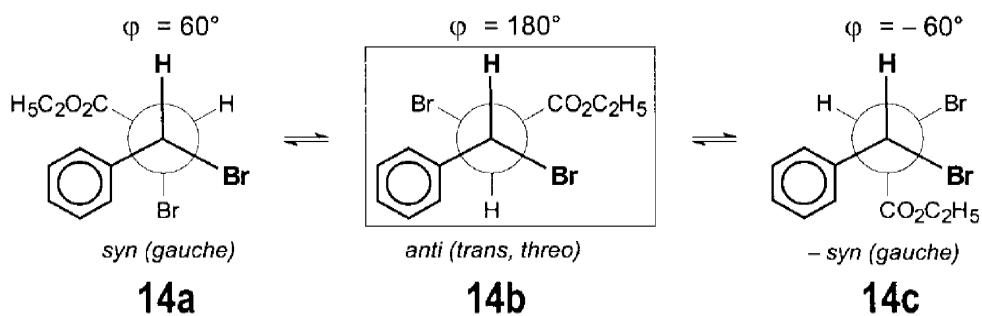


Figure 2.19. ${}^1\text{H}$ NMR spectrum of ethyl dibromodihydrocinnamate (**14**) [CDCl_3 , 25°C , 90 MHz, CW recording]

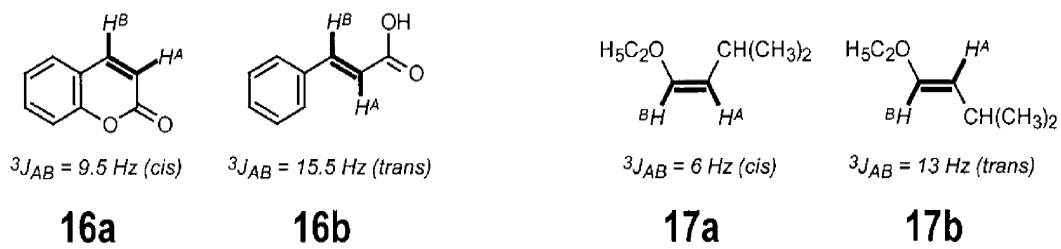


Table 2.10. $^3J_{HH}$ coupling constants (Hz) and relative configuration ^{2,3}. The coupling path is shown in bold

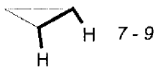
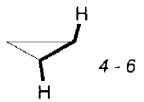
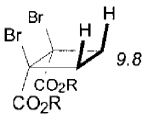
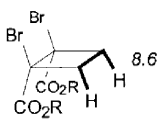
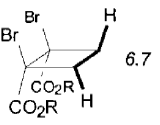
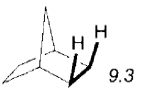
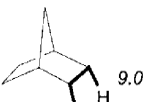
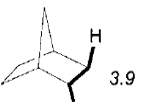
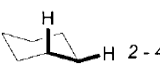
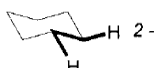
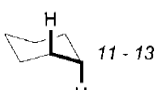
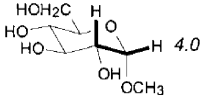
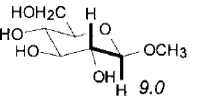
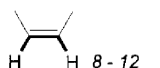
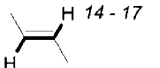
	<i>cis-</i>	<i>trans-</i>
<i>Cyclopropanes</i>	 <p>7 - 9</p>	 <p>4 - 6</p>
<i>Cyclobutanes</i>	 <p>9.8</p>	 <p>8.6</p>
	 <p>6.7</p>	
<i>Norbornanes</i>	 <p>9.3</p> <p><i>exo-exo-</i></p>	 <p>9.0</p> <p><i>endo-endo-</i></p>
		 <p>3.9</p> <p><i>endo-exo-</i></p>
<i>Cyclohexanes</i>	 <p>2 - 4</p> <p><i>axial-equatorial</i></p>	 <p>2 - 4</p> <p><i>diequatorial</i></p>
		 <p>11 - 13</p> <p><i>diaxial</i></p>
<i>Pyranoses</i>	 <p>4.0</p>	 <p>9.0</p>
<i>Alkenes</i>	 <p>8 - 12</p>	 <p>14 - 17</p>

Table 2.11. $^3J_{CH}$ coupling constants (Hz) and relative configuration ¹⁶. The coupling path is shown in bold

<i>Cyclohexane derivatives and pyranoses</i>				
<i>cis-</i>	 H 2.1	 H 4.3	 0 - 2 H	
<i>trans-</i>	 H 8.1	 9.0 H	 H 5 - 6	
<i>Carbon hybridisation</i>			<i>Alkenes</i>	
<i>cis-</i>	 7.5 H	 7.8 H	 11.9 H	 14.7 H
<i>trans-</i>	 12.6 H			
<i>Electronegative substituents</i>				
<i>cis-</i>	 9.1 H	 4.6 H		
<i>trans-</i>	 15.5 H	 8.9 H		
<i>Steric interactions</i>				
<i>cis-</i>	 10.1 H	 9.5 H	 11.0 H	
<i>trans-</i>	 15.9 H	 15.1 H	 11.0 H	