

EKSAMENSOPPGAVE

Fag: IRK31015 Instrumentell analyse 2

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Grupper: 3. klasse kjemi	Dato: 14.12.2015	Tid: 09:00 – 13:00
Antall oppgavesider: 7	Antall vedleggssider: 9	
Hjelpemidler: "Book of data" eller andre formelsamlinger Kalkulator		
KANDIDATEN MÅ SELV KONTROLLERE AT OPPGAVESETTET ER FULLSTENDIG		

Vedlegg 1: Kromatografiparametere	til bruk i oppgave 1 og 3
Vedlegg 2: Typiske fragmenter i MS	til bruk i oppgave 5 og 7
Vedlegg 3: Typiske fragmenter mistet, MS	til bruk i oppgave 5 og 7
Vedlegg 4: Typiske absorpsjoner i IR	til bruk i oppgave 7
Vedlegg 5: Oversikt IR	til bruk i oppgave 7
Vedlegg 6: Oversikt NMR	til bruk i oppgave 6 og 7
Vedlegg 7: 13-regel og Karbon-hydrogenekvivalenter	til bruk i oppgave 7

Oppgave 1

Optimalisering av en analyse fokuserer hovedsakelig på:

- 1) Å øke separasjon ved å påvirke vandringshastighet for komponenter
- 2) Å øke effektivitet som igjen gir smalere bånd

a) Noen aktuelle parametere for optimalisering er K_c , k , α , N og H .

- i) Gi en forklaring på parameterne og angi hvilke som representerer separasjon/ vandringshastighet og hvilke som representerer effektivitet.
- ii) Hvorfor er K_c lite brukt i praksis?
- iii) Hvorfor er H mer informativ enn N ?

b) Van Deemter ligningen som beskriver båndspredning er gitt ved:

$$H = A + \frac{B}{u} + C_S u + C_M u$$

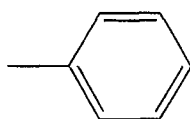
- i) Gi en beskrivelse på prosessene som to av leddene representerer, og hvorfor mobilfasehastigheten påvirker disse som angitt i ligningen. Det er valgfritt hvilke to ledd som beskrives.
- ii) Hvilken informasjon får man fra van Deemter ligningen / van Deemter plot?

Oppgave 2

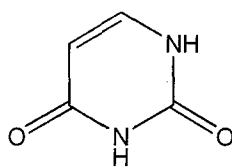
- a) Beskriv prinsipp for adsorpsjonskromatografi og fordelingskromatografi.
- b) Silika er en mye brukt stasjonærfase i adsorpsjonskromatografi.
 - i) Beskriv aktive grupper for silika, og hvilke typer interaksjon mellom silika og komponenter som er viktig for adsorpsjon. Angi og begrunn om sure eller basiske forbindelser blir meste retardert.
 - ii) Hva menes med C18 silika? Hvordan lages den, hva innebærer end-capping og for hvilken type kromatografi er den mye brukt?

Oppgave 3

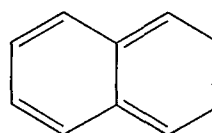
a) Følgende komponenter skal separeres ved omvendt fase HPLC:



Toluene



Uracil



Naphthalene

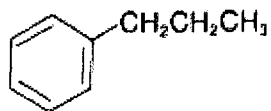
- i) Angi i hvilken rekkefølge komponentene elueres. Rekkefølgen skal begrunnes.
 - ii) Det benyttes en blanding av vann og acetonitrill (AcN) som mobilfase. Angi hvordan og hvorfor retensjonstiden til komponentene påvirkes når andelen acetonitrill i blandingen økes. Vil retensjonstiden påvirkes likt for alle komponentene?
 - iii) Angi en passende detektor for analysen. Valget skal begrunnes.
- b) For å optimalisere analysen i a) tester man ulike mobilfase-hastigheter og ulike blandingsforhold av vann og acetonitrill i mobilfasen.
- i) Ta utgangspunkt i oppløsningsevnen R_S , og forklar på generelt grunnlag hvordan de ulike leddene (k , α og N) påvirkes av enten mobilfasehastighet eller sammensetning.
 - ii) Hvorfor er det bedre å bruke oppløsningsevnen R_S i stedet for selektivitetsfaktoren α for å beskrive separasjon av topper?
 - iii) Hvilken verdi må R_S ha for at to topper skal være baselinjeseperert?

Oppgave 4

- a) Foreslå og begrunn kort en metode for hver av følgende tilfeller:
 - 1) Separere en blanding av vannløselige proteiner med høy molmasse.
 - 2) Erstatte kalsium (Ca^{2+}) i hardt vann med natrium (Na^+).
- b) Beskriv injeksjonsmetodene «splittless» og «cool-on-column» for GC. Beskriv både den fysiske injektoren, og hvordan injeksjonen fungerer. For hvilke typer forbindelser bruker man cool-on-column injeksjon?
- c) EI og CI er to ioniseringsmetoder for MS. Hvordan skjer ioniseringen for de to metodene, og angi en viktig forskjell mellom metodene angående molekyliontoppen.

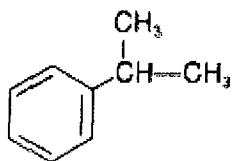
Oppgave 5

MS spekter (A, B og C) til følgende forbindelser er vist nedenfor:



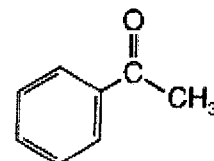
M.W. = 120

Propylbenzen



M.W. = 120

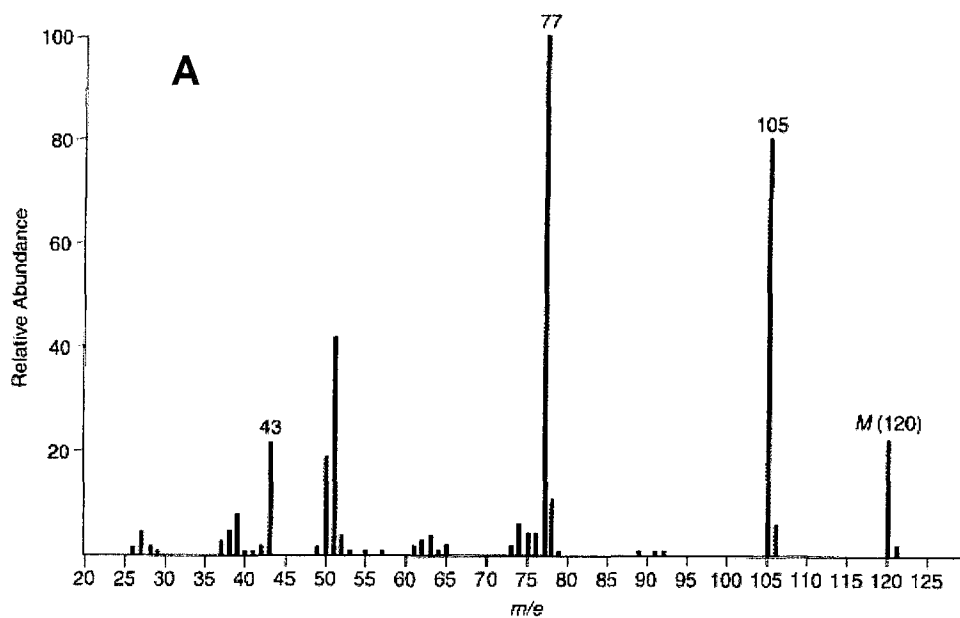
Isopropylbenzen

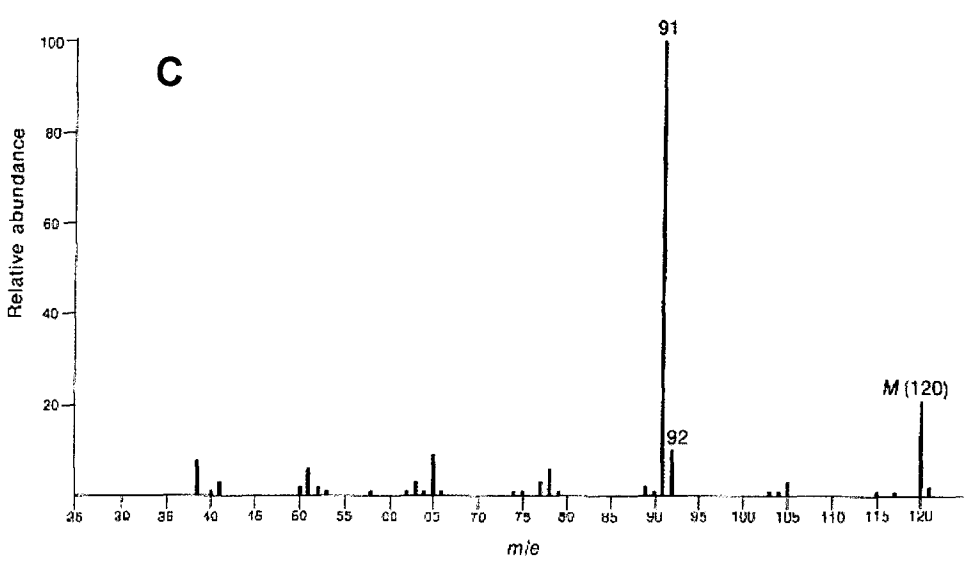
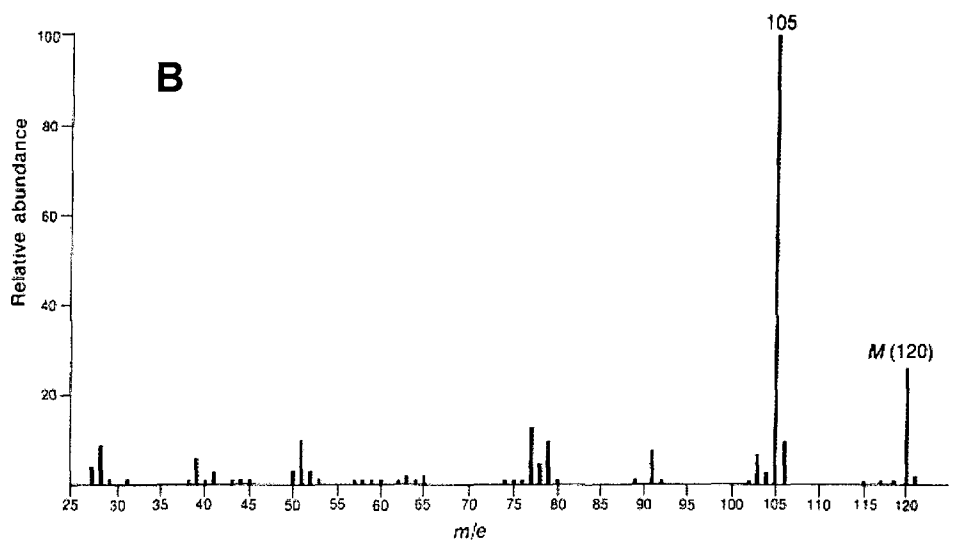


M.W. = 120

Acetofenon

Angi hvilket spekter som tilhører hvilken forbindelse. Begrunn dette ved fragmentering for hver forbindelse og sentrale topper i spektrene. Angi kort «regler» for fragmenteringen som foretas.

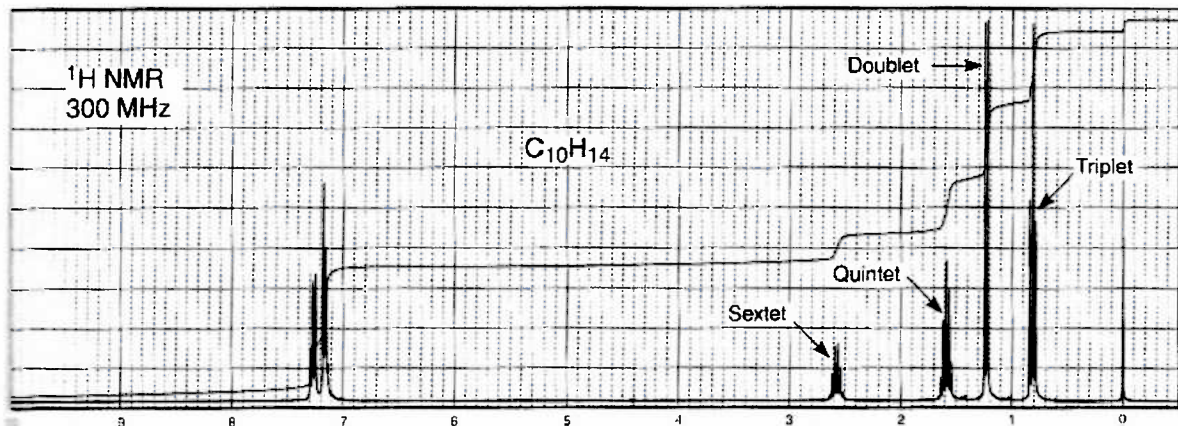




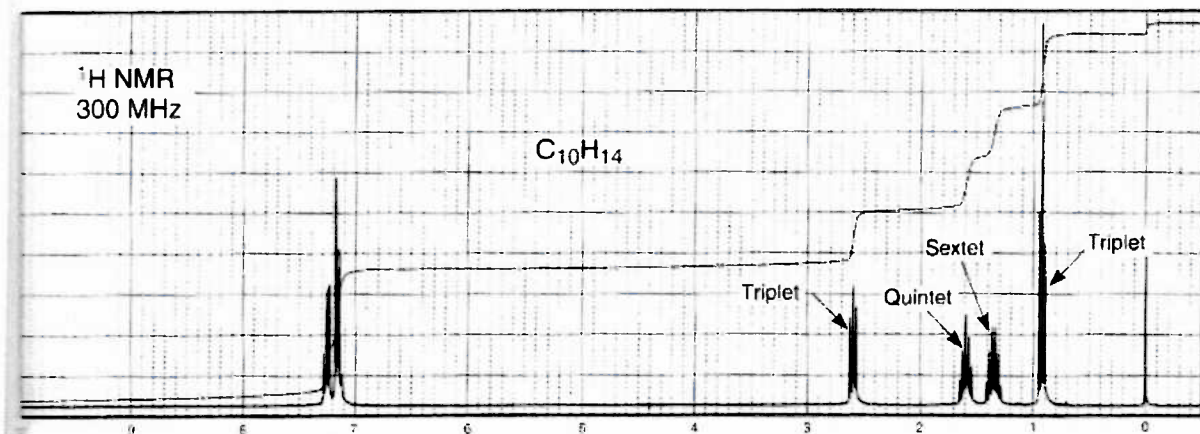
Oppgave 6

Under er det vist 2 NMR-spekter (A og B) som tilhører isomere monosubstituerte aromatiske hydrokarboner med formel $C_{10}H_{14}$. Tegn struktur for A og B, og begrunn valgt struktur med toppene i hvert spekter (hvert topp skal kobles til strukturene). For hver topp, med unntak av toppene over 7ppm og TMS, skal splittingsmønster forklares.

A



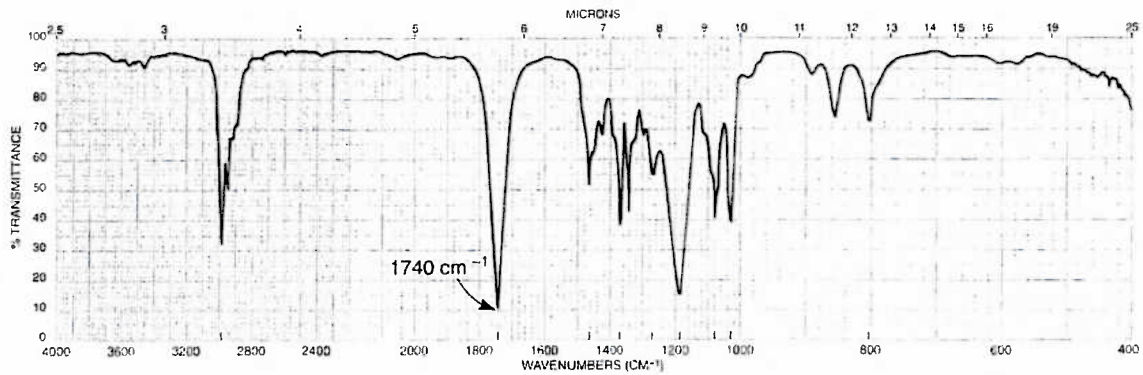
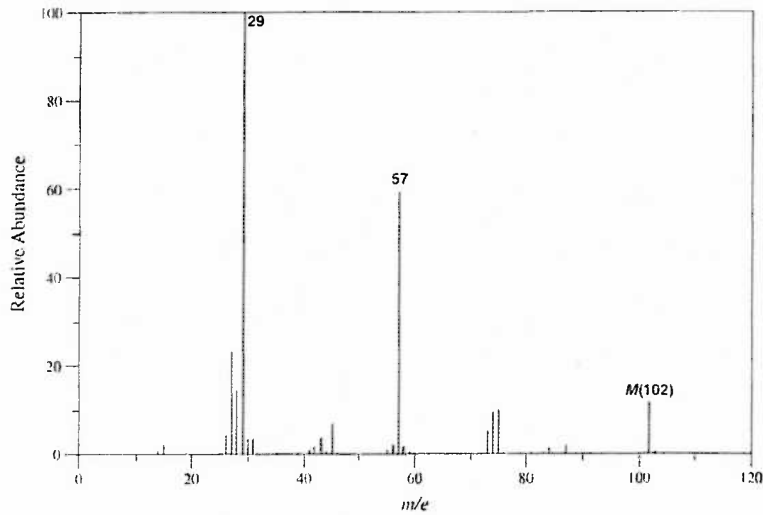
B



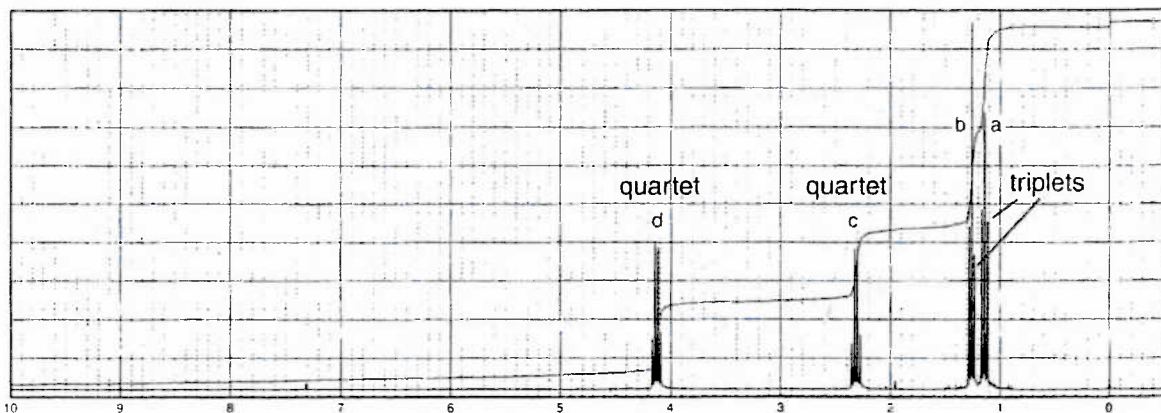
Oppgave 7

En forbindelse har MS-, IR- og NMR-spekter som vist under.

- Finn molekylformel ved bruk av "13-regelen" og beregning av hydrogenindeks/umettethet. Vis beregninger.
- Foreslå struktur basert på spektrene.
- Begrunn struktur ut fra topper i alle spektrene. Angi relevante topper for MS og IR. For NMR skal både splittingsmønster og relativ plassering for alle topper forklares.



^1H



Kromatografi: Viktige parametre og sammenhenger

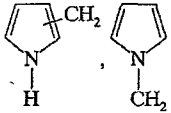
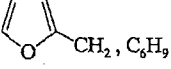

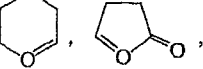

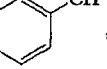

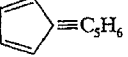
Parameter	Matematisk uttrykk	Forhold til andre størrelser etc.
Lineær mobilfasehastighet	$u = \frac{L}{t_0}$	L er lengde av kolonne
Volum av mobilfase	$V_M = t_0 F$	F er volumetrisk hastighet i ml/sek
Retensjonsfaktor	$k = \frac{t_R - t_0}{t_0}$	$k = \frac{n_s}{n_m}$, $k = K \times \frac{V_s}{V_M}$
Fordelingskonstant	$K = k \times \frac{V_M}{V_s}$	$K = \frac{C_s}{C_M}$
Separasjonsfaktor	$\alpha = \frac{t_2 - t_0}{t_1 - t_0}$	$\alpha = \frac{k_2}{k_1} = \frac{K_2}{K_1}$ også kalt selektivitetsfaktor
Oppløsningsevne	$R_s = \frac{t_2 - t_1}{\frac{1}{2}(t_{w1} + t_{w2})}$	$R_s = \frac{1}{4}(\alpha - 1)\sqrt{N} \left(\frac{\bar{k}}{1 + \bar{k}} \right)$ \bar{k} er snittverdi av k_1 og k_2
Platetallet	$N = 16 \left(\frac{t_R}{t_w} \right)^2$	$N = 5.54 \left(\frac{t_R}{t_{w0.5}} \right)^2$
Platehøyden	$H = \frac{L}{N}$	

APPENDIX B COMMON FRAGMENT IONS

All fragments listed bear +1 charges. To be used in conjunction with Appendix C. Not all members of homologous and isomeric series are given. The list is meant to be suggestive rather than exhaustive.

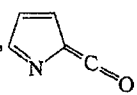
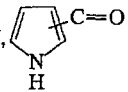
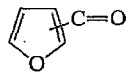
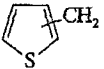
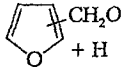
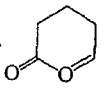
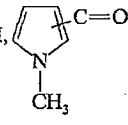
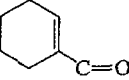
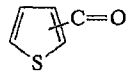
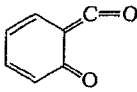
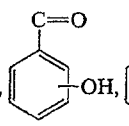
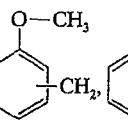
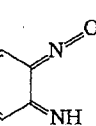
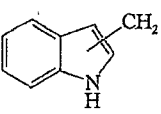
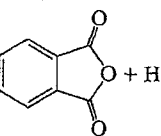
Appendix II of Hamming and Foster (1972). Table A-7 of McLafferty's (1993) interpretative book, and the high-resolution ion data of McLafferty (1982) are recommended as supplements.

m/z Ions^a

14 CH ₂	70 C ₃ H ₁₀
15 CH ₃	71 C ₃ H ₁₁ , C ₃ H ₇ C=O
16 O	72 C ₂ H ₅ C(=O)CH ₂ + H, C ₃ H ₇ CHNH ₂ , (CH ₃) ₂ N=C=O, C ₂ H ₅ NHCHCH ₃ and isomers
17 OH	73 Homologs of 59, (CH ₃) ₃ Si
18 H ₂ O, NH ₄	74 CH ₂ CO ₂ CH ₃ + H
19 F, H ₃ O	75 CO ₂ C ₂ H ₅ + 2H, C ₂ H ₅ CO ₂ + 2H, CH ₂ SC ₂ H ₅ , (CH ₃) ₂ CSH, (CH ₃ O) ₂ CH, (CH ₃) ₂ SiOH
26 C≡N, C ₂ H ₂	76 C ₆ H ₄ (C ₆ H ₄ XY)
27 C ₂ H ₃	77 C ₆ H ₅ (C ₆ H ₅ X)
28 C ₂ H ₄ , CO, N ₂ (air), CH=NH	78 C ₆ H ₅ + H
29 C ₂ H ₅ , CHO	79 C ₆ H ₅ + 2H, ⁷⁹ Br ^b
30 CH ₂ NH ₂ , NO	80 CH ₃ SS + H, H ⁷⁹ Br ^b ,
31 CH ₂ OH, OCH ₃	
32 O ₂ (air)	81  , C ₆ H ₉
33 SH, CH ₂ F	82 (CH ₂) ₄ C≡N, C ₆ H ₁₀ , C ³⁵ Cl ₂ ^b
34 H ₂ S	83 C ₆ H ₁₁ , CH ³⁵ Cl ₂ ^b , 
35 ³⁵ Cl ^b	85  , C ₆ H ₁₃ , C ₄ H ₉ C=O, Cl ³⁵ ClF ₂ ^b
36 H ³⁵ Cl ^b	86 C ₃ H ₇ C(=O)CH ₂ + H, C ₄ H ₉ CHNH ₂ and isomers
39 C ₃ H ₃	87 C ₃ H ₇ CO ₂ , Homologs of 73, CH ₂ CH ₂ CO ₂ CH ₃
40 CH ₂ C=N, Ar (air)	88 CH ₂ CO ₂ C ₂ H ₅ + H
41 C ₃ H ₅ , CH ₃ C=N + H, C ₂ H ₂ NH	89 CO ₂ C ₃ H ₇ + 2H, 
42 C ₃ H ₆ , C ₂ H ₂ O	90  , CH ₃ CHONO ₂
43 C ₃ H ₇ , CH ₃ C=O, C ₂ H ₂ N	91 (C ₆ H ₅)CH ₂ , (C ₆ H ₅)CH + H, (C ₆ H ₅)C + 2H, (CH ₂) ₄ ³⁵ Cl ^b , (C ₆ H ₅)N
44 CH ₂ C(=O)H + H, CH ₃ CHNH ₂ , CO ₂ (air), NH ₂ C=O, (CH ₃) ₂ N	92  -CH ₂ , (C ₆ H ₅)CH ₂ + H
45 CH ₃ CH(OH), CH ₂ CH ₂ OH, CH ₂ OCH ₃ , C(=O)OH	
46 NO ₂	
47 CH ₂ SH, CH ₃ S	
48 CH ₃ S + H	
49 CH ₂ ³⁵ Cl ^b	
51 CH ₂ F ₂ , C ₄ H ₃	
53 C ₄ H ₅	
54 CH ₂ CH ₂ C≡N	
55 C ₄ H ₇ , CH ₂ =CHC=O	
56 C ₄ H ₈	
57 C ₄ H ₉ , C ₂ H ₅ C=O	
58 CH ₃ C(=O)CH ₂ + H, C ₂ H ₅ CHNH ₂ , (CH ₃) ₂ NCH ₂ , C ₂ H ₅ NHCH ₂ , C ₂ H ₅ S	
59 (CH ₃) ₂ COH, CH ₂ OC ₂ H ₅ , CO ₂ CH ₃ , NH ₂ C(=O)CH ₂ + H, CH ₃ OCHCH ₃ , CH ₃ CHCH ₂ OH, C ₂ H ₅ CHOH	
60 CH ₂ CO ₂ H + H, CH ₂ ONO	
61 CH ₃ CO ₂ + 2H, CH ₂ CH ₂ SH, CH ₂ SCH ₃	
65 C ₅ H ₅	
66 H ₂ S ₂ ,  ≡C ₅ H ₆	
67 C ₅ H ₇	
68 CH ₂ CH ₂ CH ₂ C≡N	
69 C ₅ H ₉ , CF ₃ , CH ₃ CH=CHC=O, CH ₂ =C(CH ₃)C=O	

APPENDIX B (Continued)

m/z Ions^a

- 93 $\text{CH}_2^{79}\text{Br}^b$, C_7H_9 , $(\text{C}_6\text{H}_5)\text{O}$, 
- 94 $(\text{C}_6\text{H}_5)\text{O} + \text{H}$, 
- 95 
- 96 $(\text{CH}_2)_5\text{C}\equiv\text{N}$
- 97 C_7H_{13} , 
- 98  + H
- 99 C_7H_{15} , $\text{C}_6\text{H}_{11}\text{O}$, 
- 100 $\text{C}_4\text{H}_9\text{C}(=\text{O})\text{CH}_2 + \text{H}$, $\text{C}_5\text{H}_{11}\text{CHNH}_2$
- 101 $\text{CO}_2\text{C}_4\text{H}_9$
- 102 $\text{CH}_2\text{CO}_2\text{C}_2\text{H}_7 + \text{H}$
- 103 $\text{CO}_2\text{C}_4\text{H}_9 + 2\text{H}$, $\text{C}_5\text{H}_{11}\text{S}$, $\text{CH}(\text{OCH}_2\text{CH}_3)_2$
- 104 $\text{C}_2\text{H}_5\text{CHONO}_2$
- 105 $\text{C}_6\text{H}_5\text{C}=\text{O}$, $\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2$, $\text{C}_6\text{H}_5\text{CHCH}_3$
- 106 $\text{C}_6\text{H}_5\text{NHCH}_2$
- 107 $\text{C}_6\text{H}_5\text{CH}_2\text{O}$, $\text{HO}(\text{C}_6\text{H}_4)\text{CH}_2$, $\text{C}_2\text{H}_4^{79}\text{Br}^b$
- 108 $\text{C}_6\text{H}_5\text{CH}_2\text{O} + \text{H}$, 
- 109 
- 111 
- 119 CF_3CF_2 , $(\text{C}_6\text{H}_5)\text{C}(\text{CH}_3)_2$, $\text{CH}_3\text{CH}(\text{C}_6\text{H}_4)\text{CH}_3$, $\text{CO}(\text{C}_6\text{H}_4)\text{CH}_3$
- 120 
- 121 C_9H_{13} , , , 
- 122 $\text{C}_6\text{H}_5\text{CO}_2 + \text{H}$
- 123 $\text{F}(\text{C}_6\text{H}_4)\text{C}=\text{O}$, $\text{C}_6\text{H}_5\text{CO}_2 + 2\text{H}$
- 125 $\text{C}_6\text{H}_5\text{SO}$
- 127 I
- 128 HI
- 130 
- 131 C_3F_5 , $\text{C}_6\text{H}_5\text{CH}=\text{CHC}=\text{O}$
- 135 $(\text{CH}_2)_4^{79}\text{B}^b$
- 138 $\text{CO}_2(\text{C}_6\text{H}_4)\text{OH} + \text{H}$
- 139 $^{35}\text{Cl}(\text{C}_6\text{H}_4)\text{C}=\text{O}^b$
- 141 CH_2I
- 147 $(\text{CH}_3)_2\text{Si}=\text{O}-\text{Si}(\text{CH}_3)_3$
- 149  + H
- 154 $(\text{C}_6\text{H}_5)_2$

^a Ions indicated as a fragment + nH (n = 1, 2, 3, ...) are ions that arise via rearrangement involving hydrogen transfer.

^b Only the more abundant isotope is indicated.



APPENDIX C COMMON FRAGMENTS LOST

This list is suggestive rather than comprehensive. It should be used in conjunction with Appendix B. Table 5-19 of Hamming and Foster (1972) and Table A-5 of McLafferty (1993) are

recommended as supplements. All of these fragments are lost as neutral species.

Molecular Ion Minus	Fragment Lost (Inference Structure)
1	H·
2	2H·
15	CH ₃ ·
16	O (ArNO ₂ , amine oxides, sulfoxides); ·NH ₂ (carboxamides, sulfonamides)
17	HO·
18	H ₂ O (alcohols, aldehydes, ketones)
19	F·
20	HF
26	CH≡CH·, ·CH≡N
27	CH ₂ =CH·, HC≡N (aromatic nitrites, nitrogen heterocycles)
28	CH ₂ =CH ₂ , CO, (quinones) (HCN + H)
29	CH ₃ CH ₂ ·, (ethyl ketones, ArCH ₂ CH ₂ CH ₃), ·CHO
30	NH ₂ CH ₂ ·, CH ₂ O (ArOCH ₃), NO (ArNO ₂), C ₂ H ₆
31	·OCH ₃ (methyl esters), ·CH ₂ OH, CH ₃ NH ₂
32	CH ₃ OH, S
33	HS· (thiols), (·CH ₃ and H ₂ O)
34	H ₂ S (thiols)
35	Cl·
36	HCl, 2H ₂ O
37	H ₂ Cl (or HCl + H)
38	C ₃ H ₂ , C ₂ N, F ₂
39	C ₃ H ₃ , HC ₂ N
40	CH ₃ C≡CH
41	CH ₂ =CHCH ₂ ·
42	CH ₂ =CHCH ₃ , CH ₂ =C=O, H ₂ C ^{H₂} CH ₂ , NCO, NCNH ₂
43	C ₃ H ₇ · (propyl ketones, ArCH ₂ -C ₃ H ₇), CH ₃ C· (methyl ketones, CH ₃ C ^O G, where G = various functional groups), CH ₂ =CH-O·, (CH ₃ · and CH ₂ =CH ₂), HCNO
44	CH ₂ =CHOH, CO ₂ (esters, anhydrides), N ₂ O, CONH ₂ , NHCH ₂ CH ₃
45	CH ₃ CHOH, CH ₃ CH ₂ O· (ethyl esters), CO ₂ H, CH ₃ CH ₂ NH ₂
46	(H ₂ O and CH ₂ =CH ₂), CH ₃ CH ₂ OH, ·NO ₂ (ArNO ₂)
47	CH ₃ S·
48	CH ₃ SH, SO (sulfoxides), O ₃
49	·CH ₂ Cl
51	·CHF ₂
52	C ₄ H ₄ , C ₂ N ₂
53	C ₄ H ₅
54	CH ₂ =CH-CH=CH ₂
55	CH ₂ =CHCHCH ₃

APPENDIX C (Continued)

Molecular Ion Minus	Fragment Lost (Inference Structure)
56	$\text{CH}_2=\text{CHCH}_2\text{CH}_3$, $\text{CH}_3\text{CH}=\text{CHCH}_3$, 2CO
57	$\text{C}_4\text{H}_9\cdot$ (butyl ketones), $\text{C}_2\text{H}_5\text{CO}$ (ethyl ketones, $\text{EtC}=\text{OG}$, G = various structural units)
58	$\cdot\text{NCS}$, ($\text{NO} + \text{CO}$), CH_3COCH_3 , C_4H_{10}
59	$\text{CH}_3\text{OC}\cdot$, CH_3CNH_2 , 
60	$\text{C}_3\text{H}_7\text{OH}$, $\text{CH}_2=\text{C}(\text{OH})_2$ (acetate esters) ^a
61	$\text{CH}_3\text{CH}_2\text{S}\cdot$, 
62	(H_2S and $\text{CH}_2=\text{CH}_2$)
63	$\cdot\text{CH}_2\text{CH}_2\text{Cl}$
64	C_5H_4 , S_2 , SO_2
68	$\text{CH}_2=\overset{\text{CH}_3}{\text{C}}-\text{CH}=\text{CH}_2$
69	$\text{CF}_3\cdot$, $\text{C}_5\text{H}_9\cdot$
71	$\text{C}_5\text{H}_{11}\cdot$
73	$\text{CH}_3\text{CH}_2\text{OC}\cdot$
74	$\text{C}_4\text{H}_9\text{OH}$
75	C_6H_3
76	C_6H_4 , CS_2
77	C_6H_5 , CS_2H
78	C_6H_6 , CS_2H_2 , $\text{C}_5\text{H}_4\text{N}$
79	$\text{Br}\cdot$, $\text{C}_5\text{H}_5\text{N}$
80	HBr
85	$\cdot\text{CClF}_2$
100	$\text{CF}_2=\text{CF}_2$
119	$\text{CF}_3-\text{CF}_2\cdot$
122	$\text{C}_6\text{H}_5\text{COOH}$
127	$\text{I}\cdot$
128	HI

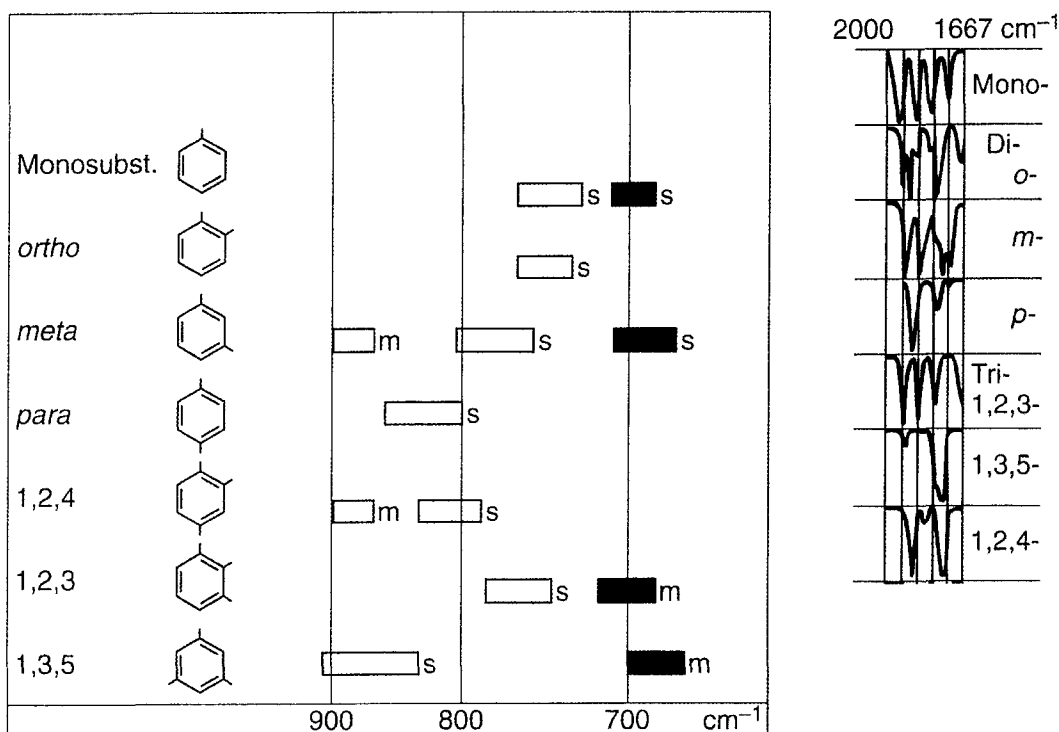
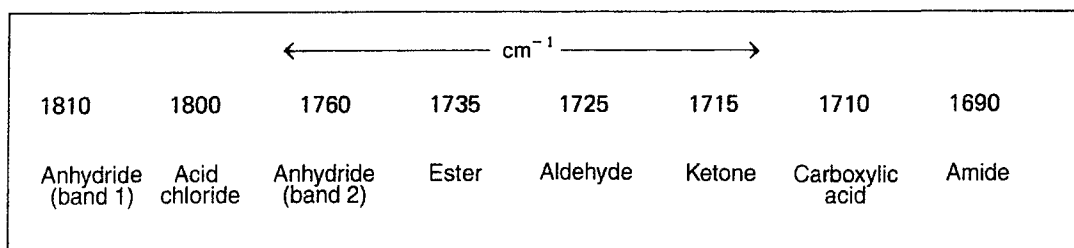
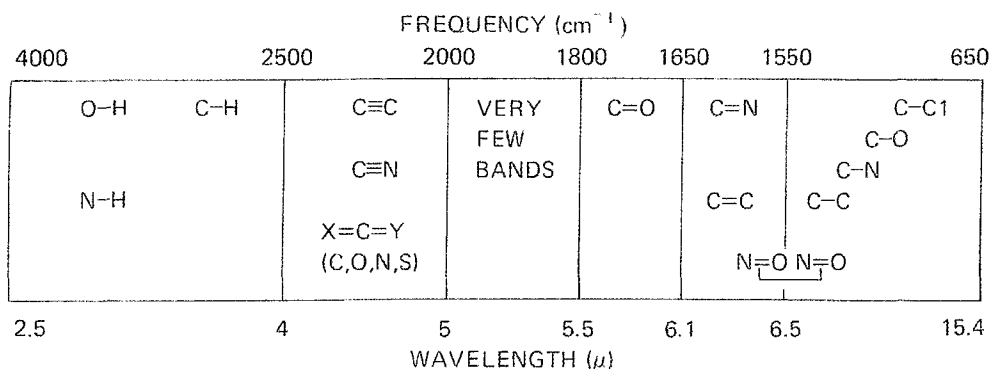
^a McLafferty rearrangement.

TABLE 2-3 A Simplified Correlation Chart

Type of Vibration		Frequency (cm ⁻¹)	Wavelength (μ)	Intensity	
C-H	Alkanes (stretch)	3000-2850	3.33-3.51	s	
	-CH ₃ (bend)	1450 and 1375	6.90 and 7.27	m	
	-CH ₂ - (bend)	1465	6.83	m	
	Alkenes	(stretch)	3100-3000	3.23-3.33	m
		(out-of-plane bend)	1000-650	10.0-15.3	s
	Aromatics	(stretch)	3150-3050	3.17-3.28	s
		(out-of-plane bend)	900-690	11.1-14.5	s
	Alkyne (stretch)	ca. 3300	ca. 3.03	s	
	Aldehyde		2900-2800	3.45-3.57	w
			2800-2700	3.57-3.70	w
C-C	Alkane	not interpretatively useful			
C=C	Alkene	1680-1600	5.95-6.25	m-w	
	Aromatic	1600 and 1475	6.25 and 6.78	m-w	
C≡C	Alkyne	2250-2100	4.44-4.76	m-w	
C=O	Aldehyde	1740-1720	5.75-5.81	s	
	Ketone	1725-1705	5.80-5.87	s	
	Carboxylic Acid	1725-1700	5.80-5.88	s	
	Ester	1750-1730	5.71-5.78	s	
	Amide	1670-1640	6.00-6.10	s	
	Anhydride	1810 and 1760	5.52 and 5.68	s	
	Acid Chloride	1800	5.56	s	
C-O	Alcohols, Ethers, Esters, Carboxylic Acids, Anhydrides	1300-1000	7.69-10.0	s	
O-H	Alcohols, Phenols				
	Free	3650-3600	2.74-2.78	m	
	H-Bonded	3500-3200	2.86-3.13	m	
	Carboxylic Acids	3400-2400	2.94-4.17	m	
N-H	Primary and Secondary Amines and Amides (stretch)	3500-3100	2.86-3.23	m	
	(bend)	1640-1550	6.10-6.45	m-s	
C-N	Amines	1350-1000	7.4-10.0	m-s	
C=N	Imines and Oximes	1690-1640	5.92-6.10	w-s	
C≡N	Nitriles	2260-2240	4.42-4.46	m	
X=C=Y	Allenes, Ketenes, Isoocyanates, Isothiocyanates	2270-1950	4.40-5.13	m-s	
N=O	Nitro (R-NO ₂)	1550 and 1350	6.45 and 7.40	s	
S-H	Mercaptans	2550	3.92	w	
S=O	Sulfoxides	1050	9.52	s	
	Sulfones, Sulfonyl Chlorides, Sulfates, Sulfonamides	1375-1300 and	7.27-7.69 and	s	
		1200-1140	8.33-8.77	s	
C-X	Fluoride	1400-1000	7.14-10.0	s	
	Chloride	800-600	12.5-16.7	s	
	Bromide, Iodide	<667	>15.0	s	

TABLE 2-4 Base Values for Absorptions of Bonds

OH	3600 cm ⁻¹	2.8 μ	C≡C	2150 cm ⁻¹	4.6 μ
NH	3500	2.9	C=O	1715	5.8
CH	3000	3.3	C=C	1650	6.1
C≡N	2250	4.4	C-O	1100	9.1



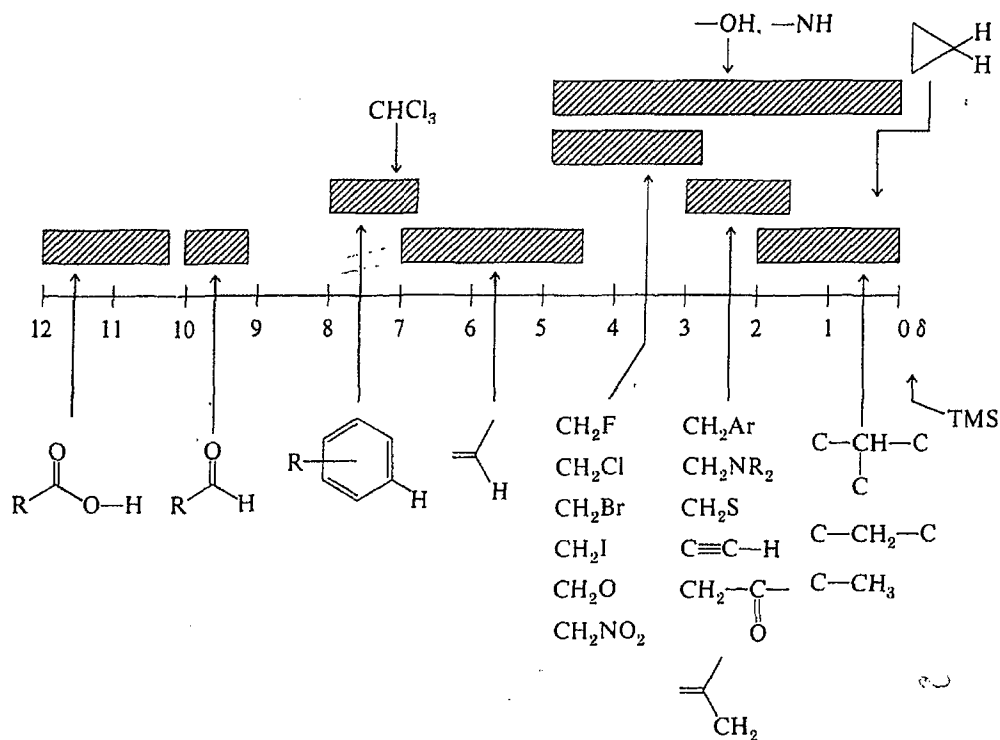
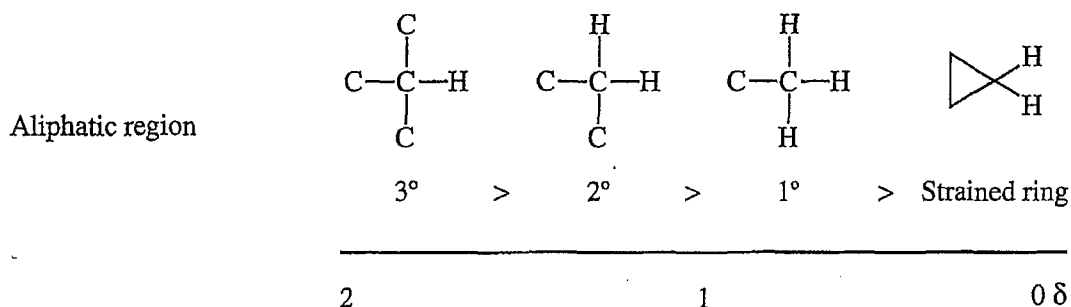


FIGURE 3.20 A simplified correlation chart for proton chemical shift values.

Fordeling i alifatisk region (CH, CH₂, CH₃)



13-Regel og Tabell karbon-hydrogenekvivalenter

Vedlegg 7

13-regel: $\frac{M}{13} = n + \frac{r}{13}$ og $U = \frac{(n-r+2)}{2}$

Tabell over karbon-hydrogenekvivalenter for en del atomer

Adder	Trekk fra	Adder ΔU
C	H ₁₂	7
H ₁₂	C	-7
O	CH ₄	1
O ₂	C ₂ H ₈	2
O ₃	C ₃ H ₁₂	3
N	CH ₂	½
N ₂	C ₂ H ₄	1
S	C ₂ H ₈	2
³⁵ Cl	C ₂ H ₁₁	3
⁷⁹ Br	C ₆ H ₇	-3
⁷⁹ Br	C ₅ H ₁₉	4
F	CH ₇	2
Si	C ₂ H ₄	1
P	C ₂ H ₇	2
I	C ₉ H ₁₉	0
I	C ₁₀ H ₇	7