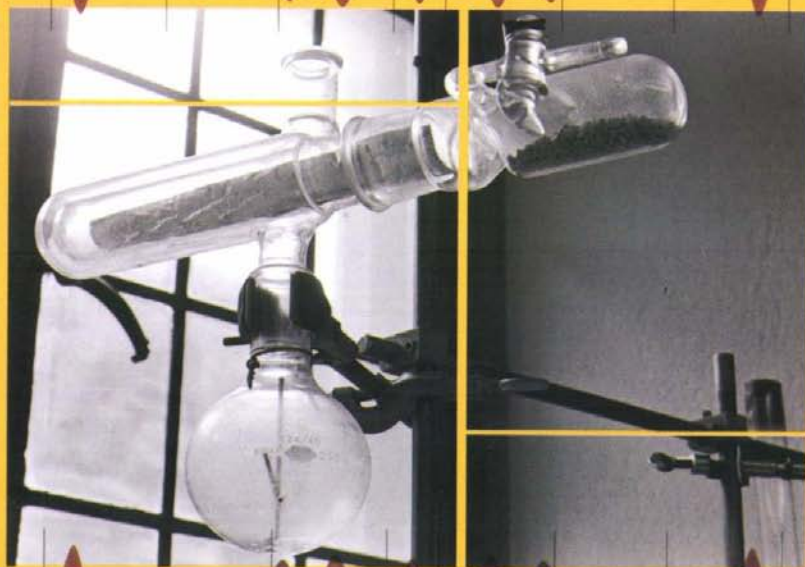


A Handbook of Spectroscopic Data

Chemistry

(UV, IR, PMR, ^{13}C NMR and
Mass Spectroscopy)

B.D.Mistry



*A Handbook of
Spectroscopic Data*
CHEMISTRY
(UV, IR, PMR, ¹³CNMR and Mass Spectroscopy)

B.D. Mistry
*B.K.M. Science College,
Valsad - (Gujarat)*

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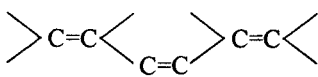
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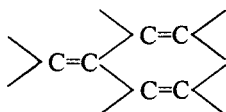
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
Ultraviolet Spectroscopy

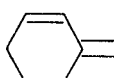
1.1 Calculating Absorption Maxima of Unsaturated Compounds

Dienes and trienes : If the compound is suspected to be a conjugated or substituted diene, its wavelength of maximum absorption can be predicted with the help of Table 1. 1. To be able to use this table, one must first learn to recognize different types of dienes, conjugations, double bonds, etc. These are as follows:

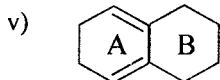
i)  A linear conjugation; for example, 1,3,5 hexatriene, isoprene, etc.

ii)  A cross conjugation.

iii)  A cyclic diene; for example, cyclohexadiene, cyclohepta 1,3- diene, etc.

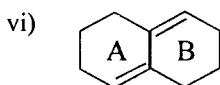
iv)  A semicyclic diene; one of the double bonds forms part of a ring and the other is exocyclic, or outside the ring. When only one of the two sp² hybridized carbons of a double bond is a part of the ring under

consideration, such a double bond is called an exocyclic double bond.



A homoannular diene is one in which the two double bonds are conjugated and are in a single ring.

Note that both double bonds are exocyclic to ring B.



A heteroannular diene is a conjugated system in which the two double bonds belong to two different rings. However, these double bonds are also exocyclic, one of them being exo-to ring A and the other exo-to ring B.

Table 1.1: Woodward's and Fieser's rules for Diene absorption (ethanol solution)

i)	Base value for an unsubstituted, conjugated, acyclic or heteroannular diene	214 nm
ii)	Base value for an unsubstituted, conjugated homoannular diene	253 nm
	Increments for	
iii)	Extra double bonds in conjugation (for each C=C)	+ 30 nm
iv)	Exocyclic double bond (effect is two fold if bond is exocyclic to two rings)	+5nm
v)	Substituents on sp ² hybridised carbon atom, per substituent	
	a) O-acyl (-O-CO-R or -O-CO-Ar)	0 nm
	b) Simple alkyl (-R) or ring residue	+5nm
	c) Halogen (-Cl, -Br)	+5nm
	d) O-alkyl (-OR)	+6nm
	e) S-alkyl (-SR)	+ 30 nm
	f) N-alkyl, (-NRR')	+ 60 nm
vi)	Solvent correction	0 nm

The following points are to be noted:

- ♦ The cyclic homoannular base values refer to a six membered ring only. For other rings the values are:

Five membered ring (C ₅)	228 nm
Seven membered ring (C ₇)	241 nm
- ♦ Accuracy of prediction is ± 5 nm
- ♦ If there is more than one possibility for calculating λ_{\max} , the highest λ_{\max} value usually agrees with the observed value.

Limitations

- ♦ Agreement is quite good for acyclic and six-membered ring polyenes but not so for other rings in some cases.
- ♦ Steric strain can also affect the position (λ_{\max}) of the band, sometimes very greatly if the strain is high. A simple example of this is 1,2 dimethylene cyclohexane, which gives a strong UV band at λ_{\max} 220 nm (ϵ 10,050) which is quite different from the calculated value.

Polyenes : The above rules (Table 1.1) holds fairly well for unsaturated compounds containing up to four conjugated double bonds. However, for systems of extended conjugation, such as those found in carotenoid pigments, Fieser and Kuhn have suggested equations to calculate the basic λ_{\max} and ϵ_{\max} of UV absorption.

$$\lambda_{\max} \text{ (in hexane)} = 114 + 5M + n(48.0 - 1.7n) - 16.5R_{\text{endo}} - 10R_{\text{exo}}$$

$$\epsilon_{\max} \text{ (in hexane)} = 1.74 \times 10^4 n$$

Where

n = number of conjugated double bonds

M = number of alkyl or alkyl like substituents on the conjugated system.

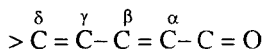
R_{endo} = number of rings with endocyclic double bonds in the conjugated system.

R_{exo} = number of rings with exocyclic double bonds.

1.2 Calculating Absorption Maxima of Carbonyl Compounds

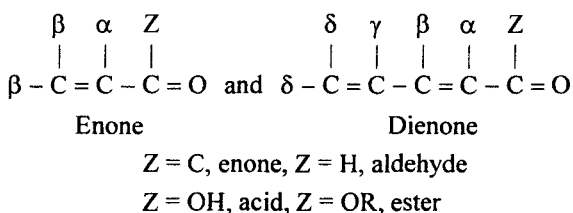
The basic chromophore containing a $>C=C<$ (–ene) conjugated with a $>C=O$ (–one), as in

$> \overset{\beta}{\text{C}} = \overset{\alpha}{\text{C}} - \text{C} = \text{O}$ is called an enone. If a carbonyl group is conjugated with two double bonds (–diene), such as



The compound is known as a dienone. In the case of cyclic compounds, the ethylenic double bonds conjugated with the carbonyl may be homoannular or heteroannular.

Table 1.2: Rules of Enone and Dienone absorption



Parent enone (acyclic or rings larger than 5 members)		215nm
5-membered cyclic enone		205nm
Aldehydes		210nm
Acid and Esters		195nm
Increments for Double bond extending conjugation (for each one)		+ 30nm
Homodiene component		+ 39nm
Exocyclic double bond (or any $>\text{C}=\text{C}<$ endocyclic to 5- or 7-member ring in a case of acid and ester)		+ 5nm
Alkyl group, ring residue	α	+ 10nm
	β	+ 12nm
	γ	
	and higher	+ 18nm
Hydroxyl (–OH)	α	+ 35nm
	β	+ 30nm
	γ	50nm
Alkoxy (–OCH ₃)	α	+ 35nm
	β	+ 30nm
	γ	+ 17nm
	δ	31nm

Acetoxy ($-\text{O}-\text{COCH}_3$)	α, β or δ	+ 6nm
Dialkyl amino ($-\text{NR}_2$)	β	+ 95nm
Chlorine ($-\text{Cl}$)	α	+ 15nm
	β	+ 12nm
Thioalkyl ($-\text{SR}$)	β	+ 85nm
Bromine ($-\text{Br}$)	α	+ 25nm
	β	+ 30nm
Solvent correction (see table below)		variable

Solvent Corrections (Enones)

Solvent	Correction
Ethanol	0
Methanol	0
Water	-8 nm
Chloroform	+ 1 nm
Dioxane	+ 5 nm
Ether	+ 7 nm
Hexane	+ 11 nm
Cyclohexane	+ 11 nm

Accuracy of prediction ± 5 nm.

1.3 Calculating Absorption Maxima of Aromatic Molecules

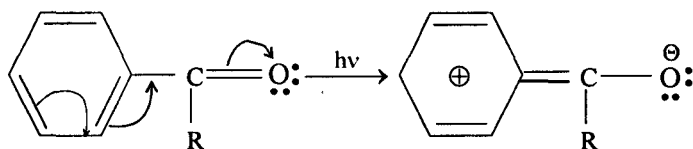
There are two types of aromatic molecules: benzenoid and nonbenzenoid. Their spectra show considerable resemblance. In fact, the presence or absence of certain features in UV spectra, such as a low intensity band (known as a fine structure band) at or about 255 nm, is often used to detect the aromatic character of an unknown substance.

Benzene Chromophore

The simplest aromatic compound is benzene. It has a ring current of π electrons, which shows strong $\pi \rightarrow \pi^*$ absorptions at 184 nm (ϵ_{max} 60,000), and at 204 nm (ϵ_{max} 7900). (This is called a primary band.) Benzene exhibits a low intensity band at 256 nm (ϵ_{max} 200) (Known as a secondary or fine-structure band), with a series of fine-structure bands between 230 and 270 nm). Any substitution on the benzene ring, irrespective of its electronic character

(electron-donating or electron-withdrawing character) shift the primary band (204 nm) to longer wave lengths. With polar substituents, e.g. $-\text{NR}_2$, $-\text{OH}$, etc. which allow for the $n \rightarrow \pi$ conjugation and $-\text{C}=\text{O}$ and $-\text{NO}_2$ where polarisability is of importance, absorption due to electron transfer transitions is apparent. These two types of transfer can be expressed as shown below:

Chromophore substituents:



Auxochrome substituents:

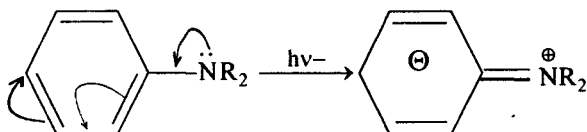


Table 1.3: Scotts rules for calculation of λ_{max} of the ET (electron transfer) band of aromatic carbonyl compounds

$\begin{array}{c} \text{Ar}-\text{C}-\text{Z} \\ \\ \text{O} \end{array}$			
Parent chromophore : $\text{Ar}=\text{C}_6\text{H}_5$			
$\text{Z} = \text{Alkyl or ring residue, (e.g.; ArCOR)}$		246 nm	In heterocyclic chemistry model compounds are essential for the interpretation of most spectra. No rules are available for the prediction of the wavelength maxima of aromatic compounds except in the case of acetophenone is taken as the parent chromophore, and increments allotted on the usual basis (Table 1.3)
$\text{Z} = \text{H, (Ar CHO)}$		250 nm	
$\text{Z} = \text{OH, Oalk, (ArCOOH and ArCOOR)}$		230 nm	
Increment for each substituent on Ar:			
- Alkyl or ring residue	o-, m-	+ 3 nm	
	p-	+ 10 nm	
- OH, -Oalk	o-, m-	+ 7 nm	
	p-	+ 25 nm	
- O ⁻ (oxyanion)	o-	+ 11 nm	
	m-	+ 20 nm	
	p-	+ 78 nm ^a	

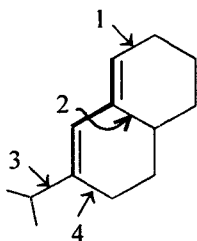
- Cl	o-, m-	+ 0 nm
	p-	+ 10 nm
- Br	o-, m-	+ 2 nm
	p-	+ 15 nm
- NH ₂	o-, m-	+ 13 nm
	p-	+ 58 nm
- NHCOCH ₃	o-, m-	+ 20 nm
	p-	+ 45 nm
- NHCH ₃	P-	+ 73 nm
- N(CH ₃) ₂	o-, m-	+ 20 nm
	p-	+ 85 nm

*This value may be decreased markedly by steric hindrance to coplanarity.

Let us now apply the rules in Table 1.1, 1.2, and 1.3 to a few known compounds and compare the resulting values of λ_{\max} with the values observed experimentally.

I. Dienes

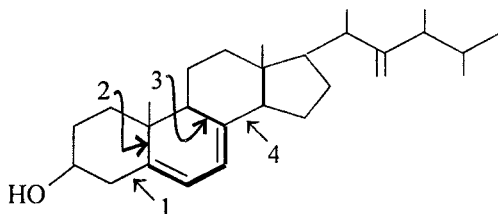
(1) Abietic acid



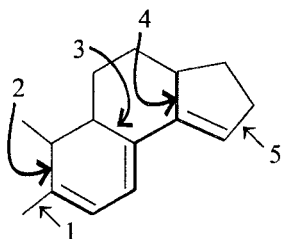
Basic heteroannular diene	214 nm
Exocyclic double bonds (1 × 5)	05 nm
Substituents R (4 × 5)	20 nm
	<hr/>
Calculated λ_{\max}	239 nm
Observed	241 nm

[Chromophore is shown by **heavy lines**; numbers indicate substituents.]

(2) Ergosterol



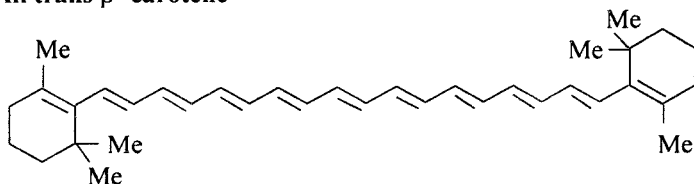
Basic homoannular diene	253 nm
Exocyclic double bonds (2×5)	10 nm
Substituents R (4×5)	20 nm
Calculated λ_{\max}	283 nm
Observed	282 nm

3. 3, β -Acetoxyergosta-5,7,14,22-tetraene

In compounds containing both homoannular and heteroannular double bonds, the diene system which requires least energy for excitation (i.e. the one with the longer wavelength of absorption) is used as a base.

Basic homoannular diene	253 nm
Exocyclic double bonds (3×5)	15 nm
Substituents R (5×5)	25 nm
Extra double bond in conjugation	30 nm
Calculated λ_{\max}	323 nm
Observed	319 nm

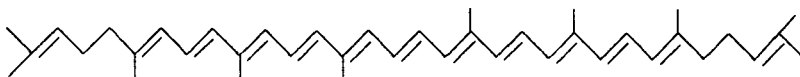
II. Polyenes

(1) All trans β -carotene

Basic λ_{\max} value		114 nm
M = number of alkyl substituents, 5×10	add	50 nm
n = number of conjugated double bonds, $11 \times [48 - (1.7 \times 11)]$	add	322.3 nm
R_{endo} = number of rings with endocyclic double bonds, 2×16.5 , subtract		33.0 nm
R_{exo} = number of rings with exocyclic double bonds, 0×10 , subtract		00.0 nm
Calculated λ_{\max}		<u>453.30 nm</u>
Observed		452.00 nm
$\epsilon_{\max} = 1.74 \times 11 \times 10^4$		
$= 19.1 \times 10^4$ (calculated)		
$= 15.2 \times 10^4$ (observed*)		

* The equation for calculating ϵ_{\max} is semi-empirical, the value calculated does not always correspond well with the observed value.

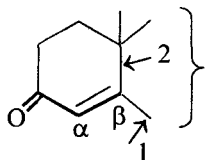
(2) All trans lycopene



Basic λ_{\max}		114 nm
M = 5×8	add	40 nm
n = $11 \times 148 - (1.7 \times 11)$	add	322.3 nm
(Note: Double bonds at ends are not in conjugation with others)		
R_{endo}	subtract	00.0 nm
R_{exo}	subtract	00.0 nm
Calculated λ_{\max}		<u>476.30 nm</u>
Observed		474.00 nm
$\epsilon_{\max} = 1.74 \times 11 \times 10^4$		
$= 19.1 \times 10^4$ (calculated)		
$= 18.6 \times 10^4$ (observed)		

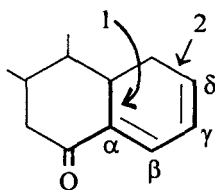
III. Enones

(1) Cholest-4-en-3-one

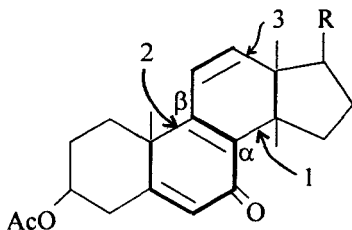


Parent base	215 nm
Substituents β , β (2×12) add	24 nm
Exocyclic = C< add	05 nm
	<hr/>
Calculated $\lambda_{\max}^{\text{EtOH}}$	244 nm
Observed	241 nm

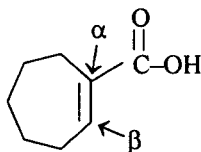
(2) Cholesta-2,4-dien-6-one



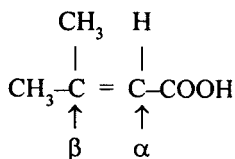
Parent base		215 nm
Extended conjugation	add	30 nm
Homoannular component	add	39 nm
Substituents α (1×10)	add	10 nm
δ (1×18)	add	18 nm
		<hr/>
Calculated $\lambda_{\max}^{\text{EtOH}}$		312 nm
Observed		314 nm

(3) 3, β -Acetoxy-7-oxolanosta-5,18,11-triene

Parent base		215 nm
Extended conjugation	add	30 nm
Homoannular component	add	39 nm
Exocyclic double bond	add	5 nm
Substituents α (1×10)	add	10 nm
β (1×12)	add	12 nm
δ (1×18)	add	18 nm
Calculated $\lambda_{\max}^{\text{EtOH}}$		<u>329 nm</u>
Observed		327 nm

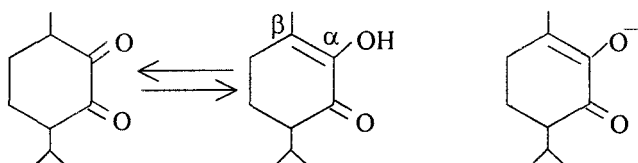
(4) Cycloheptene-1-carboxylic acid

Parent base		195 nm
Substituents α (1×10)	add	10 nm
β (1×12)	add	12 nm
C=C endocyclic to 7-member ring,	add	05 nm
Calculated $\lambda_{\max}^{\text{EtOH}}$		<u>222 nm</u>

(5) 3-Methyl-2-butenic acid

Parent base		195 nm
Substituents α (1×10)		10 nm
β (1×12)		12 nm
Calculated		<u>217 nm</u>
Observed value		216 nm

Dicarbonyl compounds

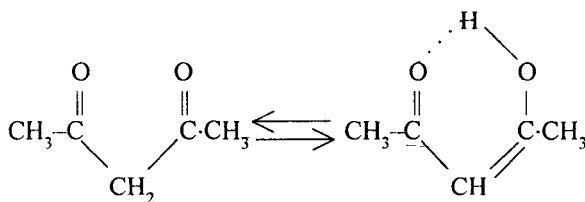


Diosphenol

Parent base	215 nm
Substituents 2β (2×12)	24 nm
α -OH (1×35)	35 nm
Calculated $\lambda_{\max}^{\text{EtOH}}$	<u>274 nm</u>
Observed $\lambda_{\max}^{\text{EtOH}}$	270 nm

In cyclic α -diketones, the enolic form is generally more stable than the keto form and therefore, the absorption is related to that of an α , β -unsaturated carbonyl system. Six-membered cyclic α -diketone known generally as diosphenols, exist in solution largely in the enolised form. In strong alkaline solution the absorption shifts to about 50 nm to longer waves, due to the formation of the enolate ion, to enable diosphenol structures to be characterised.

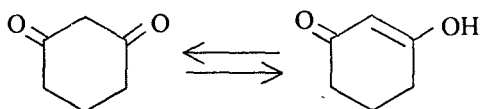
Acetyl acetone exists in the enolic form to the extent of about 90% in solution in non-polar solvents and the absorption directly depends on the concentration of the enol tautomer.

Acetyl acetone
 $\alpha\beta$ -diketone

$\lambda_{\max}^{\text{Isooctane}}$ 272,	ϵ_{\max} 12,000
$\lambda_{\max}^{\text{H}_2\text{O}}$ 274,	ϵ_{\max} 2050

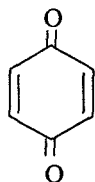
However, in the case of acetyl acetone agreement with the calculated wavelength (257 nm) is indifferent. This may be due to the fact that the strong internal hydrogen bond forces the carbonyl group and the double bond into a configuration different from that which is present in cyclic structures, e.g., diosphenol exists almost entirely in the enolic form.

1,3-cyclohexanedione, absorbs at 253 nm (ϵ_{\max} 22,000) in ethanol



1,3-Cyclohexanedione

The formation of enolate ion in alkaline solution in these cases also shifts the strong absorption band. Quinones represent α -, or vinylogous α -diketones. The spectrum of p-benzoquinone is thus found to be similar with that of a typical α , β -unsaturated ketone with the strong K-band appearing at 242 nm and a weak R-band near 434 nm.



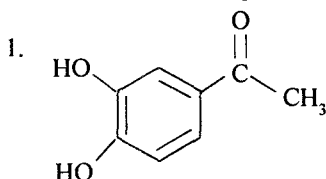
$$\lambda_{\max}^{\text{hexane}} = 242 \text{ nm } (\epsilon 24,000)$$

$$(\pi \rightarrow \pi^* \text{ K-band})$$

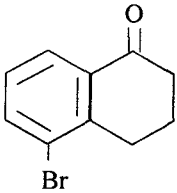
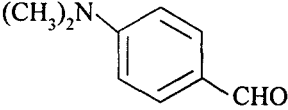
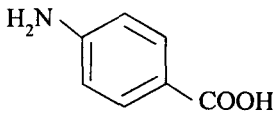
$$\left. \begin{array}{l} 281 \text{ nm } (\epsilon 400) \\ 434 \text{ nm } (\epsilon 20) \end{array} \right\} \begin{array}{l} n \rightarrow \pi^* \\ \text{R-band} \end{array}$$

The colour of the simpler members is due to the weak $n \rightarrow \pi^*$ transition which is also present in α -diketones. The $n \rightarrow \pi^*$ transitions of α -diketones in the diketo form gives rise to two bands one in the usual region near 290 nm ($\epsilon \sim 30$) and a second ($\epsilon 10 \sim 30$) which stretches into the visible 340–440 nm region to give yellow colour to some of these compounds.

IV. Aromatic carbonyl compounds



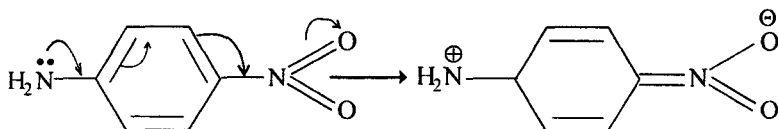
Base value	246 nm
OH in m	07 nm
OH in p	25 nm
	<hr/>
	278 nm

2.		Base value Br in m -CH ₂ in o	246 nm 02 nm 03 nm <hr style="width: 50%; margin-left: auto; margin-right: 0;"/> 251 nm
3.		Base value NMe ₂ in p	250 nm 85 nm <hr style="width: 50%; margin-left: auto; margin-right: 0;"/> 335 nm
4.		Base value NH ₂ in p	230 nm 58 nm <hr style="width: 50%; margin-left: auto; margin-right: 0;"/> 288 nm

Another approach to predicting, the λ_{\max} of the primary band of substituted benzenes involves the use of Table 1.5. This table has been successfully used with disubstituted compounds when the following rules are used:



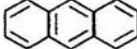
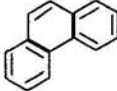
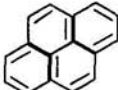
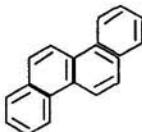
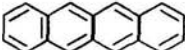
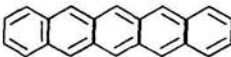
I. Para substitution:

- a. Both groups are either electron donating or electron withdrawing: Only the effect of the group causing the larger shift is used. For example, the λ_{\max} of *p*-nitrobenzoic acid would be expected to be the same as that of nitrobenzene, $\sim(203.5 + 65.0) = \sim 268.5$ (in alcohol solvent).
- b. One group is electron donating and the other electron withdrawing: The shift in the primary band of such a disubstituted benzene is usually greater than the sum of the shifts caused individually by the two groups. Such large shifts in *p*-disubstituted benzenes are attributed to interaction resonance, as illustrated below:



2. Ortho and Meta substitution: The shift effects are additive.

Table 1.4: Absorption characteristics of some polycyclic aromatic compounds

Compound	λ_{\max} , nm	ϵ_{\max}	λ_{\max} , nm	ϵ_{\max}	λ_{\max} , nm	ϵ_{\max}
 Benzene	184	47,000	203	7,400	255	230
 Naphthalene	220	1,10,000	275	5,600	314	316
 Anthracene	252	2,00,000	375	7,900	•	•
 Phenanthrene	252	50,000	295	13,000	330	250
 Pyrene	240	89,000	334	50,000	352	630
 Chrysene	268	1,41,000	320	13,000	360	630
 Naphthacene	278	1,30,000	473	11,000	•	•
 Pentacene			580	12,600		

• These weak bands are usually submerged by strong adjacent bands.

Table 1.5: Calculation of the Primary Band ($\pi \rightarrow \pi^*$ Transition) of substituted Benzenes (CH₃OH solvent)

Base Value: 203.5 nm

Substituent	Shift	Substituent	Shift
-CH ₃	3.0	-NH ₂	26.5
-CN	20.5	-NHCOCH ₃	38.5
-CHO	46.0	-NO ₂	65.0
-COCH ₃	42.0	-OH	7.0
-COOH	25.5	-O ⁻	31.5
-Br	6.5	-OCH ₃	13.5
-Cl	6.0		

Absorption Characteristics of Disubstituted Benzenes:

Compound	$\pi \rightarrow \pi^*$ Transition K Band		B Band	
	λ_{\max} (nm)	ϵ_{\max}	λ_{\max} (nm)	ϵ_{\max}
o-NO ₂ Phenol	279	6,600	351	3,200
m-NO ₂ Phenol	274	6,000	333	1,960
p-NO ₂ Phenol	318	10,000		Submerged
o-NO ₂ Aniline	283	5,400	412	4,500
m-NO ₂ Aniline	280	4,800	358	1,450
p-NO ₂ Aniline	381	13,500		Submerged

Table 1.6: Absorption characteristics of Aromatic systems and their substituted derivatives

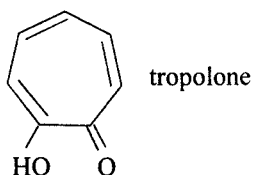
Compound	Solvent	Primary band		Secondary band		
		$\pi \rightarrow \pi^*$ Transition K Band		$\pi \rightarrow \pi^*$ Transition B Band		$n \rightarrow \pi^*$ Transition R Band
		λ_{\max} (nm)	ϵ_{\max}	λ_{\max} (nm)	ϵ_{\max}	λ_{\max} (nm)
Benzene	Hexane	204	7,900	256	200	
Toluene	Methanol(2%)	206.5	7,000	261	225	
o-Xylene	Methanol	210	8,300	263	300	

Compound	Solvent	Primary band		Secondary band			
		$\pi \rightarrow \pi^*$		$\pi \rightarrow \pi^*$		$n \rightarrow \pi^*$	
		Transition		Transition		Transition	
		K Band		B Band		R Band	
		λ_{\max} (nm)	ϵ_{\max}	λ_{\max} (nm)	ϵ_{\max}	λ_{\max} (nm)	ϵ_{\max}
m-Xylene	Methanol	212	7,200	265	300		
p-Xylene	Methanol	212	8,000	274	460		
Benzaldehyde	Ethanol	244	15,000	280	1500	328	20
Acetophenone	Ethanol	240	13,000	278	1,100	319	50
Benzophenone	Ethanol	252	20,000			325	180
Nitrobenzene	Hexane	252	10,000	280	1,000	330	125
Benzonitrile	Water	224	13,000	271	1,000		
Diphenyl Sulfoxide	Alcohol	232	14,000	262	2,400		
Methyl phenyl sulfone	Alcohol	217	6,700	264	977		
Biphenyl	Alcohol	246	20,000	Submerged			
2,2'-Dimethyl biphenyl		222		270	800		
Diphenyl- methane	Ethanol	-	-	262	500		
Styrene	Hexane	244	12,000	282	450		
Phenylacetylene	-	236	12,500	278	650		
Stilbene (cis)	Alcohol	283	12,300	Submerged			
Stilbene (trans)	Alcohol	295	25,000	Submerged			
Cinnamic acid (cis)		268	10,700				
(trans)		272	15,900				
1-Phenyl-1,3- butadiene (cis)	Isooctane	268	18,500				
(trans)	Isooctane	280	27,000				
1,3-Pentadiene							
(cis)	Alcohol	223	22,600				
(trans)	Alcohol	223.5	23,000				

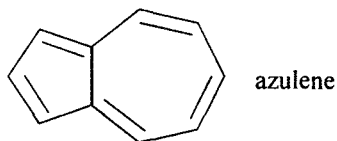
Compound	Solvent	Primary band		Secondary band			
		$\pi \rightarrow \pi^*$		$\pi \rightarrow \pi^*$		$n \rightarrow \pi^*$	
		Transition		Transition		Transition	
		K Band		B Band		R Band	
		λ_{\max} (nm)	ϵ_{\max}	λ_{\max} (nm)	ϵ_{\max}	λ_{\max} (nm)	ϵ_{\max}
Chlorobenzene	Ethanol	210	7,600	265	240		
Thiophenol	Hexane	236	10,000	269	700		
Anisole	Methanol (2%)	217	6,400	269	1,480		
Phenol	Water	210.5	6,200	270	1,450		
Phenolate anion	Alkali (aq)	235	9,400	287	2,600		
o-Catechol	Water (P ^{H3})	214	6,300	276	2,300		
o-Catecholate anion	Water (P ^{H11})	236.5	6,800	292	3,500		
Aniline	Water	230	8,600	280	1,430		
Aniliniumcation	Acid (aq)	203	7,500	254	160		
Acetanilide	Water	238	10,500	-	-		
Diphenyl ether	Cyclohexane	255	11,000	272	2,000		
Naphthalene	Ethanol	275	5,700	312	250		
Anthracene	Ethanol	375	8,000				
Tetracene (Naphthacene)	Ethanol	474	13,000				
Pentacene	Ethanol	580	15,000				
Pyridine	Hexane	257	2,750	270	450		
Quinoline	Cyclohexane	270	3,161	315	2,500		
Isoquinoline	Cyclohexane	265	4,170	313	1,800		
Acridine	Ethanol	358	10,000				
				Band I	Band II		
Furan	Cyclohexane	200	10,000	252	1 ^a		
Pyrrrole	Hexane	209	6,730	240	300 ^a		
Thiophene	Hexane	231	7,100	269.5	1.5 ^a		
Pyrazole	Ethanol	214	3,160	-	-		

^a These weak bands may be due to impurities rather than a forbidden transition ($n \rightarrow \pi^*$) of a hetero aromatic molecule.

Spectra of nonbenzenoid aromatic hydrocarbons show considerable resemblance to spectra of benzenoid compounds. Tropolone and its derivatives show absorption in the region 220 - 250 nm (ϵ_{\max} ca 30,000) and 340 - 375 nm (ϵ_{\max} ca 8,000); the latter absorption is characterized by the group of fine structure bands typical of aromatic systems.



Azulene and its derivatives have complicated spectra consisting of a number of relatively intense bands throughout most of the ultraviolet region (up to 360 nm) and a number of relatively weak bands throughout most of the visible region (500 - 700 nm). As a consequence of the latter, azulene and most of its derivatives are blue.



1.4: Approximate lower cutoff wavelengths* for commonly used solvents in UV-visible spectroscopy of organic substances

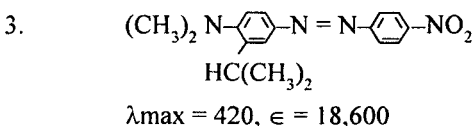
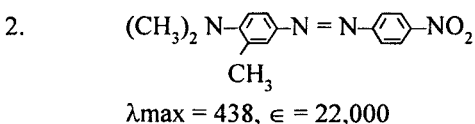
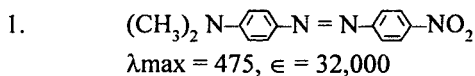
Solvent	Cutoff wavelength, nm	Solvent	Cutoff wavelength, nm
	<u>200-250</u>		<u>250-300</u>
Acetonitrile	210	Benzene	280
n-Butanol	210	Carbon tetrachloride	265
Chloroform	245	N,N-Dimethylformamide	270
Cyclohexane	210	Methyl formate	260
Decahydronaphthalene	200	Tetrachloroethylene	290
1, 1-Dichloroethane	235	Xylene	295
Dichloromethane	235		

Solvent	Cutoff wavelength, nm	Solvent	Cutoff wavelength, nm
Dioxane	225		
Dodecane	200		<u>300-350</u>
Ethanol	210	Acetone	330
Ethyl ether	210	Benzonitrile	300
Heptane	210	Bromofon-n	335
		Pyridine	305
Hexane	210		
Methanol	215		
Methylcyclohexane	210		<u>350-400</u>
isooctane	210		
isopropanol	215		
Water	210	Nitromethane	380

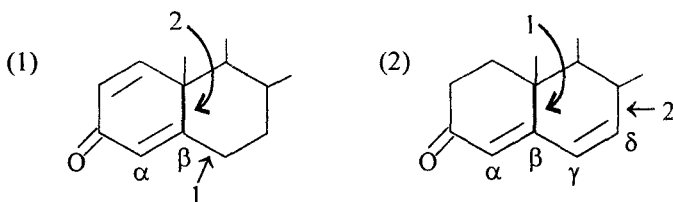
* **Cutoff wavelengths:** i.e. useful wavelength range is beyond the indicated wavelength.

Exercises and problems:

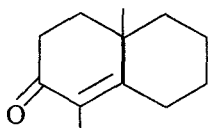
- (1) Explain the differences in the electron spectra of compounds (2) and (3) compared to compound (1)



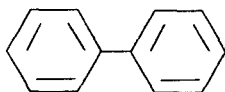
- (2) Identify which one of the following two isomers has the electronic absorption band with $\lambda_{\text{max}} = 241 \text{ nm}$ and $\epsilon_{\text{max}} = 18000$



- (3) Which structural features may produce a bathochromic or a hypsochromic effect in an organic compound.
- (4) Aniline absorbs at 230 nm ($\epsilon 8600$), however, in acid solution the main absorption band is seen at 203 nm ($\epsilon 7500$) and is comparable with benzene. Explain.
- (5) o-Nitrophenol gives a UV band at λ_{max} 350 nm when the spectrum is recorded in 0.1 N HCl solution, but the band is observed at λ_{max} 415 nm in 0.1 N NaOH solution. Explain.
- (6) Optical whiteners are used to make white clothes appear brighter. Can you suggest an explanation for the brightening action?
- (7) Explain the substitution pattern on the following enone and calculate the position of K band.

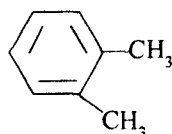


- (8) The position of absorption of acetone shifts in different solvents: 279 nm (hexane); 272 nm (ethanol) and 264.5 (water). Explain.
- (9) At what wavelength the coloured compounds absorb?
- (10) Biphenyl shows the following UV absorption data. In its 2,2'-dimethyl derivative however, the absorption pattern becomes almost similar to o-xylene. Explain.



Biphenyl

K-Band, $\lambda_{max} \rightarrow 252,$



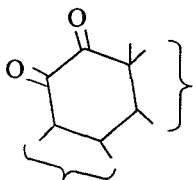
o-xylene

$\epsilon_{\max} \rightarrow 19,000$ $\lambda_{\max} 262$

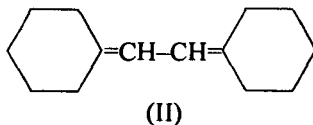
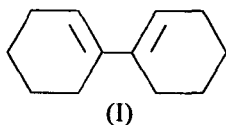
planar conformation

 $\epsilon_{\max} 270$

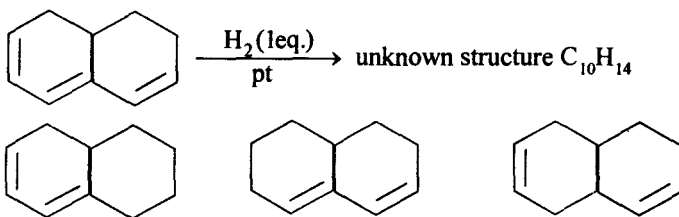
- (11) How will you confirm the presence of α -diketone system in the following steroid?



- (12) Why the λ_{\max} for the diene (I) is observed at lower nm than (II)



- (13) The following triene on partial hydrogenation gives three products. Which are separated by glc. How UV spectroscopy and application of Woodward-Fieser rules will help to identify the products.



Answers to the problems

- (1) In compound (1) the unshared electron pair of the nitrogen atom in the dimethylamino group is conjugated with the benzene ring ($n \rightarrow \pi^*$ conjugation). While in compound (2) this conjugation cannot be complete owing to the methyl group at the ortho position.

When methyl at the ortho position is replaced by a more bulky group, namely, isopropyl, the peak wavelength is shifted still further (owing to full violation of conjugation) to shorter wavelengths ($\lambda = 420 \text{ nm}$), with an accompanying drop of the band intensity ($\epsilon = 18,600$).

- (2) For isomer 1 we find

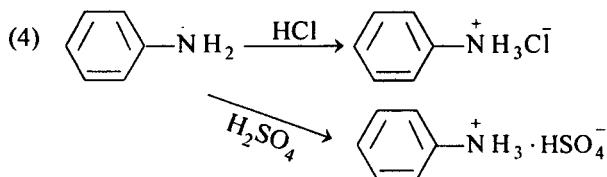
$$\begin{aligned} \lambda &= 215 \text{ nm} \\ &+ \frac{24 \text{ nm} (2 \times 12)}{239 \text{ nm}} \end{aligned}$$

For isomer 2 $\lambda = 215 \text{ nm}$

$$\begin{aligned} &+ 12 \text{ nm} (\beta\text{-substituent}) \\ &+ 18 \text{ nm} (\delta\text{-substituent}) \\ &+ 30 \text{ nm} (\text{extra double bond in conjugation}) \\ &+ \frac{05 \text{ nm} (\text{exocyclic double bond})}{280 \text{ nm}} \end{aligned}$$

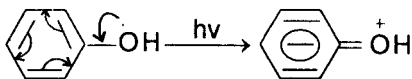
Hence, the absorption spectrum has been measured for isomer I.

- (3) A bathochromic shift (red shift) may occur by a change of medium or by the presence of an auxochrome. A hypsochromic shift (blue shift) may be caused by a change of the medium or by such structural changes like removal of conjugation.



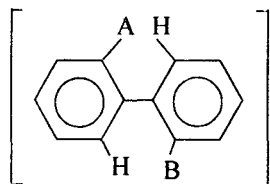
Due to the removal of conjugation of the lone pair of electrons on the nitrogen atom of aniline with the π -bond system of the benzene ring on protonation, the main absorption band is seen at 203 nm ($\epsilon = 7500$) and is comparable with benzene.

- (5) In 0.1 N HCl solution o-Nitrophenol gives a UV band at λ_{\max} 350 nm due to n- π conjugation



Conversion of a phenol to the corresponding anion (i.e. in 0.1 N NaOH solution) results in a bathochromic shift of the E_2 and B bands and an increase in ϵ_{\max} because the nonbonding electrons in the anion are available for interaction with the π electron system of the ring. Therefore band is observed at 415 nm in 0.1 N NaOH soln.

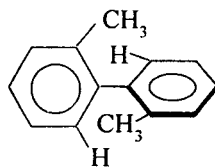
- (6) Singlet excited state of the brightening agent is converted into triplet state which emits radiation in the visible range.
- (7) One α -substituent, two β -ring residues and one exocyclic double bond: $215 + 10 + 24 + 5 = 254$ nm.
- (8) This is the expected shift of the $n \rightarrow \pi^*$ transition of acetone to shorter wavelength (blue shift) by changing to solvents of increased polarity.
- (9) Longer than 400 nm.
- (10) Although biphenyl is slightly twisted, the angle of twist is small, therefore, conjugation between the rings is not affected. Biphenyl thus shows a very intense absorption band at 252 nm (K-Band). Biphenyl derivatives with bulky substituents in the ortho positions are more stable in twisted conformations than in the planar conformation, which suffers serious non-bonded compressions from the juxtaposed substituents. The loss of conjugation in the twist conformation of 2, 2'-dimethylbiphenyl is reflected in its UV spectral data, which now structurally is like two moles of o-xylene.



Planar conformation

(A = CH_3 and B = CH_3)

2,2'-Dimethylbiphenyl

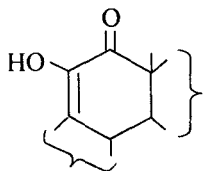


Twist conformation

2,2'-dimethylbiphenyl

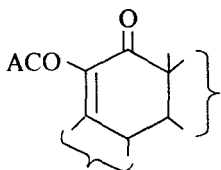
B-Band λ_{\max} 270, ϵ_{\max} 800

- (11) It will largely exist in the enolic form as revealed by the observed λ_{\max} 281 nm (ϵ_{\max} 9,700) which matches with the Cal. λ_{\max} (on enolisation the double bond becomes exocyclic to one ring). On acetylation the spectrum is restored to that calculated for the system now with OAC in the α -position. Further confirmation will come from the measurement of the spectrum of the enolised form in alkaline solution which will show the expected bathochromic shift of some 50 nm, i.e., 281 nm \rightarrow 330 nm.



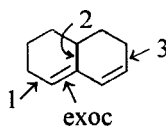
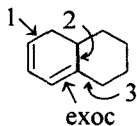
$$\lambda_{\max}^{\text{obs}} = 281 \text{ nm } (\epsilon_{\max} 9700)$$

$$\lambda_{\max}^{\text{calc}} = 215 + 2 \times 12 + 5 + 35 = 279 \text{ nm.}$$



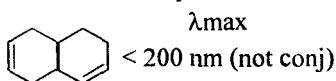
$$(215 + 2 \times 12 + 5 + 6 \text{ (OAC)}) = 250 \text{ nm}$$

- (12) In both the dienes, there are 4 ring residues as substituents. In diene (II), the two double bonds are exocyclic, thus in it λ_{\max} will be higher by $2 \times 5 = 10$ nm.
- (13) The markedly differed values are expected from each of the structures.



base value	253 nm
3 alkyl substituents 3×5	15 nm
exocyclic C=C	05 nm
Calculated or expected	<u>273 nm</u>

	214 nm
	15 nm
	05 nm
	<u>234 nm</u>



□□□

Infrared Spectroscopy

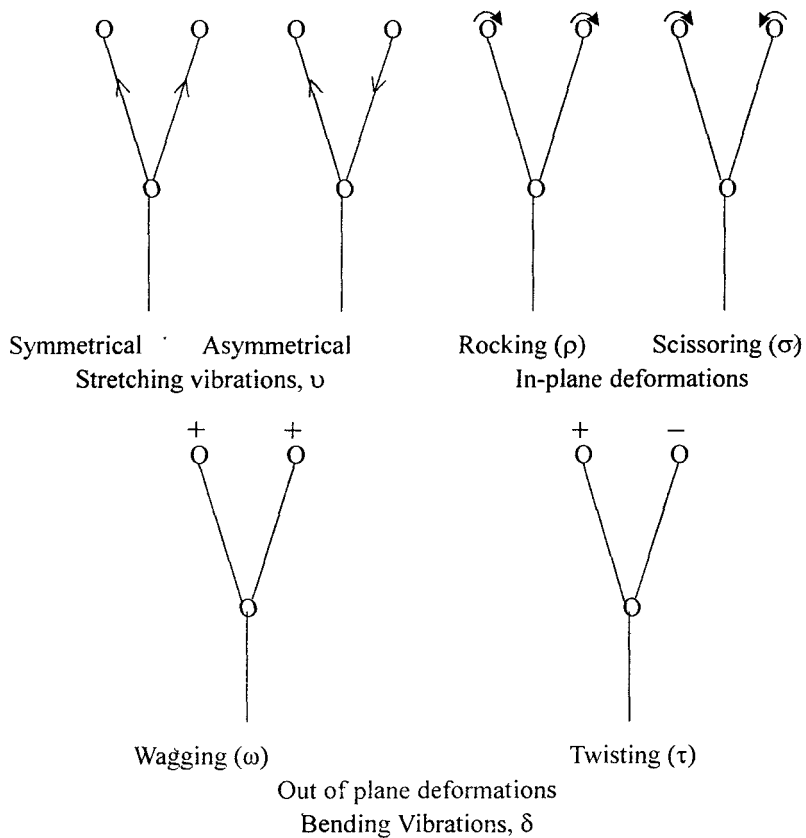


Table 2.1a: Characteristic infrared absorption frequencies of common classes of organic compounds

Type	Vibration mode	Frequency. cm^{-1}	Wave length, μ	Relative intensity*
1. Alkanes				
-CH ₃	C-H str., asym.	2975-2950	3.36-3.39	m.
	C-H str., sym.	2880-2860	3.47-3.50	m.
	C-H def., asym.	1470-1435	6.80-6.97	s.
	C-H def., sym.	1385-1370	7.22-7.30	m., sh.
-C(CH ₃) ₂	C-H def.	1385-1365	7.22-7.33	s., d.
	Skeletal	1175-1140 840-790	8.51-8.77 11.90-12.66	s., br. m.
-C(CH ₃) ₃	C-H def.	1395-1365	7.17-7.33	s, d. ratio 1:2
	Skeletal	1255-1200 750-720	7.97-8.33 13.33-13.89	s., br., d. s., br.
-CH ₂ -	C-H str., asym.	2940-2915	3.40-3.45	m. strong if several
	C-H str., sym.	2870-2845	3.49-3.52	m. -CH ₂ - present
	C-H, Scissoring	1480-1440	6.76-6.94	m.
	C-H, twisting & wagging	Ca. 1250	Ca. 8.00	m.
	Skeletal, if	750-720	13.33-13.89	s.
	-(CH ₂) ₄ or more			
CH ₃	C-H str.	3080-3040	3.25-3.29	v.
-in cyclopropane	Skeletal	1020-1000	9.80-10.00	m.
-C-H	C-H str.	2900-2880	3.45-3.47	w.
	C-H def	Ca. 1340	Ca. 7.45	w.
2. Alkenes				
See Table 2.2a & 2.2b				
3. Alkynes and allenes C-H str.				
Terminal/		3310-3300	3.02-3.03	m.
monosubstituted	C-H def.	600-650	16.7-15.4	s.
(RC≡CH)	C≡C str.	2140-2100	4.67-4.76	w.
Nonterminal/	} C≡C str.	2260-2190	4.42-4.57	v.
unsymmetrically				
disubstituted				
R ₁ C≡CR ₂				

Allenes (C=C=C)	C≡C type str.,			
	antisym.	1970-1950	5.08-5.13	m.
	C-C type str., sym.	1060	9.43	m.

4. Aromatic hydrocarbons

See Table 2.3

5. Alcohols and phenols

Free -OH	O-H str.	3650-3590	2.74-2.79	v., sh.
Intermolecularly hydrogen bonded (Change on dilution)				
Dimeric (Single bridge compounds)	O-H str.	3550-3450	2.82-2.90	v., sh.
Polymeric	O-H str.	3400-3230	2.94-3.10	s., br.
Intramolecularly hydrogen bonded (no change on dilution)				
single bridge compounds	O-H str.	3570-3450	2.80-2.90	v., sh.
chelate compounds	O-H str.	3200-2500	3.1-4.0	w., br.
Primary C-O-H	O-H def.	1350-1260	7.40-7.94	s.
	C-O str.	1075-1000	9.30-10.00	s.
Secondary C-O-H	O-H def.	1350-1260	7.40-7.94	s.
	C-O str.	1120-1030	8.93-9.71	s.
Tertiary C-O-H	O-H def.	1410-1310	7.09-7.63	s.
	C-O str.	1170-1100	8.55-9.09	s.
Phenols	O-H def.	1410-1310	7.09-7.63	s.
	C-O str.	1230-1140	8.13-8.77	s.

6. Ethers and epoxides

Acyclic CH ₃ -O-CH ₃	R-O-R str.asym.	1150-1070	8.70-9.35	s.
	C-H str.	2830-2815	3.54-3.55	m.
Aryl and aralkyl	Ar-O-R str.,			
	Ar-O-Ar asym.	1260-1200	7.98-8.33	v-s
	= C-H str.	3150-3050	3.18-3.28	w.
Conjugated	C-O-C str.	1275-1200	7.84-8.33	v.

t-butyl	$\begin{array}{c} \text{C} \\ \\ \text{C}-\text{C}-\text{O str.} \\ \\ \text{C} \end{array}$	920-800	10.87-12.50	s.
Cyclic	C-O str.	1140-1070.	8.77-9.35	s.
-O-CH ₂ -O	C-O str.	Ca. 940	Ca. 10-65	s.
	C-H str.	Ca. 2780	Ca. 3.65	v.
Epoxides	C-O str.	1260-1240	7.94-8.07	s.
trans	C-O str.	950-860	10.53-11.63	v.
cis	C-O str.	865-785	11.56-12.74	m.

7. Carbonyl compounds

For C=O stretching vibrations of acid chlorides, acid anhydrides, carboxylic acids, esters, aldehydes, ketones, amides and salts, see tables 2.4 and 2.5.

Vibrations other than C = O stretching vibrations

a) Anhydrides

Cyclic	C-O str.	1310- 1210	7.63-8.26	s.
Acyclic	C-O str.	1175-1045	8.51-9.57	s.

b) Carboxylic acids

Free OH	O-H str.	3550-3500	2.82-2.86	m.
Bonded OH	O-H str.	3333-2500	3.00-4.00	w., br.
	fine structure bands	2700-2500	3.70-4.00	w.
All OH	O-H def.	955-890	10.47-11.24	v.
Solid fatty acids	CH ₂ vib.	1350-1180	7.40-8.48	w.

characteristic
pattern

-COOH	C-O str. plus			
	O-H def.	1440-1395	6.94-7.17	w.
		1320-1210	7.58-8.26	s.
Carboxylate ion	O=C-O str., asym.	1610-1550	6.21-6.45	s.
	O=C-O str., sym.	1420-1300	7.04-7.69	m.

c) Esters

Formates	C-O str.	1200-1180	8.33-8.48	
Acetates	C-O str.	1250-1230	8.00-8.13	s.
Propionates and higher esters	C-O str.	1200-1170	8.33-8.55	s.

Esters of aromatic acids	C-O str.	1300-1250	7.69-8.00	s.
Vinylic and phenolic acetates	C-O str.	1220-1200	8.20-8.33	s.
Esters of α , β unsat. aliphatic acids	C-O str.	1310-1250	7.63-8.00	s.
d) Aldehydes	C-H str., asym.	2880-2650 975-780	3.47-3.77 10.26-12.82	w.-m., d. w.
e) Ketones				
CH ₃ -CO	CH ₃ def.	1360-1355	7.35-7.38	s.
CH ₂ -CO-	-CH ₂ def.	1435-1405	6.97-7.12	s.
	C=O str., overtone	3550-3200	2.82-3.13	w.
f) Amides				
primary, free NH	N-H str.	3540 - 3480 3420-3380	2.83-2.88 2.92-2.96	s. s.
bonded NH	N-H str.	3360-3320 3220-3180	2.98-3.01 3.11-3.15	m. m.
Free or bonded NH	N-H def. plus C-N str.	1650-1620 (amide II band) 1620-1590 (amide II band)	6.06- 6.17 6.17-6.29	s. s.
Secondary, free NH	N-H, cis str. N-H, trans str.	3440-3420 3460-3430	2.91-2.93 2.89-2.92	s. s.
bonded NH	N-H, cis str. N-H, trans str. N-H, cis and trans. str. N-H def. (amide V band)	3180-3140 3330-3270 3100-3070 Ca.700 (amide V band)	3.15-3.19 3.00-3.06 3.23-3.26 Ca 14.30	m. m. w. conc. dependent
Acyclic compound	N-H def. plus C-N str. N-H def. plus C-N str. (amide II band)	1305-1200 (amide III band) 1570-1515 (amide II band) 1550-1510 (amide II band)	7.67-8.33 6.37-6.60 6.45-6.62	m. s. s.

770-620	13.00-16.13	m.
(amide IV band)		
630-530	15.87-18.87	s.
(amide VI band)		

8. Amines, amino acids and their salts see table 2.6

9. Unsaturated nitrogen compounds

a) Nitriles

saturated alkyl	$C \equiv N$ str.	2260-2240	4.42-4.46	m.
α , β unsaturated				
alkyl	$C \equiv N$ str.	2235-2215	4.47-4.51	s., v.
Aryl	$C \equiv N$ str.	2240-2220	4.46-4.50	m.
Iso-	$C \equiv N$ str.	2185-2120	4.52-4.72	s.

b) Oximes, pyridines, quinolines, purines, pyrimidies etc.

Acyclic saturated, (alkyl compounds)	$C=N$ str.	1690-1640	5.92-6.10	v.
Acyclic α , β unsat. compounds	$C=N$ str.	1665-1630	6.01-6.14	v.
Cyclic α , β unsat. compound (such as thiazoles)	$C=N$ str.	1660-1480	6.02-6.67	v.
Pyridines	$C=N$ str.	1580-1550	6.33-6.45	w.
	$=C-H$ str.	3070-3020	3.26-3.31	s.
	Ring $C-H$ def.	Ca. 1200	Ca. 8.33	s.
		1100-1000	9.09-10.00	s.
	$C=C$ str.	1650-1580	6.06-6.35	m.
Pyrimidines and	$=C-H$ str.	3060-3010	3.27-3.32	s.
Purines	Ring $C-H$ def.	1000-960	10.00-10.42	m.
		825-775	12.12-12.90	m.
	$C=N$ str.	1580-1520	6.33-6.58	m.
Pyrroles	$N-H$ str.	3440-3400	2.91-2.94	m.
	$C=C$ str.	1565-1500	6.39-6.67	v., d.
Oximes	$C=N$ str.	1690-1620	5.92-6.17	v.
	$O-H$ str.	3650-3500	2.74-2.86	v.
Azo compounds	$-N=N$ str.	1630-1575	6.14-6.35	v.
Carbodiimides	$-N=C=N$ str.	2155-2130	4.64-4.70	s.
Isocyanates	$-N=C=O$ str.	2275-2240	4.40-4.46	s., -v.
Azides	$-N=N=N$ str.	2170-2080	4.61-4.81	s.

10. Compounds containing nitrogen-oxygen bond

Nitrates (O-NO ₂),	NO ₂ str.. asym	1590-1500	6.29-6.67	s.
nitramines.nitro	NO ₂ , str.. sym.	1390-1250	7.20-8.00	w.
(compounds CC-NO ₂)	C-N vib.	920-830	10.88-12.05	m., -s
Nitroso compounds	(R-C-N=O)			
alkyl, aromatic	N=O str.	1550-1500	6.45-6.67	s.
(α-halogeno, aliphatic	N=O str.	1620-1560	6.17-6.47	s.
Nitrites (R-O-N=O)				
trans form	N=O str.	1680-1650	5.95-6.05	v., -s,
	N-O str.	815-750	12.27-13.33	s.
	O-N=O def.	625-565	16.00-17.70	s.
Cis form	N = O str.	1625-1610	6.16-6.21	v., s.
	N-O str.	850-810	11.76-12.35	s.
	O-N=O def.	690-615	14.49-16.26	s.
	overtone	3360-3220	2.98-3.11	m.
Nitrosamines	N=O str.	1500-1480	6.67-6.76	s.Vapor
				phase
(R-N-N=O)		1460-1440	6.85-6.94	s. solution
				phase
	N-N str.	Ca. 1050	Ca. 9.52	s.
	N-N = 0 def.	Ca. 660	Ca. 15.15	s.
Azoxy comp.	N-O str.	1310-1250	7.63-8.00	m., -s.
(R-N-N-O)				

11. Sulfur compounds

	S-H str.	2600-2550	3.85-3.92	w.
	C-S str.	700-570	14.18-17.54	w.
	C= S str.	1675-1130	5.97-8.85	s.
Thioketone	C= S str.	1250-1020	8.0-9.8	s
Thioamide	C= S str.	1300-1100	7.69-9.9	s.
Covalent sylfates	S=O str., sym..	1440-1350	6.94-7.41	s.
(RO) ₂ SO ₂	S=O str., asym.	1230-1150	8.13-8.70	s.
Covalent sylfonates	S=O str. sym.	1420- 1330	7.04-7.52	s.
(R ₁ -O-SO ₂ -R ₂)	S=O str.. asym.	1200-1145	8.33-8.73	s.
Sulfonyl chlorides	S=O str., sym.	1375-1340	7.27-7.46	s.
(R-SO ₂ Cl)	S=O str.. asym.	1190-1160	8.40-8.62	s.
Sylfonamides	S=O str.. sym.	1370-1300	7.30-7.69	s.

(R-SO ₂ -N)	S=O str. asym.	1180-1140	8.48-8.77	s.
Sulfones	S=O Str., Sym.	1350-1300	7.41-7.69	v., -s.
(R ₂ SO ₂)	S=O str., asym	1160-1120	8.62-8.93	v., -s.
Sulfonic acids	S=O str., sym.	1260-1150	7.94-8.70	s.
(RSO ₃ H)	S=O str., asym.	1080-1010	9.26-9.90	s.
Sulfites (RO) ₂ SO	S=O str.	1220-1170	8.20-8.55	s.
Sulfoxides (R-SO-R)	S=O str.	1070-1030	9.35-9.71	s.

12. Phosphorus compounds

P-OH	O-H str.	2700-2560	3.70-3.90	w.
	P-H str.	2440-2350	4.10-4.26	m.
	P-C def.	1450-1280	6.90-7.81	m.-s.
	P=O str.	1350-1150	7.41-8.70	v.-s.
	P-O str.	1240-900	8.07-10.10	v.
P-O-P	P-O str.	1000-870		s.
		~ 700		w.
P-O-C (aliph)		1050-970		s.
		830-740		s. (may be absent)
P-O-C (arom)		1260-1160		s.
		994-855		s.

13. Halogen compounds

Polyfluorinated	C-F str.	1400-1100	7.14-9.10	v. -s., mlt.
Difluorinated	C-F str.	1250-1050	8.00-9.50	v. -s., d.
Monofluorinated	C-F str.	1110-1000	9.01-10.00	s.
Polychlorinated	C-Cl str.	800-700	12.50-14.30	v. -s.
C-Cl equatorial	C-Cl str.	780-750	12.80-13.33	s.
C-Cl axial, other monochlorinated	C-Cl str.	Ca. 650	Ca. 15.40	s.
C-Br equatorial	C-Br str.	750-700	13.33-14.29	s.
C-Br axial	C-Br str.	690-550	14.50-18.20	s.
Other monobromides	C-Br str.	650-560	15.40-17.85	s.
Iodides	C-I str.	Ca. 500	Ca. 20.00	s.

14. Silicon and boron compounds

	B-H str.	2220-1600	4.51-6.25	v., mlt.
	B-C def.	1460-1280	6.85-7.81	v.
	Si-H str.	2280-2080	4.39-4.81	v.-s.
	Si-H def.	800-950	12.5-10.53	s.

SiOH	O-H str.	3700-3200	2.7-3.12	s.
	Si-O	830-1110	12.05-9.01	s.
	Si-F str.	800-1000	12.5-10.0	s
	Si-C def.	Ca. 1260	Ca. 7.94	v. -s.
	Si-C str.	840-755	11.90-13.25	v.-s.

str.*=stretching sym.=symmetric s=strong absorption w=weak absorption
 def. = deformation asym.=asymmetric m.=medium absorption v.=variable intensity
 sh.=sharp peak d.=doublet br.=broad absorption mlt.=multiplet

Table 2.1b Correlations of infrared absorption and structure of organic compounds

Frequency range	Wavelength range	Intensity	Type and group	Bond
4000-3001				
3676-3584	2.72-2.79	v., sh.	Alcohols, phenols, free OH	O-H str.
3650-3496	2.74-2.86	v.	Oximes (R-C = NOH)	O-H str.
3595-3425	2.78-2.92	v., sh.	R-OH, Ar-OH, intramolecular hydrogen bonded	O-H str.
3550-3500	2.82-2.86	m.	Carboxylic acids, free OH	O-H str.
3550-3450	2.82-2.90	v., sh.	R-OH, Ar-OH, dimeric	O-H str.
3550-3205	2.82-3.12	w.	Ketones, C=O overtone	C=O str.
3540-3380	2.83-2.96	s., d.	Primary amides, free NH	N-H str.
3500-3300	2.86-3.03	v., d.	Primary amines, free NH secondary amines	N-H str.
3460-3435	2.89-2.91	s.	Sec. amides, free NH (trans)	N-H str.
3360-3220	2.98-3.11	m.	Nitrites (R-O-N=O) overtones	N=O str.
3440-3420	2.91-2.93	s.	Sec. amides, free NH(cis)	N-H str.
3440-3400	2.91-2.94	m.	Pyrroles	N-H str.
3400-3300	2.94-3.03	v.	Imines	N-H str.
3400-3230	2.94-3.10	s., br.	R-OH, Ar-OH, polymeric	O-H str.

3400-3200	2.94-3.13	m. d	Amino acid salts	NH ₂ str.
3400-3095	2.94-3.23	m.	Amines, imines, associated	N-H str.
3390-3255	2.95-3.07	m.	Amido acids	N-H str.
3380-3150	2.96-3.18	m., mlt.	Charged amine derivatives	NH ₃ ⁺ str.
3360-3180	2.97-3.15	m., d.	Amides, bonded NH (primary)	N-H str. N-H str.
3330-3270	3.00-3.06	m.	Sec. amides, bonded (trans)	N-H str.
3310-3300	3.02-3.03	m.	Alkynes (RC≡CH)	C-H str.
3300-2500	3.00-4.00	w., br.	R-COOH, bonded OH	O-H str.
3200-1700	3.13-5.88	w., br.	R-OH, Ar-OH, chelate	O-H str.
3175-3135	3.15-3.19	m.	Sec. amides, bonded NH (cis)	N-H str.
3150-3050	3.18-3.28	w.	Ethers -CH=C-O- and C=CH-O-	C-H str.
3130-3030	3.20-3.30	m.	Amino acids, hydrochlorides	NH ₃ ⁺ str.
Ca. 3100	ca. 3.23	v.	Tropolones	O-H str.
3100-3070	3.23-3.26	w.	Amides, bon. NH (cis)	N-H str.
3095-3075	3.23-3.25	m.	Alkenes (CHR=CH ₂)	RC-H str.
3085-3040	3.24-3.29	v.	Alkanes (-CH ₂ -, cyclopropane)	C-H str.
3085-3030	3.24-3.30	w.-m, mlt.	Aromatic homocyclic (=C-H)	C-H str.
3075-3020	3.25-3.31	s.	Pyridines, quinolines (=C-H)	C-H str.
3060-3010	3.27-3.32	s.	Pyrimidines, purines (=C-H)	C-H str.
3050-2995	3.28-3.34	w.	Ethers, epoxides	OC-H str.
3040-3010	3.29-3.32	m	Alkenes (CHR=CH ₂ , CHR ₁ =CHR ₂ , cis or trans, CR ₁ R ₂ =CH ₂)	C-H str.
3030-2500	3.30-4.00	w., mlt.	Amino acid hydrochlorides	

3000-2001

2975-2950	3.36-3.39	m.	Alkanes ($-\text{CH}_3$)	C-H str.
2940-2915	3.40-3.43	m.	Alkanes ($-\text{CH}_2-$)	C-H str.
2905-2875	3.44-3.48	w.	Alkanes ($-\text{CH}-$)	C-H str.
2880-2860	3.47-3.50	m.	Alkanes ($-\text{CH}_3$)	C-H str.
2880-2650	3.47-3.77	w.-m., d.	Aldehydes ($-\text{CHO}$)	C-H str.
2870-2845	3.49-3.52	m.	Alkanes ($-\text{CH}_2-$)	C-H str.
2835-2815	3.53-3.55	m.	Ethers ($-\text{O}-\text{CH}_3$)	C-H str.
Ca. 2825	ca. 3.54	m.	Alkyl acetals	C-H str.
2825-2760	3.54-3.62	m.-s.	Amines (N-methyl)	C-H str.
2780-2400	3.60-4.17	v.	Deuterated R-OH, Ar-OH	O-D str.
ca. 2780	ca. 3.60	v.	Ethers ($\text{O}-\text{CH}_2-\text{O}-$)	C-H str.
2760-2530	3.62-3.95	w.	Amino acids	
ca. 2700	ca. 3.70	s.	Charged amine derivatives	NH_2^+ rck.
2700-2560	3.70-3.90	w., b.	Organo-phosphorus compounds	O-H str,
2640-2360	3.79-4.24	w.	Amido acids,	
2600-2400	3.85-4.15	v.	Deuterated amines, imines	N-D str.
2590-2550	3.86-3.92	w.	Organo-sulfur compounds	S-H str.
2500-2325	4.00-4.30	s.	Charged amines ($\text{C}=\text{NH}^+$)	NH^+ str.
2280-2260	4.39-4.43	s.	Diazonium salts ($\text{R}-\text{C}=\text{N}=\text{N}^+$)	
2280-2080	4.39-4.81	v.	Organo-silicon compounds	Si-H str.
2275-2240	4.40-4.46	v.	isocyanates	$\text{N}=\text{C}=\text{O}$ str.
2260-2240	4.43-4.46	w.-m.	Saturated nitrites	$\text{C}\equiv\text{N}$ str.
2240-2220	4.46-4.51	m.-s.	Aryl nitrites	$\text{C}\equiv\text{N}$ str.
2235-2215	4.47-4.52	s.	Acyclic α . β unsat. nitriles	$\text{C}\equiv\text{N}$ str.
2220-1600	4.51-6.25	v., mlt.	Boron compounds	B-H str.
2200-1800	4.55-5.56	w.-m.	Charged amine derivatives	NH^+ vib.

2185-2120	4.58-4.72	s.	Isonitriles	$C\equiv N$ str
2160-2120	4.63-4.72	s.	Azides ($-N=N=N$)	$-N=N=N$ str.
2155-2150	4.64-4.69	s.	Carbodiimides	$N=C=N$ str.
2140-2100	4.67-4.76	w.	Alkynes ($RC\equiv CH$)	$C\equiv C$ str.
2140-2080	4.67-4.81	w.	Amino acids	NH_3^+ str.
Ca. 2100	ca. 4.76	w.	Deuterated alkanes	$C-D$ str.
<u>2000-1501</u>				
ca. 2000	ca. 5.00	w.	Amino acid hydrochlorides	
1970-1950	5.08-5.13	m.	Allenes ($C=C=C$)	$C\equiv C$ type str.
1945-1835	5.14-5.45	w.	Amido acids	
1870-1830	5.35-5.46	s.	Acid anhydrides, 5 ring	$C=O$ str.
1850-1810	5.40-5.53	s.	Acid anhydrides, conj. 5 ring	$C=O$ str.
1850-1800	5.40-5.56	m.	Alkenes ($CHR=CH_2$) overtone	$C-H$ str.
1840-1800	5.44-5.56	s.	Acid anhydride, acyclic	$C=O$ str.
1820-1810	5.50-5.53	s.	Acyl peroxides	$C=O$ str.
1820-1780	5.50-5.62	s.	conj.acyclic acid anhydrides	$C=O$ str.
1815-1785	5.51-5.60	s.	Acid halides	$C=O$ str.
1805-1780	5.54-5.62	s.	Aroyl peroxides esters, lactone	$C=O$ str.
1800-1780	5.56-5.62	s.	$(R-CO-O-)_2$	$C=O$ str.
1800-1780	5.56-5.62	m	Alkenes ($CR_1R_2=CH_2$), overtone	$C-H$ str.
1800-1770	5.56-5.65	s.	Conj. acid halides	$C=O$ str.
1800-1770	5.56-5.65	s.	Vinylic phenolic esters	$C=O$ str.
1800-1760	5.56-5.68	s.	Acid anhydride, 5 ring	$C=O$ str.
1795-1740	5.57-5.75	s.	Acid anhydrides, conj. 5 ring	$C=O$ str.
1790-1720	5.59-5.81	s.	Ureas ($-CO-NH-CO-$), amide I	$C=O$ str
1785-1755	5.60-5.70	s.	$(RCO-O-)_2$	$C=O$ str.
1780-1770	5.62-5.65	s.	Fused - ring β lactams, amide I	$C=O$ str.

1780-1760	5.62-5.68	s.	Ketones. 4 ring, sat. γ lactone	C=O str.
1780-1740	5.62-5.75	s.	Acyclic acid anhydrides	C=O str.
1760-1730	5.68-5.78	s.	Simple β lactams	C=O str.
1760-1720	5.68-5.81	s.	Conj. acyclic anhydrides	C=O str.
1755-1740	5.70-5.75	s.	α keto esters, α diesters	C=Ostr.
1755-1730	5.70-5.78	s.	α -amino acid hydrochloride	C=O str.
1755-1720	5.70-5.81	s.	Dicarboxylic α -amino acids	C=O str.
1750-1740	5.71-5.75	s.	Ketones. 5 ring	C=O str.
1750-1735	5.71-5.76	s.	γ -keto esters, diesters, nonenolic β -keto esters	C=O str.
1750-1735	5.71-5.76	s.	Sat. aliphatic esters, α -lactones	C=O str.
1745-1725	5.73-5.80	s.	CO-O-CH ₂ -CO-	C=O str.
1750-1700	5.71-5.88	s.	Fused ring γ lactams	C=O str.
1740-1720	5.75-5.81	s.	Sat. aliphatic aldehydes	C=O str.
1740-1715	5.75-5.83	s.	α -halogeno carboxylic acids	C=O str.
1735-1700	5.76-5.88	s.	Urethanes	C=O str.
1730-1710	5.78-5.85	s.	-CO-CO-	C=O str.
1730-1700	5.78-5.88	s.	Amino acid hydrochlorides	C=O str.
1730-1715	5.78-5.83	s.	α , β unsat., aryl esters	C=O str.
1730-1700	5.78-5.88	s.	Dicarboxylic amino acids	C=O str.
1725-1705	5.80-5.87	s.	-CO-CH ₂ -CH ₂ -CO-	C=O str.
1725-1700	5.80-5.88	s.	Sat. aliphatic acids, dimer, acyclic, CH ₂ -CO-CH ₂ -ketones	C=Ostr.
1725-1695	5.80-5.90	s.	α -amido acids	C=O str.
1720-1700	5.81-5.88	s.	Ketones. 6-ring	C=O str.
1715-1700	5.83-5.88	s.	Ketones. 7-ring	C=O str.
1715-1695	5.83-5.90	s.	Aryl aldehydes	C=O str.
1715-1680	5.83-5.95	s.	α , β unsat. acids	C=O str.
1710-1690	5.85-5.92	s.	Carbamates. amide I band	C=O str.
1710-1670	5.85-5.99	s.	-CO-NH-CO-, amide I band	C=O str.
1705-1685	5.78-5.93	s.	α , β unsat. aldehydes	C=O str.
ca. 1700	ca. 5.88	s.	Simple γ lactams, amide I band	C=O str.

1700-1680	5.88-5.95	s.	Aryl carboxylic acids.	C=O str.
1700-1665	5.88-6.01	s	dimer. aryl ketones secondary amide. amide I band	C=O str.
1695-1660	5.90-6.02	s.	α , β unsat. acyclic or 6 ring ketones	C=O str.
ca. 1690	ca. 5.92	s.	Primary amides, amide I band	C=O str.
1690-1670	5.92-5.99	w.	$CR_1R_2=CR_3R_4$ alkenes	C=C str.
1690-1670	5.92-5.99	s.	o-hydroxy (amino) benzoates	C=O str.
1690-1655	5.92-6.04	s.	Quinones, 2 CO's in same ring	C=O str.
1690-1635	5.92-6.01	v.	oximes, oxazines, oxazolines, oxazolones, azomethines, acyclic C=N	C=N str.
ca. 1680	ca. 5.95	s.	Large-ring cyclic lactams	C=O str.
1680-1660	5.95-6.02	s.	Conj. polyene aldehydes	C=O str.
1680-1650	5.95-6.06	s.	Intramolecular H-bonded carboxylic acids	C=O str.
1680-1650	5.95-6.06	v.	Nitrites (R-O-N=O trans)	N=O str.
1680-1630	5.95-6.14	s.	sec. amides, amide I band	C=O str.
1680-1620	5.95-6.17	v.	Nonconj. alkenes	C=C str.
1675-1665	5.97-6.00	v.	Alkenes, $CR_1R_2=CHR_3$	C=C str.
ca. 1675	ca. 5.97	s.	Thioesters	C=S str.
1670-1660	5.99-6	s	Cross-conj. dienones	C=O str.
1670-1645	5.99-6.08	s.	Intramolecular OH H-bonded ($-C=C-CHO$ type) aldehydes	C=O str.
1670-1630	5.99-6.14	s.	Tertiary amides. amide I band	C=O str.
1665-1635	6.01-6.12	v.	Alkenes ($CHR_1=CHR_2$ -cis)	C=C str.
1665-1630	6.01-6.14	v.	Oximes, Oxazines, etc.	C=N str.

ca. 1660	ca. 6.02	s.	Ureas (NH-CO-NH), amide I band	C=O str
1660-1640	6.02-6.10	v.	Alkenes (CR ₁ R ₂ =CH ₂)	C=C Str.
1660-1610	6.02-6-21	w.	Amino acids containing NH ₂ group. amino acid I band	NH ₃ ⁺ def.
1660-1580	6.02-6.33	s.	Alkenes conj. with C=O or C=C	C=C str.
1660-1480	6.02-6.76	v.	Thiazoles (cyclic α, β sat. C=N)	C=N str.
1655-1635	6.04-6.12	s.	Enolic β-keto esters, chelated	C=O str.
1655-1635	6.04-6.12	s.	Quinones, 2 CO's in 2 rings	C=O str.
1655-1610	6.04-6.21	s.	o-CO-C ₆ H ₄ -OH (or NH ₂), H-bonded	C=O str.
1655-1610	6.04-6.21	s.	Nitrates (RONO ₂), asym. vibration	NO ₂ str.
ca. 1650	ca. 6.06	s.	Primary amides, amide I band	C=O str.
1650-1590	6.06-6.31	s.	Prim. amides, amide II band, combination NH def. + CN str. NH def. + CN str.	
1650-1620	6.06-6.17	s.	Amido acids, amide I band-	C=C + C = N str.
1650-1580	6.06-6.33	m.	pyrimidines, quinolines	
1650-1580	6.06-6.33	m.-s.	Prim. amines	NH def.
1650-1550	6.06-6.45	w.	Sec. amines	NH def.
1645-1640	6.08-6.10	v.	Alkenes (CHR=CH ₂)	C=C str.
1640-1605	6.10-6.23	s.	Alkyl nitroguanidines, asym. NO ₂ vibrations	NO ₂ str.
1640-1535	6.10-6.52	s., d.	Ketones (-CO-CH ₂ -CO or -CO-C=C-OH)	C=O str.
1630-1575	6.14-6.35	v.	Azo compounds	N=N str.
ca. 1625	ca. 6.16	s.	Alkenes, phenyl conj. C=C	C=C str.

1625-1610	6.16-6.21	v.	Nitrites (RON=O cis form)	N=O str.
1625-1575	6.16-6.35	v.	Aromatic homocyclic comp.	C=C i-p vib.
1620-1600	6.17-6.25	s.	Tropolones	C=O str.
1620-1600	6.17-6.25	s.	Amido acids, amide I band	
1620-1590	6.17-6.31	s.	Prim. amides, amide II band, combination	NH def. + CN str.
			NH def. + CN str.	
1620-1560	6.17-6.41	s.	Nitroso compounds, α halogeno	N=N str.
1620-1560	6.17-6.41	m.-s.	Charged amine derivatives	NH ₂ ⁺ def.
1610-1590	6.21-6.29	w.	Amino acid hydrochlorides	NH ₃ ⁺ def.
1610-1550	6.21-6.45	s.	Carboxylate ion, asym. str.	
Ca. 1600	ca. 6.25	m.	Charged amine derivatives	NH ₃ ⁺ def.
1600-1575	6.25-6.35	s.	α , α -dihalogenonitro compounds	NO ₂ str.
1600-1560	6.15-6.41	s.	Amino acid salts, all amino acids with ionized carboxyl	C=O str.
1590-1575	6.29-6.36	v.	Aromatic homocyclic comp. C=C	i-p str.
1590-1575	6.29-6.36	s.	Nitroureas	NO ₂ str.
1585-1530	6.31-6.54	s.	Saturated nitramines	NO ₂ str.
1580-1570	6.33-6.37	s.	α -halogenonitro compounds	NO ₂ str.
1580-1550	6.33-6.45	w.	Nitrogen heterocycles, combination, C=C and C=N str.	C=C + C=N str.
1580-1520	6.33-6.58	m.	Pyrimidines and purines, combination, C=C and C=N str.	C=C+C=N str.
1570-1515	6.37-6.60	s.	Sec. acyclic amides, amide II band, combination NH def. and CN str.	NH def. + CN str.

1570-1500	6.37-6.67	s.	All amido acids, amido II band	N-H def.
ca. 1565	ca. 6.39	v.	Pyrroles	C=C str.
1565-1545	6.39-6.47	s.	Prim. and sec. nitro compounds	NO ₂ str.
ca. 1550	ca. 6.45	s.	Tertiary aliphatic nitroso compounds, vapor phase	N=O str.
1550-1510	6.45-6.62	s.	Aromatic nitro compounds	
1550-1485	6.45-6.73	v.	Amino acids cont. NH ₂ group, amino acid II band	NH ₃ ⁺ def.
1550-1510	6.45-6.62	s.	Sec. acyclic amides, amides II band	NH def. + CN str.
1550-1485	6.45-6.73	v.	Amino acid hydrochlorides	NH ₃ ⁺ def.
1545-1530	6.47-6.54	s.	Tert. nitro compounds	NO ₂ str.
1530-1510	6.54-6.62	s.	α, β-unsat. nitro compounds	NO ₂ str.
1525-1475	6.56-6.78	v.	aromatic homocyclic comp. C=C	i-p vib.
1510-1480	6.62-6.76	m.	Pyridines, quinolines, combination C=C and C=N str.	C=C+C=N str.
ca. 1500	ca. 6.67	v.	Pyrroles	C=C str.
ca. 1500	ca. 6.67	s.	Aromatic nitroso compounds	N=O str.
ca. 1500	ca. 6.67	s.	Amine salts	NH def.
<u>1500-1001</u>				
1500-1440	6.67-6.94	s.	Nitrosamines (RNN=O)	N=O str.
1485-1445	6.74-6.92	m.	Alkanes (-CH ₂ -)	C-H def.
1470-1430	6.80-7.00	m.	Alkanes (-CH ₃)	C-H def.
ca. 1467	ca. 6.81	m.	Alkanes, CH ₂ scissor	C-H def.
ca. 1460	ca. 6.85	m.	Alkanes. asym CH ₃	C-H def.
1455 (ca.)	ca. 6.87	m.	Alkanes, alicyclic CH ₂ scissor	C-H def.
ca. 1450	ca. 6.90	m.	Aromatic multiple bond	C=C str.

1430-1400	7.0-7.14	v.	Ketones, esters, α -methylene C-H scissor	C-H def.
1430-1350	7.00-7.41	s.	Sulfites	S=O str.
1420-1410	7.04-7.09	s.	Alkenes ($RCH=CH_2$ or $R_1R_2C=CH_2$)	C-H def.
1420-1390	7.04-7.20	w.	Alcohols	O-H def.
1410-1310	7.10-7.60	s.	Phenols, tert. alcohols	O-H def.
1400-1300	7.15-7.69	s.	Carboxylic acids, ionic	
1400-1000	7.15-10.0	s.	Halogen comp., fluorides	C-F str.
1395-1385	7.17-7.22	m., d.	Alkane, tert. butyl	C-H def.
1390-1360	7.20-7.35	m., d.	Alkane, geminal dimethyl, isopropyl, tert. butyl sym. CH_3 bending	CH_3 def.
1380-1370	7.25-7.30	s.	Alkane, $-CH_3$	C-H def.
1380-1310	7.25-7.30	s.	Aliphatic nitro compounds	NO_2 str.
1370-1340	7.30-7.46	s.	Sulfonyl chlorides	S=O str.
1370-1300	7.30-7.70	s.	Aromatic nitro compounds	NO_2 str.
ca. 1365	ca. 7.33	s.	Alkane, tert. butyl	C-H def.
1360-1310	7.35-7.64	s.	Aromatic tert. amines	C-N vib.
1350-1300	7.41-7.69	s.	Sulfones, sulfonamides	S=O str.
1350-1280	7.41-7.81	s.	Aromatic sec. amines	C-N vib.
1350-1260	7.41-7.94	s.	Prim. and sec. alcohols	O-H def.
ca. 1340	ca. 7.46	w.	Alkanes	C-H def.
1340-1250	7.46-8.00	s.	Aromatic prim. amines	C-N vib.
1340-1180	7.46-8.48	w.	Azides	$-N_3$ str.
1335-1310	7.39-7.64	v.	Sulfur compounds	S=O str.
1310-1295	7.64-7.72	m.	Alkene ($R_1CH=CHR_2$) trans	C-H def.
1300-1250	7.70-8.00	s.	Nitrates	O- NO_2 vib.
1275-1200	7.84-8.33	v.	Conj. ethers	ROR str.
ca. 1270	ca. 7.88	v.	Aromatic esters	$\begin{array}{c} O \\ \\ -C-O-R \end{array}$ str.
1260-1200	7.94-8.33	v.	Aromatic ethers	R-O-Ar str.
1257-1232	7.95-8.12	v.	Aliphatic esters, CH_3COOR	

1255-1200	7.97-8.33	s., d.	Alkanes, tert. butyl	Skeletal str.
1240-1190	8.06-8.40	v.	Aromatic phosphorus comp.	P-O str.
1230-1150	8.13-8.70	s.	Sulfites	S=O str.
1210-1150	8.27-8.70	s.	Sulfonic acids	S=O str.
1220-1020	8.20-9.80	w.	Aliphatic amines	C-N vib.
ca. 1200	ca. 8.33	s.	Phenols	C-O str.
1200-1050	8.33-9.52	s.	Sulfur compounds	C=S str.
1200-1190	8.33-8.40	v.	Esters (RCOOR)	
1185-1175	8.44-8.51	v.	Esters (H-COOR)	
1185-1165	8.44-8.59	s.	Sulfonyl chlorides	S=O str.
1180-1140	8.48-8.77	s.	Sulfonamides	S=O str.
1175-1140	8.51-8.77	s.	Alkanes, geminal dimethyl	skeletal vib.
1175-1155	8.51-8.65	v.	Methyl esters (R-COOCH ₃)	
1175-1125	8.51-8.89	w.	Substituted benzenes, 1, 3-disubstituted or tri-substituted benzenes	C-H def.
1160-1140	8.62-8.77	s.	Sulfones	S=O str.
ca. 1150	ca. 8.70	s.	Tertiary alcohols	C-OH str.
1150-1070	8.70-9.35	v.	Aliphatic ethers	R-O-R str.
1120-1100	8.93-9.09	s.	Secondary alcohols	C-OH str.
1070-1030	9.35-9.71	s.	Sulfoxides	S=O str.
ca. 1060	ca. 9.40	m.	Allene (C=C=C)	
1060-1030	9.43-9.71	s.	Sulfonic acids	S=O str.
1075-1010	9.30-9.90	v.	Primary alcohols	C-OH str.
1050-990	9.52-10.1	v.	Phosphorus compounds	P-O str.
<u>1000-501</u>				
995-985	10.05-10.15	s.	Monosubstituted alkenes (RCH=CH ₂)	C-H def.
970-960	10.31-10.42	s.	Disubstituted alkenes (R ₁ CH=CHR ₂) trans	C-H def.
915-905	10.93-11.05	s.	Monosubstituted alkenes (RCH=CH ₂)	C-H def.
900-860	11.11-11.63	m.	Tetra-or penta-substituted benzene containing 1 free H	C-H def.
895-885	11.17-11.30	s.	Geminal disubstituted alkene	C-H def.

885-870	11.30-11.50	m.	1,2,4-trisubstituted benzene. another peak at 852-805	C-H def.
ca. 870	11.50 (Ca.)	m.	Pentasubstituted benzene	C-H def.
870-800	11.50-12.50	v.	Benzene ring containing two adjacent H atoms	C-H def.
840-790	11.90-12.66	s.	Trisubstituted alkenes	C-H def.
810-750	12.34-13.34	v.	Benzene ring with three adjacent H atoms	C-H def.
800-600	12.50-16.67	s.	Halides	C-Cl str.
770-735	12.98-13.61	v., s.	Benzene ring with four adjacent free H atoms	C-H def.
770-730	12.98-13.70	v., s.	Benzene ring with five adjacent free H atoms, second peak at 710-690	C-H def.
ca. 690	ca. 14.50	s.	Disubstituted alkenes (R ₁ CH=CHR ₂) cis	C-H def.
ca. 650	ca. 15.40	s.	Sulfonic acids	S=O str.
ca. 630	ca. 15.90	s.	Alkynes	C-H def.
600-500	16.60-20.00	s.	Bromides	C-Br str.
ca. 500	ca. 20.00	s.	Iodides	C-I str.

s.=strong absorption

v.=variable intensity

vib.=vibrating

bon.=bonded

m.=medium absorption

sh.=sharp peak

d.=doublet

sat.=saturated

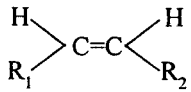
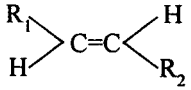
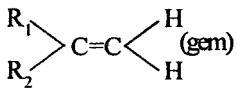
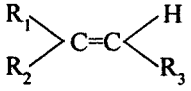
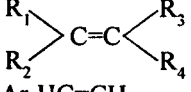
w.=weak absorption

br.=broad absorption

mlt.=multiplet

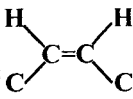
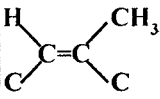
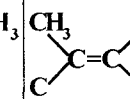
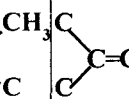
Table 2.2a: Infrared absorption frequencies of alkenes

Alkene type	Vibration mode	Frequency, cm ⁻¹	Wave length, μ	Relative intensity
RCH=CH ₂ (Vinyl)	C-H str. (CH ₂)	3095-3075	3.23-3.25	m
$\begin{array}{c} \text{H} \\ \diagdown \\ \text{C}=\text{C} \\ \diagup \\ \text{R} \end{array}$	C-H str. (CHR)	3040-3010	3.29-3.32	m
	Overtone	1850-1800	5.40-5.56	m
	C=C str.	1645-1640	6.08-6.10	v

	CH ₂ i-p def.	1430-1410	7.00-7.10	w
	CH i-p def.	1300-1290	7.69-7.75	v
	CH o-o-p def.	995-985	10.05-10.15	m
	CH ₂ o-o-p def.	915-905	10.93-11.05	s
R₁CH=CHR₂(cis)				
	C-H str.	3040-3010	3.29-3.32	m
	C=C str.	1665-1635	6.01-6.12	v
	C-H i-p def.	1430-1400	7.00-7.14	w
	C-H o-o-p def.	730-665	13.70-15.04	s
R₁CH=CHR₂(trans)				
	C-H str.	3040-3010	3.29-3.32	m
	C=C str.	1675-1665	5.97-6.01	v
	C-H i-p def.	1310-1290	7.63-7.75	w
	C-H o-o-p def.	980-960	10.20-10.42	s
R₁R₂C=CH₂ (Vinylidene)				
	C-H str.	3095-3075	3.23-3.25	m
	overtone	1800-1780	5.56-5.62	m
	C=C str.	1660-1640	6.02-6.10	v
	CH ₂ i-p def.	1420-1410	7.04-7.09	w
	CH ₂ o-o-p def.	895-885	11.17-11.30	s
R₁R₂C=CHR₃ (Trisubstituted)				
	C-H str.	3040-3010	3.29-3.32	m
	C=C str.	1675-1665	5.97-6.01	v
	C-H o-o-p def.	840-790	11.90-12.66	m
R₁R₂C=CR₃R₄ (Tetrasubstituted)				
	C=C str.	1690-1670	5.92-5.99	w
Ar-HC=CH ₂	C=C str.	~1625	~6.16	s
C=O or C=C				
Conjugated with				
C=C	C=C str.	1660-1580	6.02-6.33	s

Abbreviations: str. = stretching, i-p def. = in-plane deformation, o-o-p def. = out of plane deformation, s = strong, m = medium, w = weak, v = variable.

Table 2.2b: C=C Stretching frequencies in cyclic and acyclic systems cm^{-1}

Ring or Chain				
Chain cis	1661			
Chain trans	1676	1681	1672	1661
Three membered ring	1641		1890	1780
Four membered ring	1566		1685	1678
Five membered ring	1611	1658	1686	1657
Six membered ring	1649	1678	1685	1651
Seven membered ring	1651	1673		
Eight membered ring	1653			

All rings have cis double bonds

Table 2.3: Absorption frequencies typical of aromatic homocyclic compounds:

Aromatic compound	Vibration mode	Frequency, cm^{-1}	Wave-length, μ	Relative Intensity
Monosubstituted	=C-H str. (Multiple bands)	3080-3030	3.24-3.33	w-m
	C=C str. (ring stretching)	1604 \pm 3	6.25-6.22	v
		1585 \pm 3	6.31-6.30	v
		1510 \rightarrow 1480*	6.62 \rightarrow 6.75	v
		1452 \pm 4	6.87-6.91	v
	C-H i-p def.	1177 \pm 6(2,5 vs 3,6)	8.45-8.54	w
1156 \pm 5(3,5 vs 4)		8.61-8.69	w	
1073 \pm 4(2,6 vs 3,4,5)		9.28-9.36		
C-H o-o-p def.	1027 \pm 3(2,3 vs 5,6)	9.71-9.77	w	
	751 \pm 15	13.06-13.58	s	
	697 \pm 11	14.1-14.58	s	
1, 2-Disubstituted (four adjacent hydrogen atoms)	=C-H str. (multiple bands)	3080-3030	3.24-3.33	w-m
		1607 \pm 9	6.26-6.19	v
	C=C str. (ring stretching)	1577 \pm 4	6.33-6.36	v
		1510 \rightarrow 1460	6.85-6.62	v
		1447 \pm 10	6.87-6.96	v
C-H i-p def.	1269 \pm 17 (all clockwise)	7.77-7.99	w	

		1160 ± 4(3,5 vs 4,6)	8 59-8 65	w
		1125 ± 14(3,6 vs 4,5)	8 78-9 0	w
		1033 ± 11(3. 4 vs 5, 6)	9 58-9 78	w
	C-H o-o-p def.	751 ± 7	13 20-13 44	s
1:3 - Disubstituted (three adjacent hydrogen atoms)	=C-H str. (multiple bands)	3080-3030	3 24-3.33	w-m
	C=C str (ring stretching)	1600 → 1620	6 25 → 6.17	v
		1586 ± 5	6 29-6.32	v
		1495 → 1470	6.69 → 6 80	v
		1465 → 1430	6.83 → 6.99	v
	C-H i-p def.	1278 ± 12 (all clockwise)	7.75-7.90	w
		1157 ± 5 (2, 5 vs 4, 6)	8.60-8.68	w
		1096 ± 7 (4 vs 6)	9.07-9.18	w
		1076+7(2 vs s)	9.23-9.36	w
	C-H o-o-p def	900 → 869 (1 free H)	11 12-11.63	m
		782 ± 10 (3 adj H Wag)	12.82-12.96	s
		725 → 680 (3 adj. H wag)	13.79-14.71	m
1:4 Disubstituted (two adjacent hydrogen atoms)	=C-H str (multiple bands)	3080-3030	3.24-3.33	w-m
		1606 ± 6	6.20-6.25	v
	C=C str. (ring stretching)	1579 ± 6	6 31-6.36	v
		1520 → 1480	6 58 → 6.76	v
		1409 ± 8	7.05-7 15	v
	C-H i-p def	1258 ± 11 (all clockwise)	7.88-8 02	w
		1175 ± 6 (2, 5 vs 3,6)	8 47-8.56	w
		1117 ± 7 (2, 6 vs 3,5)	8.90-9.01	w
		1013 ± 5 (2, 3 vs 5,6)	9.82-9.92	w
	C-H o-o-p def.	817 ± 15	12.02-12.47	s
1:2:3- Trisubstituted	=C-H str. (multiple bands)	3080-3030	3.24-3.33	w-m
	C-H i-p def.	1175 → 1125	8.51 → 8.90	w
		1110 → 1070	9.01 → 9.35	w
		1070 → 1000	9.35 → 10.00	w
		1000 → 960	10.00 → 10.42	w
	C-H o-o-p def.	800 → 770	12.50 → 12.99	s
		720 → 685	13 90 → 14.60	m
1:2.4-Trisubstituted	=C-H str (multiple bands)	3080-3030	3 24-3 33	w-m
	C=C str (ring stretching)	1616 ± 8	6 15-6.22	v
		1577± 8	6 31-6 37	v
		1510 ± 8	6 60-6.66	v
		1456 ± 1	6 86-6 88	v

	C-H i-p def	1225 → 1175	8.16 → 8.51	w
		1175 → 1125	8.51 → 8.89	w
		1125 → 1090	8.89 → 9.18	w
		1070 → 1000	9.35 → 10.00	w
	C-H o-o-p def	900 → 860	11.11 → 11.63	m
		860 → 800	11.63 → 12.50	s
1.3.5-Trisubstituted	=C-H str (multiple bands)	3080-3030	3.24-3.33	w-m
	C-H i-p def.	1175 → 1125	8.51 → 8.89	w
		1070 → 1000	9.35 → 10.00	w
	C-H o-o-p def.	900 → 860	11.11 → 11.63	m
		865 → 810	11.56 → 12.30	s
		730 → 675	13.70 → 14.82	s
1:2:3 :4- Tetrasubstituted	=C-H str. (multiple bands)	3080-3030	3.24-3.33	w-m
	C-H o-o-p def	860 → 800	11.63 → 12.50	s
1:2:3:5; 1:2:4.5 and 1:2:3:4:5 substituted	=C-H str. (multiple bands)	3080-3030	3.24-3.33	w-m
	C-H o-o-p def	900 → 860	11.11 → 11.63	m

* The symbol 1510 → 1480 indicates the range, in cm^{-1} , of absorption of radiation. Usually an electron donor substituent causes absorption near 1510 cm^{-1} , while an electron acceptor substituent causes absorption near 1480 cm^{-1} .

Abbreviations: str. = stretching, i-p def. = in plane deformation, o-o-p def. = out of plane deformation, w = weak, m = medium, s = strong, v = variable, adj. = adjacent, wag = wagging.

Table 2.4: C = O stretching frequencies of carbonyl compounds

Type of carbonyl Compound	Typical examples (phase)	C=O st. fre. cm^{-1}	Value of absorption wavelength, μ
Acid anhydrides (RCOOCOR)			
a. Saturated, acyclic		1850-1800	5.41-5.56
		1790-1740	5.59-5.75
	Acetic anhydride (CCl_4)	1825 and 1754	5.48 and 5.70
b. Saturated, 5-membered ring		1870-1820	5.35-5.49
		1800-1750	5.56-5.71
	Succinic anhydride (CHCl_3)	1820 and 1776	5.49 and 5.63

c. α , β - Unsaturated and aryl, acyclic		1830-1780	5.47-5-62
		1770-1720	5.65-5-81
	Benzoic anhydride (CHCl_3)	1818 and 1740	5.50 and 5.75
d. α , β - Unsaturated, 5 membered ring		1850-1800	5.41-5.56
		1830-1780	5.47-5-62
Acid halides (RCOX)			
a. Acyl fluorides		~1850	~5.41
b'. Acyl chlorides	Acetyl chloride (CCl_4)	~1795	~5.57
		1812	5.52
	Isovaleryl chloride (Film)	1792	5.58
		~1810	~5.53
		1780-1750	5.61-5.72
		1750-1720(m)	5.72-5.82
c. Acyl bromides			
d. α , β - Unsaturated and aryl	Benzoyl chloride (CCl_4)	1739	5.75
e. COF_2		1928	5.19
f. COCl_2		1828	5.47
g. COBr_2		1828	5.47
Carboxylic acids (RCOOH)dimers			
a. Saturated aliphatic		1725-1700	5.80-5.88
	Butyric acid (monomer) (CCl_4)	1775	5.63
	Acetic acid (CCl_4)	1760	5.68
	Butyric acid (Film)	1721	5.81
	α - chloropropionic acid (Film)	1724	5.80
	n- Hexanoic acid (Film)	1698	5.89
b. α , β - unsaturated aliphatic		1715-1690	5.83-5.92
c. aryl		1700-1680	5.88-5.95
	Benzoic acid (KBr)	1678	5.96
	Salicylic acid (KBr)	1665	6.01
Esters (RCOOR)			
a. Saturated, acyclic		1750-1735	5.71-5.76

	Methyl acetate (CCl ₄)	1750	5.71
	Methyl propionate (CCl ₄)	1748	5.72
	Ethyl propionate (CCl ₄)	1736	5.76
	Propyl formate (CCl ₄)	1733	5.77
b. Saturated, cyclic			
	δ-lactones (and larger rings)	1750-1735	5.71-5.76
	γ-lactones	1780-1760	5.62-5.68
	β-lactones	~1820	~5.5
c. Unsaturated			
	vinyl ester type	1800-1770	5.56-5.65
	Vinyl acetate (CCl ₄)	1765	5.68
	α, β- unsaturated and aryl	1730-1717	5.78-5.82
	Ethyl cinnamate (CCl ₄)	1710	5.85
	α, β-unsaturated γ-lactone	1760-1740	5.68-5.75
	β-γ-unsaturated γ-lactone	~1800	~5.56
	d. α-keto esters	1755-1740	5.70-5.75
	e. β-keto esters (enolic)	~1650	~6.06
	f. Carbonates	1780-1740	5.62-5.75
Aldehydes (RCHO)			
	a. Saturated, aliphatic	1740-1720	5.75-5.81
	n-butanal (CCl ₄)	1736	5.76
	Acetaldehyde (CCl ₄)	1730	5.78
	Valeraldehyde (CCl ₄)	1730	5.78
	Isovaleraldehyde (Film)	1715	5.83
	o-Chlorobenzaldehyde (Film)	1695	5.90
	b. α, β- Unsaturated, aliphatic	1705-1680	5.87-5.95
	c. α, β- γ- δ- Unsaturated, aliphatic	1680-1660	5.95-6.02
	d. Aryl		
	p-anisaldehyde (CCl ₄)	1715-1695	5.83-5.90
	CCl ₄	1690	5.92
Ketones (RCOR)			
	a. Saturated acyclic	1725-1705	5.80-5.87
	Butanone (CCl ₄)	1724	5.80
	Acetone (CCl ₄)	1720	5.81
	2-Pentanone (CCl ₄)	1712	5.84
	Methyl isopropyl ketone Film	1709	5.85

b. Saturated, cyclic		
6-membered ring (and higher)	1725-1705	5.80-5.87
5-membered ring	1750-1740	5.71-5.75
4-membered ring	~1775	~5.63
c. α , β -Unsaturated, acyclic		
Methyl vinyl ketone (CCl_4)	1686	5.94-6.01
d. α , β -Unsaturated, cyclic		
6-membered ring (and higher)	1685-1665	5.94-6.01
5-membered ring	1725-1708	5.80-5.85
e- α , β , α^1 , β^1 -Unsaturated, acyclic	1670-1663	5.99-6.01
f. Aryl		
propiophenone (CCl_4)	1686	5.88-5.95
g. Diaryl		
Benzophenone (CHCl_3)	1669	5.99-6.02
h. α -Diketones		
	1730-1710	5.78-5.85
i. β -Diketones (enolic)		
	1640-1540	6.10-6.50
j. 1, 4-Quinones		
	1690-1660	5.92-6.02
k. Ketenes		
	~2150	~4.65
Amides		
a. Primary (RCONH_2)		
solid and concentrated solution	~1650	~6.06
dilute solution	~1690	~5.92
Acetamide (CHCl_3)	1670 and shoulder at 1716	5.97 and 5.83 (sh.)
b. Secondary (RCONHR)		
solid and concentrated solution	1680-1630	5.95-6.14
dilute solution	1700-1670	5.88-5.99
N-methyl acetamide (CCl_4)	1675 and shoulder at 1705	5.97 and 5.86 (sh.)
c. Tertiary, solid and all solutions		
N, N-dimethyl-(CCl_4) acetamide	1660 and shoulder at 1710	5.99-6.14 6.02 and 5.85 (sh.)

d. Cyclic, δ -lactams, dilute solution	~1680	~5.95
e. Cyclic, γ -lactams, dilute solution	~1700	~5.88
f. Cyclic, γ -lactams, fused to another ring, dilute solution	1750-1700	5.71-5.88
g. Cyclic, β -lactams, dilute solution	1760-1730	5.68-5.78
h. Cyclic, β -lactams, fused to another ring, dilute solution	1780-1770	5.62-5.65
i. Ureas, acyclic	~1660	~6.02
j. Ureas, cyclic, 6 membered ring	~1640	~6.10
k. Ureas, cyclic, 5-membered ring	~1720	~5.81
l. Urethanes	1740-1690	5.75-5.92
m. Imides, acyclic	~1710	~5.85
	~1700	~5.88
n. Imides, cyclic, 6-membered ring	~1710	~5.85
o. Imides, cyclic, α , β -unsaturated, 6-membered ring	~1730	~5.78
	~1670	~5.99
p. Imides, cyclic, 5-membered ring	~1770	~5.65
	~1700	~5.88
q. Imides, cyclic, α , β -unsaturated, 5-membered ring	~1790	~5.59
	~1710	~5.85

Table 2.5: Variation in frequency of vibrations of carbonyl stretching bands due to inter and intramolecular factors

Shift to higher frequency	Add cm^{-1}	Shift to lower frequency	Subtract cm^{-1}
Basic value in CCl_4 Solvent	1720	Neat solid or liquid state	10
Hydrocarbon solvents	7	CHCl_3 , CHBr_3 , CH_3CN (partially polar)	15
Ring strain		Ring strain	
Angle decreases 6 \rightarrow 5 ring	35	Angle increases 6 \rightarrow 7 to 10 ring	10

Bridged systems	15	Substitution on α -carbon	
Substitution on α -carbon (Field and inductive effects)		Each alkyl group	5
Substituent cis oriented and Coplanar		Alkyl groups substituted by amine	
–Cl, –Br, –OR	20	–NH ₂ (amide)	5
–OH, and –OAC		–NHMe (monosubstituted amide)	30
Substituent trans and nonplanar	Nil	–NMe ₂ (disubstituted amide)	55
Alkyl group substituted by electronegative atoms or groups		Intramolecular hydrogen bonding	
–H (aldehyde)	10	Weak: α or β -OH ketone	10
–OR (ester)	25	Medium: o -OH arylketone	40
–OH (monomeric acid)	40	Strong : β -diketone	100
–O–C=C (vinyl ester)	50	Intermolecular hydrogen bonding	
–Cl (acid chloride)	90	Weak: ROH....O=C<	15
–OCOR (anhydrides)	100	Strong: RCOOH dimer	45
		conjugation (depends on stereochemistry)	
		First C=C	30
		Second C=C	15
		Third C=C	Nil
		Benzene ring	20
		Vinylogous, –CO–C=C–X(X=Hor O)	40

Table 2.6: Vibration modes of amines and amino acids (frequency in cm^{-1})

Compound	N-H stretching		N-H deformation	C-N stretching	C=O stretching	C-O stretching	Other vibrations and remarks
	asym	sym					
Primary amines	3550-3350 (2.82-2.99 μ)	3450-3250 (2.90-3.08 μ)	1650-1580 (6.06-6.33 μ)	1220-1020 (ali) (8.2-9.8 μ) 1340-1250 (aro) (7.46-8.0 μ)			Shoulder at 3200 (3.12 μ), overtone of 1610 (6.21 μ) band N-H wagging strong band at 850-750 (11.76-13.34 μ)
Secondary amines	3550-3350 (2.82-2.99 μ)		1650-1550 (6.06-6.45 μ)	1350-1280 aro (7.41-7.81 μ)			N-H wagging strong band at 750-700 (13.34-14.29 μ) - N-H def. band often masked by aromatic band in aromatic compounds
Tertiary amines				1380-1260 aro (7.24-7.94 μ)			N-Me band in secondary and tertiary amines, observed at 2820-2760 (3.54-3.62 μ)
Amine hydrochloride chloride	About 3380, (2.96 μ) NH_3^+ str.		About 1600 (6.25 μ) asym.				

Compound	N-H stretching		N-H deformation	C-N stretching	C=O stretching	C-O stretching	Other vibrations and remarks
	asym	sym					
Charged amine derivatives	About 3280, (3.05 μ) NH ₃ ⁺ str. 3350-3150, NH ₃ ⁺ str. (2.99-3.17 μ) (12.5 μ) NH ₃ ⁺ solid phase		About 1300 (7.7 μ) sym. About 800 rock				
Primary amino acids	3125-3030 (3.2-3.3 μ)		1660-1610 band I (6.02-6.21 μ) 1550-1485 band II (6.45-6.74 μ)		1600-1560 ionized (6.25-6.41 μ) carboxyl str.		Weak band at 2760-2530 (3.62-3.96 μ) Medium band at 1300 (7.69 μ)
Dicarboxylic amino acids					1755-1720 (5.7-5.81 μ) unionised carboxyl str.		
Amino acid hydrochlorides	3130-3030 (3.2-3.3 μ)		1610-1590 band I (6.21-6.29 μ) 1550-1480 band II (6.45-6.75 μ)		1755-1730 (5.7-5.78 μ) Unionised carboxyl str.	1230-1215 (8.13-8.23 μ)	Series of bands between 3030 and 2500 (3.3 and 4.0 μ)
Amino acid sodium salts	3400-3200 (2.94-3.13 μ) Two bands				1600-1560 (6.25-6.14 μ) ionised carboxyl		

Table-2.7: Infrared Transmission characteristics of selected solvents and Mulling Oils(Transmission below 80% obtained with a 0-10 mm cell path is given in cm^{-1})

Solvent	Absorption (cm^{-1})
Acetone	3480-3340, 3180-2730, 1890-1060, 940-880, 805-790, 600-630
Acetonitrile	3260-2800, 2340-2180, 1600-1310, 1100-1000, 980-900, 815-740, 630-600
Benzene	3150-2960, 2000-1935, 1860-1790, 1545-1500, 1445-1365, 1190-1140, 1070-980, 865-845, 600-750
Benzonitrile	3150-2960, 2280-2160, 2000-1890, 1640-1285, 1215-1165, 1100-1000, 960-915, 600-820
Bis-2-(methyl ethyl) ether	3150-2580, 2000-1930, 1545-815, 600-635
Bromoform	3060-2960, 1190-1100, 600-800
Bromotrichloromethane	600-840
Butyl acetate	3150-2800, 1935-815, 780-755, 600-680
1-Butanol	3600-2500, 1600-600
Dibutyl ether	3040-2580, 1540-810, 775-740, 630-600
Carbondisulfide	2360-2100, 1625-1410, 690-600
Carbon tetrachloride	1570-1520, 840-720, 690-600
Chloroform	3060-2960, 1250-1180, 945-935, 830-600
Cyclohexane	3040-2580, 1510-1410, 1285-1250, 1060-1020, 910-860, 680-600

Solvent	Absorption (cm^{-1})
Cyclopentane	3060-2730, 1520-1410, 1340-1310, 925-870, 645-600
1,2-Dichloroethane	3150-2960, 1500-1435, 1370-1230, 1050-1070, 975-875, 765-600
Diethyl ether	3060-2600, 2000-1965, 1525-1000, 960-895, 870-790, 635-600
1,4-Dioxane	3060-2650, 2000-1965, 1460-1075, 940-825, 690-600
Dodecane	3060-2650, 1460-1290, 755-695, 665-600
Hexane	3060-2650, 1525-1330, 900-885, 780-720, 635-600
Tetrachloro ethylene	1060-1035, 960-885, 830-745, 680-600
1,1-Trichloro-trifluoroethane	1415-1345, 1270-780, 700-600
2,2,4-Trimethylpentane	3040-2550, 1520-1175, 1000-975, 645-600
Water	3650-2930, 1750-1580, 930-600
Mulling Oils	Absorption (cm^{-1})
Nujol®	3030-2860, 1460-1386, 720
Hexachlorobutadiene	1650-1500, 1280-1200, 1020-760
Fluorolube®	1350-650

Problems: (1) The IR spectrum of an organic compound $\text{C}_6\text{H}_7\text{N}$ shows the following bands:

3030(w); 2920(w); 2217(s); 1607(m); 1607(m); 1508(m); 817(s)

What is its structure?

C_8H_7N Index = 6* (Probably aromatic)

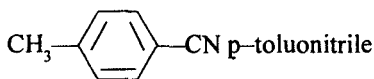
* [For a molecule ($C_wH_xN_yO_z$, the total number of rings and double bonds is obtained by the formula $R = 1/2 (2w - x + y + 2)$

Here M.F. = $C_8H_7N = R = 1/2 (16 - 7 + 1 + 2) = 6$.

The presence of one benzene ring in the structure requires atleast four unsaturation sites (3 double bonds + 1 ring)]

3030 cm^{-1} ; 1607 cm^{-1} ; 1508 cm^{-1} aromatic 2217 cm^{-1} ; CN rather than $C\equiv C$ which gives a weak band CN, C_7H_7 Index 2

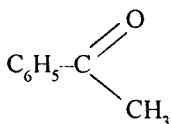
The band at 2920 cm^{-1} is weak. Since alkyl groups give a strong band in this region, it may be concluded that such groups are absent or are very few in number. This is supported by the fact that CN accounts for an index value of 2 and the remaining index (4) must be in the C_7H_7 unit. This can be a heptatriene or a phenyl ring. But the presence of a band at 2920 cm^{-1} , though weak, indicates the presence of atleast one alkyl unit, hence heptatriene ring is absent and C_7H_7 is a toluyl unit. The very strong band at 817 cm^{-1} may be ascribed to out of plane bending vibrations of two -ArH atoms and hence, the compound is a p-disubstituted benzene and the structure of the compound is



(2) Identify the structure of the compound C_8H_8O whose spectrum contains the following absorption bands:

1680(s), 1600(m), 1580(m), 1450(m), 1430(s), 1360(s), 1265(s), 755(s), 690(s) cm^{-1} .

The empirical formula suggests the following structure for the compound:



The IR spectral bands agree with this structure. The monosubstituted benzene ring has the characteristic bands at 1600, 1580, 1450, 750 and 690 cm^{-1} , the characteristic bands for the aromatic ketone are at 1680 and 1275 cm^{-1} , and those for the methyl group are at 1430 and 1360 cm^{-1} .

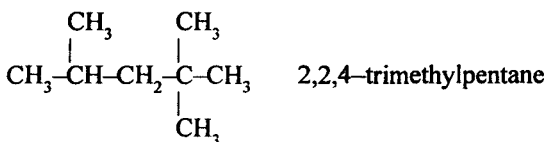
(3) Deduce the structure:

C_8H_{18} IR bands (cm^{-1}) 2960; 2860; 1460;
1395; 1385;
1375; 1365

Several bands in finger print region, i.e., a branched alkane. The latter four bands are two doublets— indicating isopropyl and tert-butyl groups

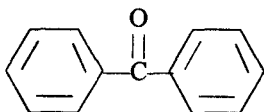
$[(\text{CH}_3)_2\text{CH}]$ $[\text{C}(\text{CH}_3)_3]\text{CH}_2$

Therefore, the compound is

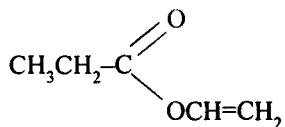


(4) From the following examples, we can readily see the usefulness of Table 2.5 in predicting the values of $\text{C}=\text{O}$ absorption bands. The wavenumbers for $\text{C}=\text{O}$ stretching vibrations for a number of compounds are calculated as follows:

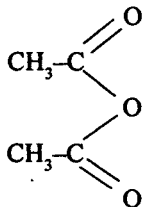
a. Benzophenone in chloroform



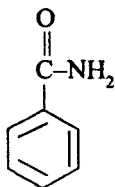
Basic value for $\text{C}=\text{O}$ absorption	1720 cm^{-1}
Shift due to benzene rings 2×20	- 40 cm^{-1}
Shift due to solvent CHCl_3	- 15 cm^{-1}
<hr/>	
Calculated	1665 cm^{-1}
Observed	1669 cm^{-1}

b. Vinyl propionate in CCl_4 

Basic value for C=O absorption	1720 cm^{-1}
Vinyl ester ($-\text{O}-\text{C}=\text{C}$) shift	+ 50 cm^{-1}
Alkyl group on a carbon	- 5 cm^{-1}
Calculated	1765 cm^{-1}
Observed	1760 cm^{-1}

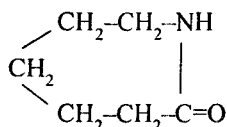
c. Acetic anhydride in CCl_4 

Basic value for C=O absorption	1720 cm^{-1}
Anhydride ($-\text{O}-\text{COR}$)	+ 100 cm^{-1}
Calculated	1820 cm^{-1}
Observed	1825 cm^{-1}

d. Benzamide in CHCl_3 

Basic value for C=O absorption	1720 cm^{-1}
Alkyl group substituted by NH_2	- 5 cm^{-1}
Alkyl group substituted by benzene	- 20 cm^{-1}
Solvent polarity effect	- 15 cm^{-1}
Hydrogen bonding about	- 15 cm^{-1}
Calculated	1665 cm^{-1}
Observed	1667 cm^{-1}

e. Caprolactam neat liquid



Basic value for C=O absorption	1720 cm ⁻¹
Alkyl group substituted by NHMe	- 30 cm ⁻¹
Alkyl group on α carbon	- 5 cm ⁻¹
seven member ring	- 10 cm ⁻¹
Neat liquid	- 10 cm ⁻¹
Calculated	1665 cm ⁻¹
Observed	1667 cm ⁻¹

(5) Suppose that you are investigating a compound with the molecular formula C₄H₆O₂. You find that it contains an ester carbonyl and -ene group. You determine this on the basis of the following bands in the IR spectrum of a CCl₄ solution of the compound. 3030 cm⁻¹ (weak), 1765 cm⁻¹ (strong), 1649 cm⁻¹ (strong), 1225 cm⁻¹ (strong) and 1140 cm⁻¹ (strong). Identify these bands, write all the possible structures which include these two groups, and identify the compound.

Answer: Identification of the bands:

3030 cm⁻¹ C-H str. in terminal RHC=CH₂ (CHR group)

1765 cm⁻¹ C=O str.

1649 cm⁻¹ C=C str. (terminal)

1225 cm⁻¹ C-O-C str. (asym.)

1140 cm⁻¹ C-O-C str. (sym.)

For a compound with the molecular formula C₄H₆O₂, only two structures with an -ene and an ester carbonyl group can be written.

(a) $\text{CH}_2 = \text{CH} - \text{C} \begin{array}{l} \text{=O} \\ \text{O} \end{array} - \text{CH}_3$ methyl acrylate (an α, β-unsaturated ester)

(b) $\text{CH}_3 - \text{C} \begin{array}{l} \text{=O} \\ \text{O} \end{array} \cdot \text{CH} = \text{CH}_2$ vinyl acetate

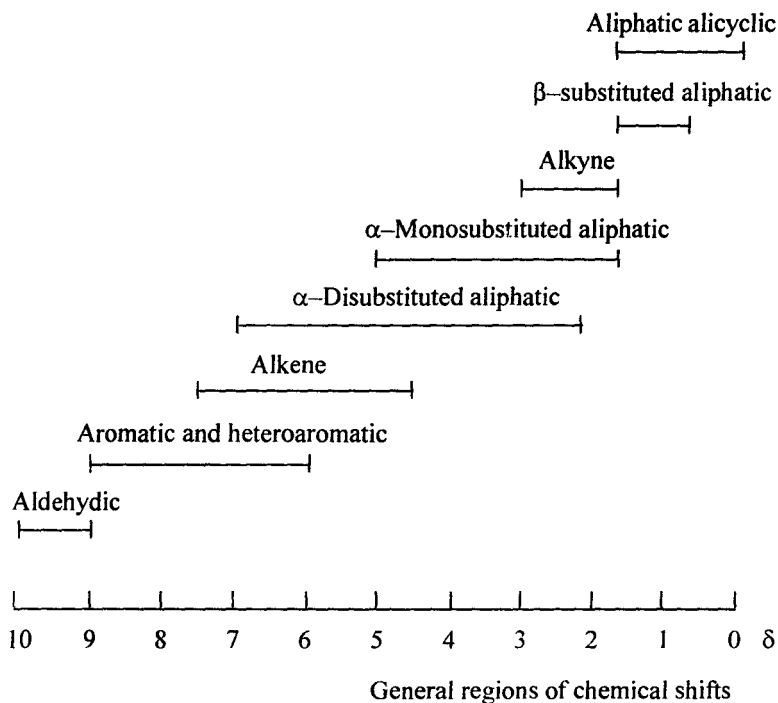
The two structures can be distinguished on the basis of their C=O stretching frequencies. We can calculate C=O stretching frequency in each case

a)	Basic value	1720 cm ⁻¹	since the observed value is 1765 cm ⁻¹ the compound is (b)
	OR (ester)	+ 25 cm ⁻¹	
	conjugation (C=C)	- 30 cm ⁻¹	
	Calculated	1715 cm ⁻¹	
b)	Basic value	1720 cm ⁻¹	
	-O-C=C (vinyl ester)	+ 50	
	Calculated	1770 cm ⁻¹	

□□□

3

Proton Magnetic Resonance Spectroscopy



3.1 Effect on shift positions of a single functional group

Table 3.1: Chemical Shifts of Methyl, Methylene and Methine protons (α to the functional groups) in δ

Functional group X	CH_3X	$-\text{CH}_2\text{X}$	$-\text{CHX}$
H	0.23	0.90	1.25
CH_3 or CH_2-	0.86	1.2	1.55
$\text{C}=\text{C}-$	1.6	2.1	
$\text{C}\equiv\text{C}-$	1.7	2.2	2.8
Ph	2.25	2.6	2.85
F	4.26	4.45	4.8
Cl	3.05	3.5	4.05
Br	2.7	3.4	4.1
I	2.16	3.15	4.25
OH	3.2	3.4	3.8
OR	3.2	3.4	3.6
OPh	3.82	4.05	4.55
OCOR	3.62	4.1	4.95
OCOPh	3.82	4.2	5.05
OTs*	3.7	3.9	4.65
CHO	2.2	2.39	2.5
COR	2.1	2.35	2.64
$\text{C}-\text{OPh}$	2.4	2.74	3.4
COOH	2.1	2.3	2.54
COOR	2.0	2.25	2.5
CONR_2	2.0	2.26	2.4
$\text{C}\equiv\text{N}$	2.15	2.45	2.85
NH_2	2.52	2.7	3.04
NR_2	2.22	2.4	2.84
NPhR	2.6	3.04	3.6
N^+R_3	2.95	3.04	3.6
NHCOR	2.95	3.34	3.8

Functional group X	CH ₃ X	-CH ₂ X	-CHX
NO ₂	4.08	4.15	4.4
N=C	2.92	3.3	4.9
N=C=O		3.3	
O-C≡N		4.6	
N=C=S	3.4	3.7	4.0
S-C≡N	2.72	3.0	3.3
O-N=O		4.8	
SH	2.1	2.6	3.1
SR	2.1	2.6	3.12
SPh	2.52		
SSR	2.4	2.72	
SOR	2.6	3.1	
SO ₂ R		3.1	
SO ₃ R	3.0		
PR ₂		2.4	
P ⁺ Cl ₃	3.32	3.4	
POR ₂		2.4	
PSR ₂		2.8	

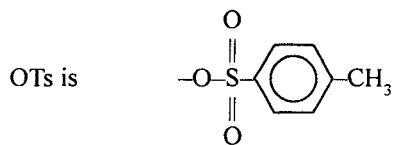
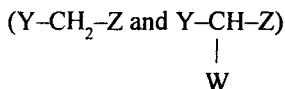


Table 3.2: Chemical shifts of Methyl, Methylene and Methine protons (β - to the functional groups) in δ

Functional group X	$\text{CH}_3\text{-C-X}$	$\text{-CH}_2\text{-C-X}$	-CH-C-X
$\text{CH}_2\text{-}$	0.86	1.2	1.55
C=C-	1.0	1.36	1.76
$\text{C}\equiv\text{C-}$	1.2	1.5	1.8
Ph	1.16	1.55	1.8
F	1.55	1.85	2.15
Cl	1.55	1.8	1.95
Br	1.8	1.85	1.9
I	1.76	1.8	2.1
OH	1.2	1.5	1.76
OR	1.2	1.5	1.76
OPh	1.3	1.55	2.0
OCOR	1.3	1.6	1.8
OCOPh	1.65	1.75	1.95
OCOCF_3	1.4	1.65	
CHO	1.1	1.65	
COR	1.05	1.55	1.95
COPh	1.16	1.56	1.9
COOR	1.16	1.7	1.9
CONR_2	1.1	1.5	1.8
$\text{C}\equiv\text{N}$	1.25	1.65	2.0
NR_2	1.05	1.45	1.7
NPhR	1.1	1.5	1.8
NR_3^+	1.4	1.75	2.05
NHCOR	1.1	1.5	1.9
NO_2	1.61	2.05	2.5
SH	1.3	1.6	1.66
SR	1.25	1.6	1.9

3.2 Effect on chemical shifts of two or three functional groups:



Shoolery's rules permit calculation of a shift position of a methylene group attached to two functional groups by the additive effect of the shielding constants in Table 3.3. The sum of the constants is added to δ 0.23, the position for CH_4

$$\therefore \delta = 0.23 + \Sigma\sigma_i$$

Thus, to calculate the shift for the $-\text{CH}_2-$ protons of $\text{C}_6\text{H}_5\text{CH}_2\text{Br}$

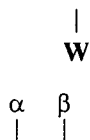
$$\begin{array}{rcl} \text{C}_6\text{H}_5 & = & 1.85 \\ \text{Br} & = & \underline{2.33} \\ & & \mathbf{4.18} \\ \text{add CH}_4 & & \underline{\mathbf{0.23}} \\ & & \mathbf{4.41} \end{array}$$

Table 3.3: Shielding constants

Functional group Y or Z	Shielding Constants σ_i
CH_3	0.47
$\text{C}=\text{C}$	1.32
$\text{C}\equiv\text{C}$	1.44
Ph	1.85
CF_2	1.21
CF_3	1.14
Cl	2.53
Br	2.33
I	1.82
OH	2.56
OR	2.36
OPh	3.23
OCOR	3.13
COR	1.70
COPh	1.84
COOR	1.55
CONH_2	1.53
CONR_2	1.59
$\text{C}\equiv\text{N}$	1.70

This chart can be used to find the shift position of a methylene group attached to two functional groups from the δ values in the box at the intersection of the horizontal and diagonal groups ("mileage chart"). The upper number in each box is an experimental value; the lower number is calculated from Shoolery's constants.

Table 3.4 can be used to calculate chemical shifts of methyl ($Y-CH_3$), methylene ($Y-CH_2-Z$), or methine ($Y-CH-Z$) groups.



Thus, the CH_2 chemical shifts in $BrCH_2CH_2OCH_2CH_2Br$ can be calculated.

CH_2 No. 1	
CH_2 (Table 3, 4, footnote a)	1.20
α -OR	2.35
β -Br	<u>0.60</u>
	4.15
CH_2 No. 2	
CH_2	1.20
α -Br	2.18
β -OR	<u>0.15</u>
	3.53
Determined: CH_2 No. 1 at $\sim\delta$ 3.80;	
CH_2 No. 2 at $\sim\delta$ 3.40	

Table 3.4: Substituent Effects on Chemical Shift C-C-H

Substituent	Type of Hydrogen ^a		
		Alpha shift	Beta shift
-C=C-	CH_3	0.78	
	CH_2	0.75	0.10
	CH		

Substituent	Type of Hydrogen ^a	Alpha shift	Beta shift
$\begin{array}{c} -C=C-C-R \\ \\ X \end{array}$	CH ₃	1.08	
(X=C or O)	CH ₃	1.40	0.35
Aryl	CH ₂	1.45	0.53
	CH	1.33	
-Cl	CH ₃	2.43	0.63
	CH ₂	2.30	0.53
	CH	2.55	0.03
-Br	CH ₃	1.80	0.83
	CH ₂	2.18	0.60
	CH	2.68	0.25
-I	CH ₃	1.28	1.23
	CH ₂	1.95	0.58
	CH	2.75	0.00
-OH	CH ₃	2.50	0.33
	CH ₂	2.30	0.13
	CH	2.20	
-OR (R is saturated)	CH ₃	2.43	0.33
	CH ₂	2.35	0.15
	CH	2.00	
$\begin{array}{c} O \quad O \\ \quad \\ -O-C-R, -O-C-OR \end{array}$	CH ₃	2.88	0.38
-OAr	CH ₂	2.98	0.43
	CH	3.43 (esters only)	
$\begin{array}{c} O \\ \\ -CR, \text{ Where R is alkyl,} \\ \text{aryl, OH, OR', H, CO, or N} \end{array}$	CH ₃	1.23	0.18
	CH ₂	1.05	0.31
	CH	1.05	
-NRR'	CH ₃	1.30	0.13
	CH ₂	1.33	0.13
	CH	1.33	

^a standard positions are CH₃, δ 0.87; CH₂, δ 1.20; CH, δ 1.55.

3.3: Chemical Shifts in Alicyclic and Heterocyclic Rings

Table 3.5: Chemical shifts in Alicyclic Rings

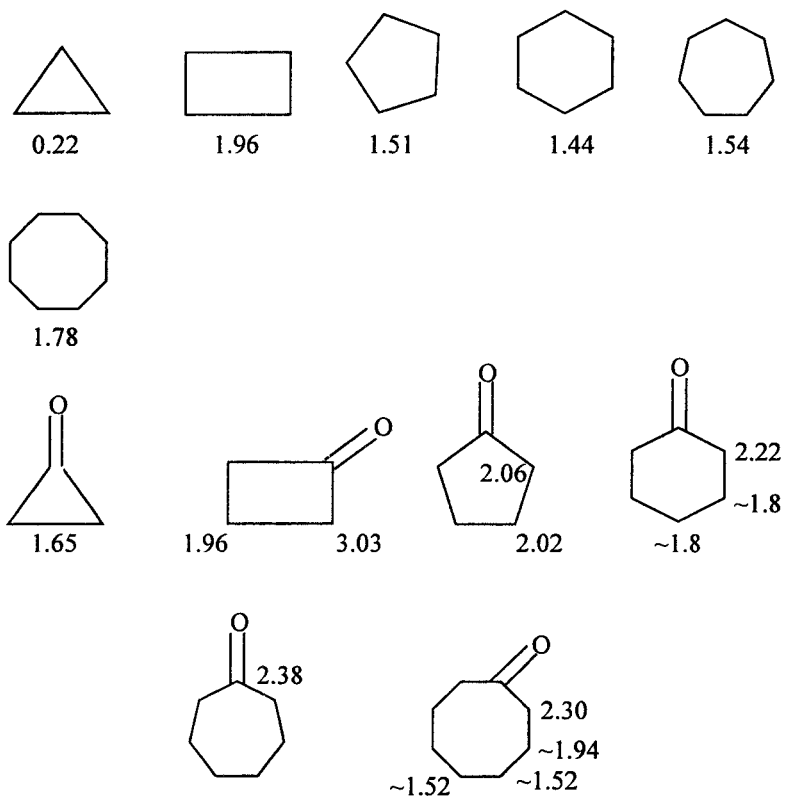
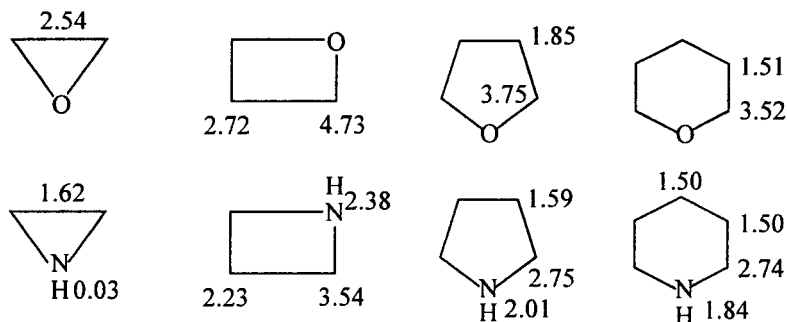
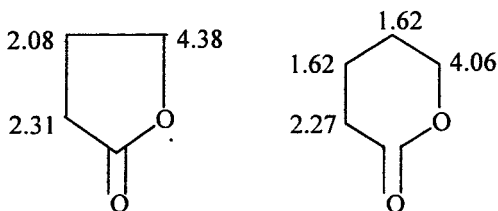
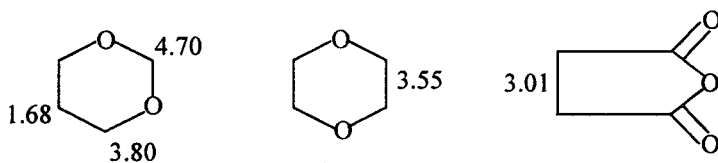
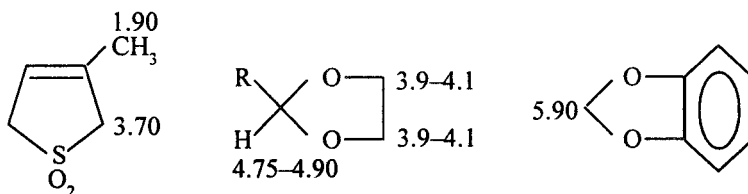
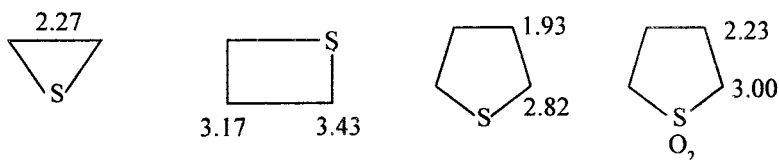
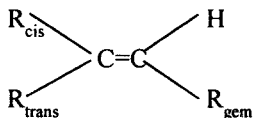


Table 3.6: Chemical Shifts in Heterocyclic Rings





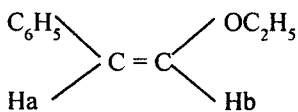
3.4: Chemical Shifts in Unsaturated and Aromatic Systems



$$\delta H = 5.25 + \sum z_i$$

i.e. $5.25 + Z_{gem} + Z_{cis} + Z_{trans}$




For example, the chemical shifts of the alkene protons in

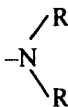
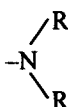


are calculated

Ha	C ₆ H ₅ gem	1.35	5.25
	OR trans	<u>-1.28</u>	<u>0.07</u>
		0.07	δ,5.32
Hb	ORgem	1.18	5.25
	C ₆ H ₅ trans	<u>-0.10</u>	<u>1.08</u>
		1.08	δ 6.33

Table 3.7: Substituent Constants (Z) for chemical shifts of substituted Ethylenes (in CCl₄)

Substituent R	Z		
	gem	cis	trans
-H	0	0	0
-Alkyl	0.44	-0.26	-0.29
-Alkyl ring ^a	0.71	-0.33	-0.30
-CH ₂ O, -CH ₂ I	0.67	-0.02	-0.07
-CH ₂ S	0.53	-0.15	-0.15
-CH ₂ Cl, -CH ₂ Br	0.72	0.12	0.07
-CH ₂ N	0.66	-0.05	-0.23
-C≡C	0.50	0.35	0.10
-C≡N	0.23	0.78	0.58
-C=C	0.98	-0.04	-0.21
-C=C conj ^b	1.26	0.08	0.01
-C=O	1.10	1.13	0.81
-C=O conj ^b	1.06	1.01	0.95
-COOH	1.00	1.35	0.74
-COOH conj ^b	0.69	0.97	0.39
-COOR	0.84	1.15	0.56
-COOR conj ^b	0.68	1.02	0.33
	1.03	0.97	1.21
	1.37	0.93	0.35
	1.10	1.41	0.99
-OR, R: aliph	1.18	-1.06	-1.28

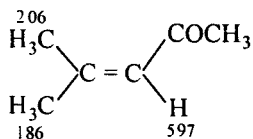
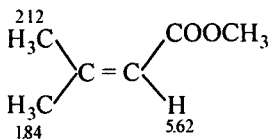
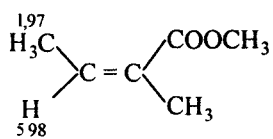
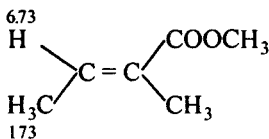
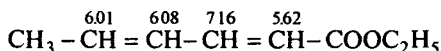
-OR, R: Conj ^b	1.14	-0.65	-1.05
-OCOR	2.09	-0.40	-0.67
-Aromatic	1.35	0.37	-0.10
-Cl	1.00	0.19	0.03
-Br	1.04	0.40	0.55
 R : aliph	0.69	-1.19	-1.31
 R : Conj ^b	2.30	-0.73	-0.81
-SR	1.00	-0.24	-0.04
-SO ₂	1.58	1.15	0.95

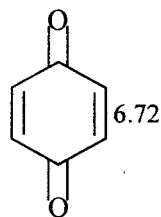
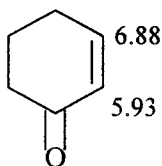
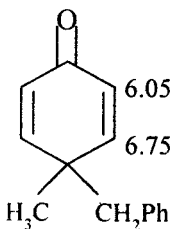
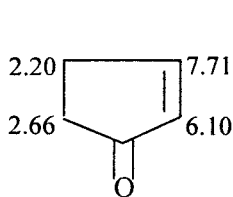
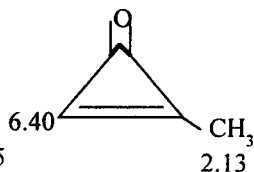
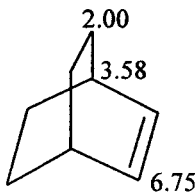
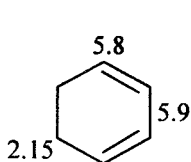
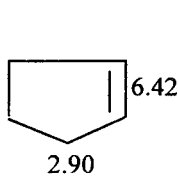
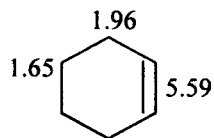
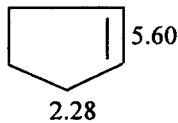
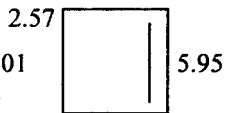
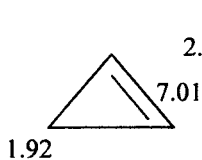
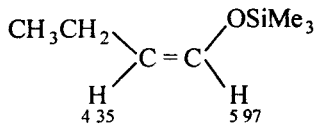
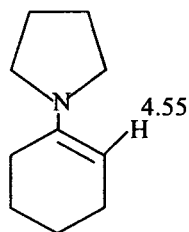
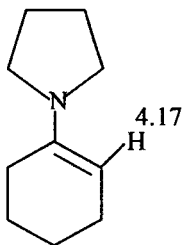
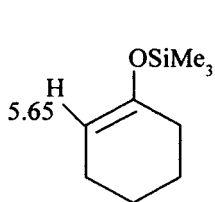
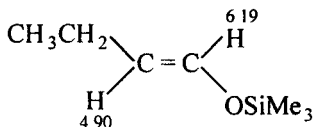
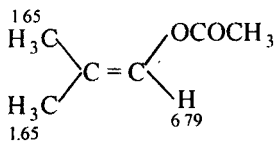
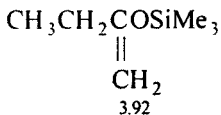
^a Alkyl ring indicates that the double bond is part of the ring

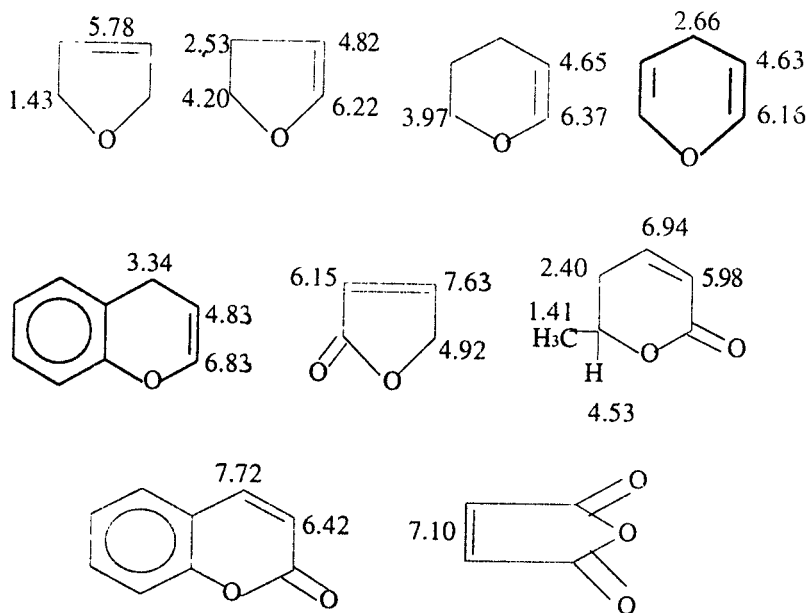


^b The Z factor for the conjugated substituent is used when either the substituent or the double bond is further conjugated with other groups.

Table 3.8: Chemical Shifts of Miscellaneous Alkenes





**Table 3.9: Chemical Shifts of Alkyne Protons**

$\text{HC}\equiv\text{CR}$	1.73–1.88
$\text{HC}\equiv\text{C}-\text{COH}$	2.23
$\text{HC}\equiv\text{C}-\text{C}\equiv\text{CR}$	1.95
$\text{HC}\equiv\text{CH}$	1.80
$\text{HC}\equiv\text{CAr}$	2.71–3.37
$\text{HC}\equiv\text{C}-\text{C}\equiv\text{CR}$	2.60–3.10

Table 3.10: Chemical Shifts of Protons on Monosubstituted Benzene Rings

Benzene	7.25
CH_3 (omp)	7.16
CH_3CH_2 (omp)	7.16
$(\text{CH}_3)_2\text{CH}$ (omp)	7.16
$(\text{CH}_3)_3\text{C}$ (o, m, p)	7.32, 7.17, 7.04
$\text{C}=\text{CH}_2$ (omp)	7.25
$\text{C}\equiv\text{CH}$ o, (mp)	7.44, 7.25
Phenyl o, m, p	7.44, 7.25, 7.16
CF_3 (omp)	7.50
CH_2Cl (omp)	7.25
CHCl_2 (omp)	7.36
CCl_3 o, (mp)	8.10, 7.50

CH ₂ OH (omp)	7.16
CH ₂ OR (omp)	7.25
CH ₂ OCOCH ₃ (omp)	7.25
CH ₂ NH ₂ (omp)	7.32
F m, p, o	7.25, 7.04, 6.95
Cl (omp)	7.25
Br, o, (pm)	7.51, 7.25
I o, p, m	7.71, 7.25, 7.04
OH m, p, o	7.04, 6.90, 6.75
OR m, (op)	7.36, 7.00
OCOCH ₃ (mp), o	7.25, 7.04
OTs ^a (mp), o	7.25, 7.04
CHO o, p, m	7.95, 7.64, 7.50
COCH ₃ o, (mp)	7.90, 7.55
COOH o, p, m	7.90, 7.44, 7.36
COOR o, p, m	8.16, 7.55, 7.44
COCl o, p, m	8.10, 7.55, 7.44
C≡N	7.55
NH ₂ , m, p, o	7.16, 6.84, 6.50
N(CH ₃) ₂ m (op)	7.16, 6.70
NHCORo	7.50
NH ₃ ⁺ o	7.64
NO ₂ o, p, m	8.23, 7.71, 7.55
SR (omp)	7.25
N=C=O (omp)	7.04

^aOTs = p – Toluenesulfonyloxy group

Table 3.11: Chemical shifts of protons on fused aromatic rings

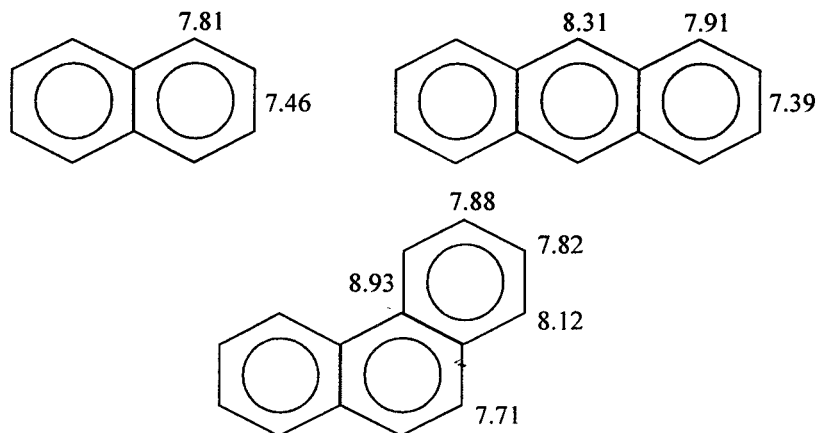
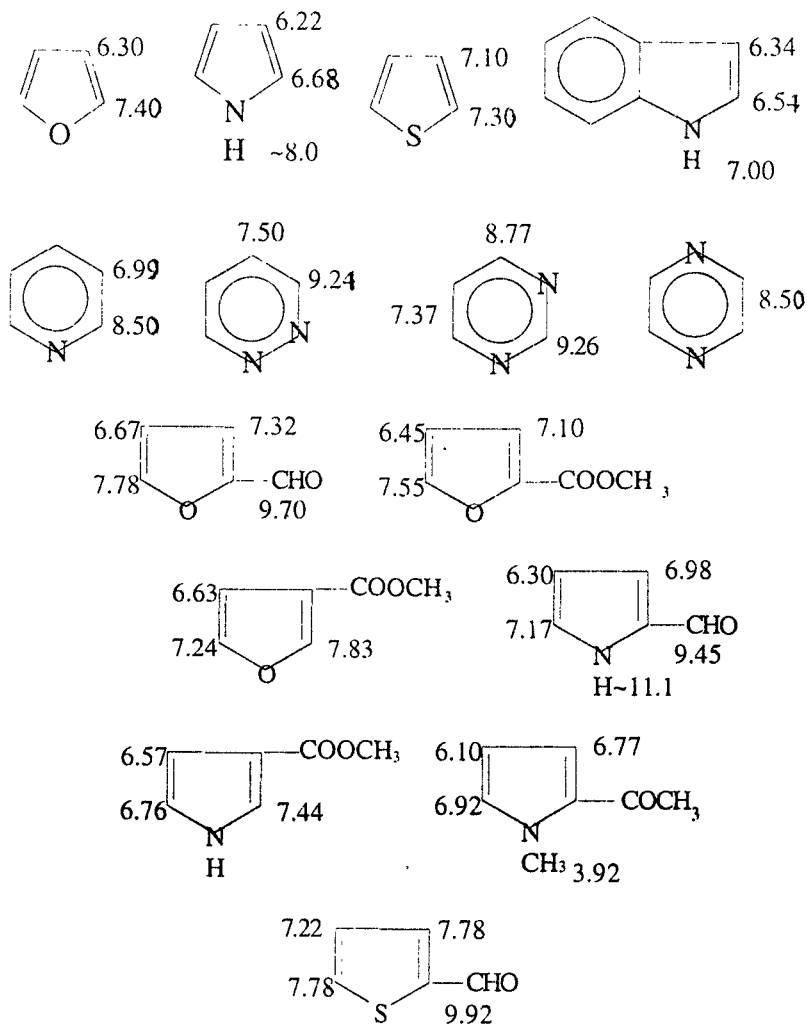
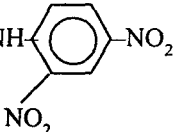


Table 3.12: Chemical shifts of protons on Heteroaromatic Rings**Table 3.13: Chemical Shifts of HC=O, HC=N, (also HC(O)₂) Protons**

RCH=O	9.70
PhCH=O	9.98
RCH=CHCH=O	9.78

HCOOR	8.05
HCONR ₂	8.05
HC(OR) ₃	5.00
RCH = NOH cis	7.25
RCH = NOH trans	6.65

RCH=N-NH-  -NO ₂	6.05
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3.5: Protons on Heteroatoms

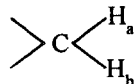
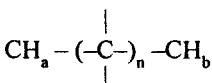
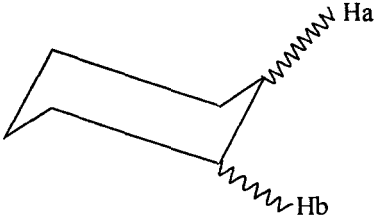
Table 3.14: Protons subject to Hydrogen Bonding Effects (protons on Heteroatoms)^a

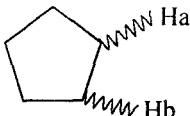
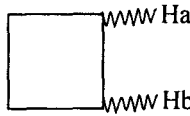
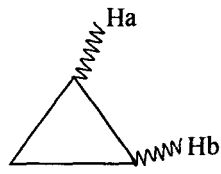
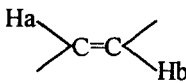
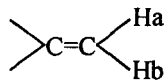
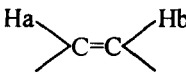
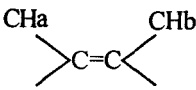
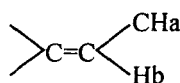
Proton	Class	δ
OH	Carboxylic acids	~13.2- ~10.0
	Sulfonic acids	12.0-10.0
	Phenols	~7.5- ~4.0
	Phenols (intramolecular H bond)	12.5-5.5
	Alcohols	4.0-0.5
	In DMSO	6.2-4.2
	Enols (cyclic α - diketones)	6.9-6.0
	Enols (β - diketones)	16.5-14.5
	Enols (β - ketoesters)	10.6-9.6
	Water (Bulk water as suspended droplets or wall films)	5.0-4.5
	Dissolved (monomeric) Water	1.5
	in acetone	2.9-2.5
	in DMSO	3.4-3.2
	Oximes	12.0-9.0

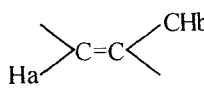
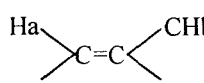
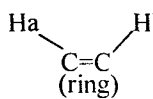
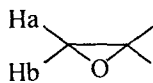
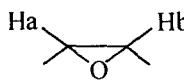
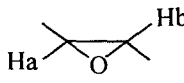
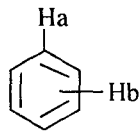
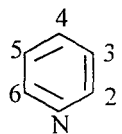
Proton	Class	δ
NH ₂ and NHR	Alkyl and cyclic amines	3.0–0.5
	Aryl amines	5.0–3.0
	Amides	8.7–5.0
	Urethanes	7.6–4.6
	Amines in trifluoroacetic acid	8.7–6.0
SH	Aliphatic mercaptans	1.7–1.3
	Thiophenols	3.6–2.8

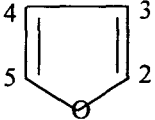
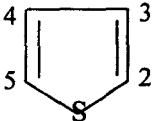
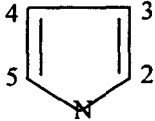
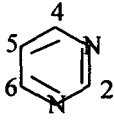
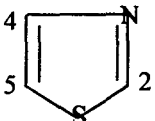
^a Solvent CDCl₃. Chemical shifts within a range are a function of concentration (The upper limit represents neat liquids, the lower limit, dilute solutions or extrapolations to infinite dilution)

3.6: Proton Spin Coupling Constants

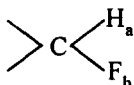
Type	Jab (Hz)	Jab Typical
Geminal 	0–30	12–15
Vicinal CH _a – CH _b (free rotation)	6–8	7
 CH _a – (–C–) _n – CH _b	0–1	0
		
ax–ax	6–14	8–10
ax–eq	0–5	2–3
eq–eq	0–5	2–3

	cis 5-10	
(cis or trans)	trans 5-10	
	cis 4-12	
(cis or trans)	trans 2-10	
	cis 7-13	
(cis or trans)	trans 4-9	
$\text{CH}_a\text{-OH}_b$ (no exchange)	4-10	5
$\begin{array}{c} \text{O} \\ \\ >\text{CH}_a\text{-CH}_b \end{array}$	1-3	2-3
$\begin{array}{c} \text{O} \\ \\ \text{C}=\text{CH}_a\text{-CH}_b \end{array}$	5-8	6
	12-18	17
	0-3	0-2
	6-12	10
	0-3	1-2
	4-10	7

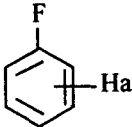
		0-3	1.5
		0-3	2
$C=CHa-CHb=C$		9-13	10
	3 member		0.5-2.0
	4 member		2.5-4.0
	5 member		5.1-7.0
	6 member		8.8-11.0
	7 member		9-13
	8 member		10-13
$HaC\equiv CHb$		9.5-9.8	9.1
$CHa-C\equiv CHb$		2-3	
$-CHa-C\equiv C-CHb$		2-3	
			6
			4
			2.5
	J (ortho)	6-10	9
	J (meta)	1-3	3
	J (para)	0-1	~0
	J (2-3)	5-6	5
	J (3-4)	7-9	8
	J (2-4)	1-2	1.5
	J (3-5)	1-2	1.5
	J (2-5)	0-1	1
	J (2-6)	0-1	~0

	J (2-3)	1.3-2.0	1.8
	J (3-4)	3.1-3.8	3.6
	J (2-4)	0-1	~0
	J (2-5)	1-2	1.5
	J (2-3)	4.9-6.2	5.4
	J (3-4)	3.4-5.0	4.0
	J (2-4)	1.2-1.7	1.5
	J (2-5)	3.2-3.7	3.4
	J (1-2)	2-3	
	J (1-3)	2-3	
	J (2-3)	2-3	
	J (3-4)	3-4	
	J (2-4)	1-2	
	J (2-5)	1.5-2.5	
	J (4-5)	4-6	
	J (2-5)	1-2	
	J (2-4)	0-1	
	J (4-6)	2-3	
	J (4-5)	3-4	
	J (2-5)	1-2	
	J (2-4)	~0	
$\text{CH}_3\text{-CH}_2\text{-X}$		6.5-7.5	
$\begin{array}{l} \text{CH}_3 \\ \diagdown \\ \text{C} \\ \diagup \\ \text{CH}_3 \end{array} \text{-CH-X}$		5.5-7.0	

Proton Fluorine



44-81

$\begin{array}{c} \\ > \text{CHa}-\text{CFb} \\ \end{array}$	3-25
$\begin{array}{c} & & \\ > \text{CHa}-\text{C}-\text{CFb} \\ & & \end{array}$	0-4
$\begin{array}{c} > \text{C}=\text{C} < \\ \text{Ha} \quad \quad \quad \text{Fb} \end{array}$	1-8
$\begin{array}{c} > \text{C}=\text{C} < \\ \text{Ha} \quad \quad \quad \text{Fb} \end{array}$	12-40
	o-6-10 m-5-6 p-2

Proton Phosphorus

$\begin{array}{c} \text{O} \\ \\ > \text{PH} \end{array}$	630-707
$(\text{CH}_3)_3\text{P}$	2.7
$(\text{CH}_3)_3\text{P}=\text{O}$	13.4
$(\text{CH}_3\text{CH}_2)_3\text{P}$	13.7 (HCCP) 0.5 (HCP)
$(\text{CH}_3\text{CH}_2)_3\text{P}=\text{O}$	16.3 (HCCP) 11.9 (HCP)
$\begin{array}{c} \text{O} \\ \\ \text{CH}_3\text{P}(\text{OR})_2 \end{array}$	10-13
$\begin{array}{c} \text{O} \\ \\ \text{CH}_3\text{C} \text{P}(\text{OR})_2 \\ \end{array}$	15-20
$\text{CH}_3\text{OP}(\text{OR})_2$	10.5-12
$\text{P}[\text{N}(\text{CH}_3)_2]_3$	8.8
$\text{O}=\text{P}[\text{N}(\text{CH}_3)_2]_3$	9.5

3.7: Chemical Shifts, Multiplicities, and Coupling Constants of Residual Protons in Commercially Available Deuterated Solvents

Compound ^a Molecular Weight	δ_{H} (mult)	J_{HD}
Acetic acid- d_4 64.078	11.53(l) 2.03 (5)	2
Acetone - d_6 64.117	2.04(5)	2.2
Acetonitrile - d_3 44.071	1.93 (5)	2.5
Benzene - d_6 84.152	7.15 (br)	
Chloroform - d 120.384	7.24(l)	
Cyclohexane - d_{12} 96.236	1.38 (br)	
Deuterium oxide 20.028	4.63 (DSS) ^b 4.67 (TSP) ^b	
1,2 - Dichloroethane- d_4 102.985	3.72 (br)	
Diethyl- d_{10} ether 84.185	3.34 (m) 1.07 (m)	
Diglyme - d_{14} 148.263	3.49 (br) 3.40 (br)	
	3.22 (5)	1.5
N, N -Dimethylformamide -d, 80.138	8.01 (br) 2.91(5)	2
	2.74 (5)	2
Dimethyl - d_6 sulphoxide 84.170	2.49 (5)	1.7

p-Dioxane - d ₈	3.53 (m)		
96.156			
Ethyl alcohol -d ₆ (anh)	5.19 (1)		
52.106	3.55 (br)		
	1.11 (m)		
Glyme - d ₁₀	3.40(m)		
100.184	3.22(5)	1.6	
Hexafluoroacetone deuterate, 198.067	5.26 (1)		
HMPT- d ₁₈	2.53 (2 × 5)	2(9.5)	
197.314			
Methyl alcohol - d ₄	4.78(1)36.067	3.30(5)	1.7
Methylene chloride -d ₂	5.32(3)	1	
86.945			
Nitrobenzene -d ₅	8.11 (br)		
128.143	7.67 (br)		
	7.50 (br)		
Nitromethane -d ₃	4.33 (5)	2	
64.059			
Isopropyl alcohol -d ₈	5.12(1)		
68.146	3.89 (br)		
	1.10 (br)		
Pyridine - d ₅	8.71 (br)		
84.133	7.55 (br)		
	7.19 (br)		
Tetrahydrofuran - d ₈	3.58 (br)		
80.157	1.73 (br)		
Toluene - d ₈	7.09 (m)		
100.191	7.00 (br)		
	6.98 (m)	2.3	
	2.09(5)		
Trifluoroacetic acid -d	11.50(1)		
115.030			

2,2,2-Trifluoroethyl alcohol - d ₃	5.02(1)	
103.059	3.88 (4 × 3)	2(9)

^a Purity (Atom % D) up to 99.96% ("100%") for several solvents.

^b DSS is 3-(trimethylsilyl)-1-propane sulfonic acid, sodium salt (or sodium 2,2-dimethyl-2-silapentane-5-sulfonate). TSP is sodium -3-trimethylpropionate -2, 2, 3, 3-d₄. Both are reference standards used in aqueous solutions.

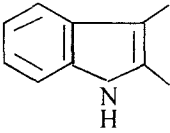
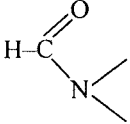
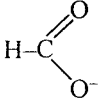
NMR table showing correlations of chemical shifts of protons

	Type and group	τ	δ
1.	TMS	10.00	
2.	-CH ₂ -Cyclopropane	9.78	0.22
3.	CH ₃ -CN	8.92-9.12	1.08-0.88
4.	CH ₃ -C-(sat.)	9.05-9.15 (8.7-9.3)	0.95-0.85 (1.3-0.7)
5.	CH ₃ -C-CO-R	8.88-9.07	1.12-0.93
6.	CH ₃ -C-N-CO-R	8.80	1.20
7.	$\begin{array}{c} \text{-N-C-} \\ \diagdown \quad \diagup \\ \text{CH}_2 \end{array}$	8.52	1.48
8.	-CH ₂ - (sat.)	8.52-8.80	1.48-1.20
9.	-CH ₂ -C-O-COR and -CH ₂ -C-O-Ar	8.50	1.50
10.	RSH,	8.5-8.9 ^a	1.5-1.1
11.	RNH ₂ (conc. less than 1 mole in inert solvent)	8.5-8.9 ^a	1.5-1.1
12.	-CH ₂ -C-C=C-	8.40-8.82	1.60-1.18
13.	-CH ₂ -CN	8.38-8.80	1.62-1.20
14.	-C-H (sat.)	8.35-8.60	1.65-1.40
15.	-CH ₂ -C-Ar	8.22-8.40	1.78-1.60
16.	-CH ₂ -C-O-R	8.19-8.79	1.81-1.21
17.	CH ₃ -C=NOH	8.19	1.81
18.	-CH ₂ -C-I	8.14-8.35	1.86-1.65

19.	$-\text{CH}_2-\text{C}-\text{CO}-\text{R}$	8.10–8.40	1.9–1.4
20.	$\text{CH}_3-\text{C}=\text{C}$	8.1–8.4	1.9–1.4
21.	$\text{CH}_3-\text{C}=\text{C}-$ $\text{O}-\text{CO}-\text{R}$	8.09–8.13	1.91–1.87
22.	$-\text{CH}_2-\text{C}=\text{C}-\text{O}-\text{R}$	8.07	1.93
23.	$-\text{CH}_2-\text{C}-\text{Cl}$	8.04–8.40	1.96–1.60
24.	$\text{CH}_3-\text{C}=\text{C}-$ COOR or CN	7.97–8.06	2.03–1.94
25.	$-\text{CH}_2-\text{C}-\text{Br}$	7.97–8.32	2.03–1.68
26.	$\text{CH}_3-\text{C}=\text{C}-\text{CO}-\text{R}$	7.94–8.07	2.06–1.93
27.	$-\text{CH}_2-\text{C}-\text{NO}_2$	7.93	2.07
28.	$-\text{CH}_2-\text{C}-\text{SO}_2-\text{R}$	7.84	2.16
29.	$-\text{C}-\text{O}$ CH	7.71	2.29
30.	$-\text{CH}_2-\text{C}=\text{C}$	7.69–8.17	2.31–1.83
31.	$\text{CH}_3-\text{N}-\text{N}-$	7.67	2.33
32.	$-\text{CH}_2-\text{CO}-\text{R}$	7.61–7.98 ^b	2.39–2.02
33.	$\text{CH}_3-\text{SO}-\text{R}$	7.50	2.5
34.	CH_3-Ar	7.50–7.75 (7.5–7.9)	2.50–2.25 (2.5–2.1)
35.	$-\text{CH}_2-\text{S}-\text{R}$	7.47–7.61	2.53–2.39
36.	$\text{CH}_3-\text{CO}-\text{SR}$	7.46–7.67	2.54–2.33
37.	$-\text{CH}_2-\text{C}\equiv\text{N}$	7.42	2.58
38.	$\text{CH}_3-\text{C}=\text{O}$	7.4–7.9 (7.4–8.1)	2.6–2.1 (2.6–1.9)
39.	$\text{CH}_3-\text{S}-\text{C}\equiv\text{N}$	7.37	2.63
40.	$\text{CH}_3-\text{CO}-\text{C}=\text{C}$ or $\text{CH}_3-\text{CO}-\text{Ar}$	7.32–8.17	2.68–1.83
41.	$\text{CH}_3-\text{CO}-\text{Cl}$ or Br	7.19–7.34	2.81–2.66
42.	$\text{CH}_3-\text{S}-$	7.2–7.9	2.8–2.1
43.	CH_3-N	7.0–7.9	3.0–2.1
44.	$-\text{C}=\text{C}-\text{C}\equiv\text{C}-\text{H}$	7.13	2.87

45.	$-\text{CH}_2-\text{SO}_2-\text{R}$	7.08	2.92
46.	$-\text{C}\equiv\text{C}-\text{H}$, nonconjugated	7.35–7.55	2.65–2.45
47.	$-\text{C}\equiv\text{C}-\text{H}$, conjugated	6.9–7.2	3.1–2.8
48.	$\text{Ar}-\text{C}=\text{C}-\text{H}$	6.95	3.05
49.	$-\text{CH}_2(\text{C}=\text{C}-)_2$	6.95–7.10	3.05–2.9
50.	$-\text{CH}_2-\text{Ar}$	6.94–7.47	3.06–2.53
51.	$-\text{CH}_2-\text{I}$	6.80–6.97	3.2–3.03
52.	$-\text{CH}_2-\text{SO}_2\text{F}$	6.72	3.28
53.	$\text{Ar}-\text{CH}_2-\text{N}$	6.68	3.32
54.	$-\text{CH}_2-\text{N}-\text{Ar}$	6.63–6.72	3.37–3.28
55.	$\text{Ar}-\text{CH}_2-\text{C}=\text{C}-$	6.62–6.82	3.38–3.18
56.	$-\text{CH}_2-\text{N}^+-$	6.60	3.40
57.	$-\text{CH}_2-\text{Cl}$	6.43–6.65	3.57–3.35
58.	$-\text{CH}_2-\text{O}-\text{R}$	6.42–7.69	3.58–2.31
59.	$\text{CH}_3-\text{O}-$	6.2–6.5 (6.0–6.7)	3.8–3.5 (4.0–3.3)
60.	$-\text{CH}_2-\text{Br}$	6.42–6.75	3.58–3.25
61.	$\text{CH}_3-\text{O}-\text{SO}-\text{OR}$	6.42	3.58
62.	$-\text{CH}_2-\text{N}=\text{C}=\text{S}$	6.39	3.61
63.	$\text{CH}_3-\text{SO}_2-\text{Cl}$	6.36	3.64
64.	$\text{Br}-\text{CH}_2-\text{C}\equiv\text{N}$	6.30	3.70
65.	$-\text{C}\equiv\text{C}-\text{CH}_2-\text{Br}$	6.18	3.82
66.	$\text{Ar}-\text{CH}_2-\text{Ar}$	6.08–6.19	3.92–3.81
67.	$\text{Ar}-\text{NH}^a_2$, $\text{Ar}-\text{NH}-\text{R}^a$, and $\text{Ar}-\text{NH}-\text{Ar}^a$	6.0–6.6 (5.7–6.7)	4.0–3.4 (4.3–3.3)
68.	$\text{CH}_3-\text{O}-\text{SO}_2-\text{OR}$	6.06	3.94
69.	$-\text{C}=\text{C}-\text{CH}_2-\text{O}-\text{R}$	6.03–6.10	3.97–3.90
70.	$-\text{C}=\text{C}-\text{CH}_2-\text{Cl}$	5.96–6.04	4.04–3.96
71.	$\text{Cl}-\text{CH}_2-\text{C}\equiv\text{N}$	5.93	4.07
72.	$\text{H}_2-\text{C}=\text{C}-\text{O}-\text{CH}_2-\text{C}=\text{C}$	5.87–6.17	4.13–3.83
73.	$-\text{C}\equiv\text{C}-\text{CH}_2-\text{Cl}$	5.84–5.91	4.16–4.09
74.	$-\text{C}=\text{C}-\text{CH}_2-\text{OR}$	5.82	4.18
75.	$-\text{CH}_2-\text{O}-\text{CO}-\text{R}$ or $-\text{CH}_2-\text{O}-\text{Ar}$	5.71–6.02	4.29–3.98

76.	$-\text{CH}_2-\text{NO}_2$	5.62	4.38
77.	$\text{Ar}-\text{CH}_2-\text{Br}$	5.57–5.59	4.43–4.41
78.	$\text{Ar}-\text{CH}_2-\text{OR}$	5.51–5.64	4.49–4.36
79.	$\text{Ar}-\text{CH}_2-\text{Cl}$	5.50	4.50
80.	$-\text{C}=\text{CH}_2$	5.37	4.63
81.	$-\text{C}=\text{CH}-$, acyclic, nonconjugated	4.3–4.9 (4.1–4.9)	5.7–5.1 (5.9–5.1)
82.	$-\text{C}=\text{CH}-$, Cyclic, nonconjugated	4.3–4.8	5.7–5.2
83.	$-\text{C}=\text{CH}_2$	4.3–4.7 (3.75–4.8)	5.7–5.3 (6.25–5.2)
84.	$-\text{CH}(\text{OR})_2$	4.80–5.20	5.20–4.80
85.	$\text{Ar}-\text{CH}_2-\text{O}-\text{CO}-\text{R}$	4.74	5.26
86.	$\text{R}-\text{O}-\text{H}$ (conc. less than one mole in inert solvent)	4.8–7.0 ^a	5.2–3.0 ^a
87.	$\text{Ar}-\text{C}=\text{CH}-$	4.60–4.72	5.40–5.28
88.	$-\text{CH}=\text{C}-\text{O}-\text{R}$	4.45–5.46	5.55–4.54
89.	$-\text{CH}=\text{C}-\text{C}\equiv\text{N}$	4.25	5.75
90.	$-\text{C}=\text{CH}-\text{CO}-\text{R}$	3.95–4.32	6.05–5.68
91.	$\text{R}-\text{CO}-\text{CH}=\text{C}-\text{CO}-\text{R}$	3.87–3.97	6.13–6.03
92.	$\text{Ar}-\text{CH}=\text{C}-$	3.72–3.77	6.28–6.23
93.	$-\text{C}=\text{C}-\text{H}$, conjugated	3.3–4.5 (2.2–4.7)	6.7–5.5 (7.8–5.3)
94.	$-\text{C}=\text{C}-\text{H}$, acyclic, conjugated	3.5–4.0 (2.9–4.5)	6.5–6.0 (7.1–5.5)
95.	$\begin{array}{c} \text{H}-\text{C}=\text{C}- \\ \quad \\ \text{H} \quad \text{CO}-\text{R} \end{array}$	3.60–3.70	6.40–6.30
96.	$-\text{C}=\text{CH}-\text{O}-\text{R}$	3.55–3.78	6.45–6.22
97.	$\text{Br}-\text{CH}=\text{C}-$	3.00–3.38	7.00–6.62
98.	$-\text{CH}=\text{C}-\text{CO}-\text{R}$	2.96–4.53	7.04–5.47
99.	$-\text{C}=\text{Ch}-\text{O}-\text{CO}-\text{CH}_3$	2.75	7.25

100.		2.6–2.7	7.4–7.3
101.	R–CO–NH	2.3–3.9 (1.5–4.5)	7.7–6.1 (8.5–5.5)
102.	Ar–CH–C–CO–R	2.28–2.62	7.72–7.38
103.	ArH, benzenoid	2.0–3.4 (0.5–4.0)	8.0–6.6 (9.5–6.0)
104.	ArH, nonbenzenoid	1.4–3.8 (1.0–6.0)	8.6–6.2 (9.0–4.0)
105.		1.9–2.1	8.1–7.9
106.		1.8–2.0	8.2–8.0
107.	–C=C–CHO, aliphatic, α , β unsat.	0.32–0.57	9.68–9.43
108.	R–CHO, aliphatic	0.2–0.3 (0.2–0.5)	9.8–9.7 (9.8–9.5)
109.	Ar–CHO	0.0–0.3 (–0.1 to 0.5)	10.0–9.7 (10.1 to 9.5)
110.	R–COOH	–1.52 to –0.97	11.52 to 10.97
111.	–SO ₃ H	–2.0 to –1.0	12.0 to 11.0
112.	–C=C–COOH	–2.18 to –1.57	12.18 to 11.57
113.	R–COOH, dimer	–2.2 to –1.0	12.2 to 11.0
114.	AR–OH, intramolecularly bonded	–2.5 to –0.5 (–5.5 to –0.5)	12.5 to 10.5 (15.5 to 10.5)
115.	AR–OH, polymeric association	2.3 to 5.5 ^a	7.7 to 4.5 ^a
116.	Enols	–6.0 to –5.0	16.0 to 15.0

Normally protons resonate within the range shown. In cases in which protons resonate outside the range, the limits are shown by values in parentheses.

^a The position of these protons depends on concentration, temperature, and the presence of other exchangeable protons. Values for amino protons depend on the basicity of the nitrogen atom.

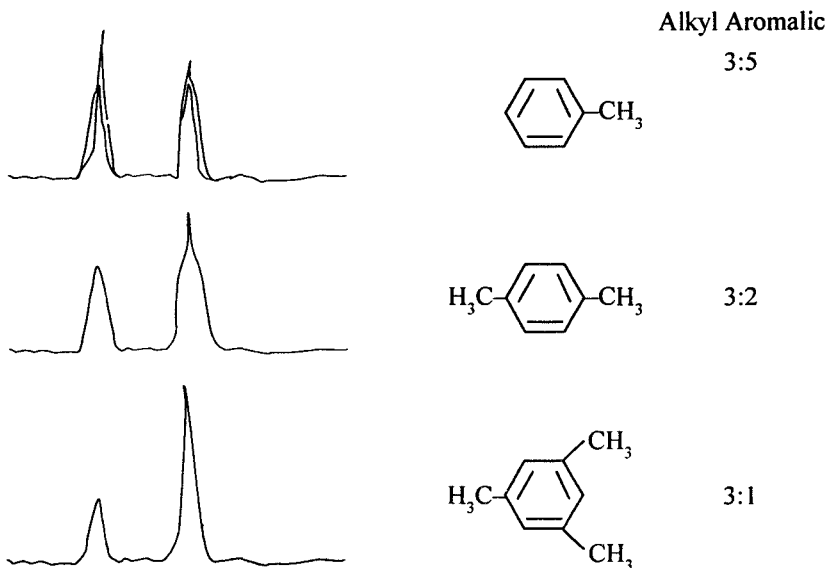
^b In these compounds R=H, alkyl, aryl, OH, OR or NH₂.

Exercises and Problems:

Problem 1. The compounds CHCl₂-CHCl₂ ($\delta=6$ ppm) and CCl₃-CH₂Cl ($\delta=3.9$ ppm) produce single NMR signals owing to the fact that their hydrogen atoms are chemically equivalent. Explain the difference between the chemical shift for these compounds.

Answer: Halogens shift the proton signal downfield and the shift is the larger, the larger the number of halogen atoms.

Problem 2. Toluene, p-xylene and mesitylene have two peaks each in their NMR spectra. Assign the spectra shown in fig. shown below (1, 2 and 3) to these compounds.



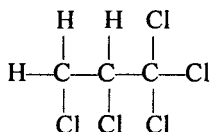
Answer: The signal with $\delta=2$ ppm is produced by the protons of the methyl group and the signal at about 7 ppm by the aromatic protons. As the lines have approximately the same width, the ratios of the peak areas are 3:5, 3:2 and 3:1 in the first, second and third spectra, respectively. Hence, the spectra can be assigned as follows: 1. Toluene, 2. p-xylene, 3. mesitylene.

Problem 3. Identify the structures of the compounds $C_3H_3Cl_5$ (1) and $C_3H_5Cl_3$ (2) with the following NMR spectra:

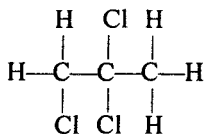
(1) Triplet ($\delta=4.52$ ppm) and doublet ($\delta=6.07$ ppm) with the peak area ratio of 1:2

(2) Singlets ($\delta=2.20$ ppm and $\delta=4.02$ ppm) with the peak area ratio of 3:2

Answer: The triplet with $\delta=4.52$ ppm and the doublet with $\delta=6.07$ ppm indicate that the methine group (1H) has a neighbour with two protons (2H). Hence the compound (1) has the following structure:



The singlets in the spectrum of the compound (2) indicate that two proton groups are separated by an aprotic group making spin-spin coupling impossible. Thus, the compound (2) has the following structure:

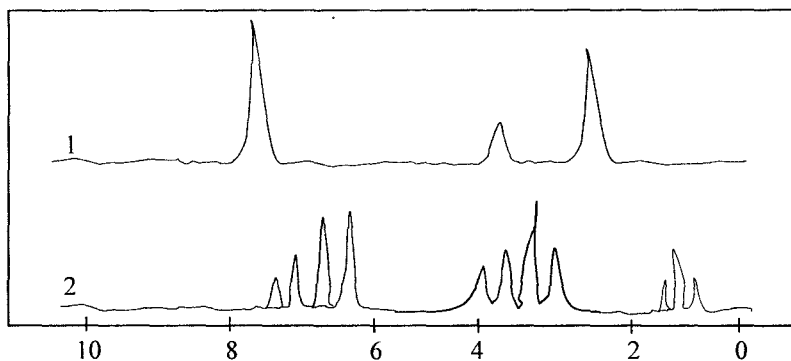


Problem 4. Fig. shown below gives two spectra for the compounds with the same empirical formula $C_8H_{10}O$. Determine the structure and explain the differences in the chemical shifts.

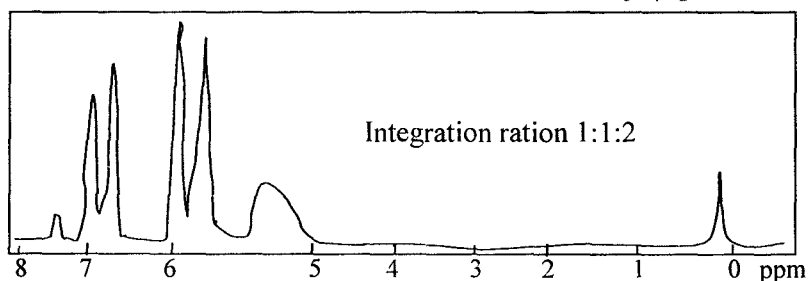
Answer: 1. $C_6H_5-CH_2-O-CH_3$ 2. $C_6H_5-O-CH_2-CH_3$

In the compound (1) the oxygen atom is linked to the groups CH_2 and CH_3 and therefore both peaks are shifted downfield (the chemical shifts are larger) and there is no spin-spin coupling between the protons of these groups.

In the compound (2) the oxygen atom affects the group CH_2 (downfield shift of the peak) and the group C_6H_5 . The aromatic protons become nonequivalent and the signal is split into a multiplet owing to their coupling.



Problem 5. Deduce the structure of the compound $C_3H_4N_2S$



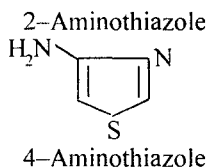
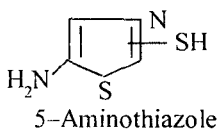
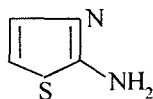
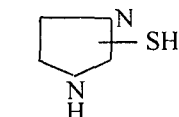
Answer: $C_3H_4N_2S$ Index = 3

doublet $\delta 7.08$ (1H) $J = 5\text{Hz}$

doublet $\delta 6.48$ (1H) $J = 5\text{Hz}$

very broad $\delta 5.61$ (2H)

The two non-equivalent protons, which are coupled to each other are in the aromatic region. With an index value of 3 and only $3C^1$ atoms, only imidazole and thiazole are the possible aromatic compounds. But the former, imidazole – thiol has four non-equivalent protons as against three observed. So the compound is aminothiazole. The J value indicates vicinal positions for the aromatic and hence the compound is 2-aminothiazole.



Problem 6. Why is an internal standard used in obtaining an nmr spectrum? Why is TMS a good standard?

In NMR spectroscopy, we are trying to determine the strength of magnetic field which is required to bring about the resonance of certain nuclei in a given compound. It is natural to expect, therefore, that a NMR spectrum would be a plot of signal strength versus magnetic field, in units of milligauss. Measuring a magnetic field is difficult. However, it is convenient to determine accurately the values of absorption frequencies ($\because \nu = \gamma H_0 / 2\pi$) of protons relative to those of a suitable standard. As only relative absorption values can be obtained, a suitable standard must be used.

The most logical standard would be a “bare proton”, having no shielding electrons, but experimentally this is not possible, and instead one uses as standards compounds having sharp resonance peaks. The chemical shift may then be expressed as the difference between the resonance frequency of the protons in the sample (ν_{sample}) and the resonance frequency of the protons in the standard (ν_{standard})

$$(\nu_{\text{sample}} - \nu_{\text{TMS}})$$

Tetramethylsilane (TMS) is commonly used as an internal reference

TMS is a good standard because

- (i) TMS is unreactive (except with con. H_2SO_4 with which it should not be used) and it does not associate with the sample.
- (ii) TMS is symmetrical, and thus gives a sharp peak of 12 equivalent protons.
- (iii) It is extremely volatile, and thus allows recovery of the pure sample.
- (iv) It is soluble in most organic solvents. Methyl protons of TMS are strongly shielded and therefore absorbs at higher field than almost all organic protons.

It also enables us to define a scale for the spectra by arbitrarily assigning a frequency value for TMS protons equal to zero.

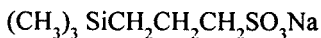
Problem 7. Which references and solvents are used to take NMR spectra of samples? Why?

To determine the resonance spectrum of the protons of an organic compound, one needs anywhere between 1 and about 30 mg of the sample. The sample is normally used in the form of its dilute solution (about 2 to 10%) in a solvent which contains no hydrogen atoms of its own.

For samples of low polarity, carbon tetrachloride, deuterated chloroform, CDCl_3 and deuterated benzene C_6D_6 , are often used. On the other hand if the sample is soluble only in polar solvents, deuterium oxide (D_2O), acetone – D_6 (CD_3COCD_3), or dimethyl sulfoxide – D_6 [$(\text{CD}_3)_2\text{SO}$] are often employed.

The internal standard used to locate the resonance frequency of most protons is tetramethyl silane (TMS) [$(\text{CH}_3)_4\text{Si}$], which one adds to the sample before recording the spectrum. TMS is commonly used as an internal reference because it is chemically inert, symmetrical, volatile and soluble in most organic solvents, it gives a single sharp absorption peak and absorbs at higher field than almost all organic protons.

TMS cannot be used as an internal reference for substances dissolved in D_2O . For aqueous solutions, the standard used is often the sodium salt of 2,2-dimethyl-2-silapentane-5-sulfonic acid or DSS.



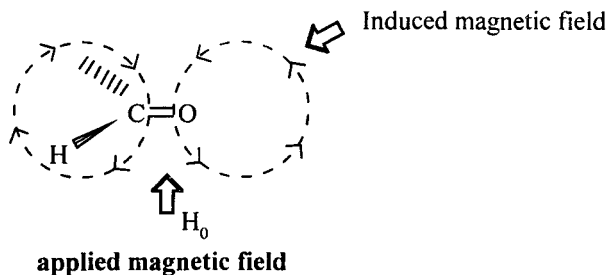
The methyl groups in this compound provide a suitable reference peak.

Acetonitrile and dioxane are also used as references in aqueous solution.

Problem 8. Explain the abnormally large shift of aldehydic proton in nmr spectra.

If molecules contain protons that are sterically oriented so that they are close to double or triple bonded groups, there will generally be a diamagnetic anisotropic effect of some kind.

The magnetic fields induced by pi electrons are directional, i.e., unsymmetrical. A measurement which varies with the direction in which the measurement is taken is said to be anisotropic. Because the effects of molecular fields induced by π electrons are direction dependent, these are, therefore termed anisotropic effects. These effects are contrasted to inductive effects, which are symmetrical around the proton.



Anisotropic effects occur in addition to the ever present molecular field, induced by sigma-bond electrons.

Thus the downfield shift of aldehyde proton (δ 9–10) is not only due to the deshielding effect of sp^2 carbon (sp^2 carbon has high s character and withdraws electrons, deshielding the hydrogen) but also due to anisotropy of the C=O. These two effects combined together deshield the attached hydrogens in these systems.

Just like in benzene, in aldehyde, the induced magnetic field (by the π -electrons) in the region where protons are located is oriented in the same direction as the applied field. A smaller field is therefore, required for resonance resulting in their deshielding. “The highly deshielded position of aldehydes is attributed to a combination of a strong inductive effect and the diamagnetic anisotropy of the carbonyl group.”

□□□

4

^{13}C NMR Spectroscopy

4.1: The ^{13}C chemical shifts of Linear and Branched Alkanes:

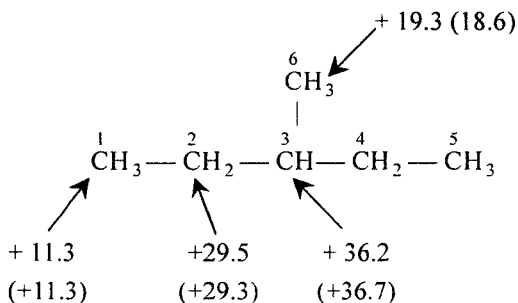
Alkane groups unsubstituted by heteroatoms absorb downfield from TMS to about 60 ppm. (Methane absorbs at 2.5 ppm upfield from TMS.) Within this range we can predict the chemical shifts of individual ^{13}C atoms in a straight chain or branched chain hydrocarbon from the data in Table 4.1 and the formula $\delta = -2.5 + \Sigma nA$.

Where δ = Predicted shift for a carbon atom.

A = Additive shift parameter.

n = number of carbon atoms for each shift parameter (-2.5 is the shift of the ^{13}C of methane).

The calculated (and observed) shifts for the carbon atoms of 3-methylpentane are



For carbon atom 1, we have 1 α -, 1 β -, 2 γ and 1 δ -carbon atoms.

$$\delta_1 = -2.5 + (9.1 \times 1) + (9.4 \times 1) + (-2.5 \times 2) + (0.3 \times 1) = + 11.3$$

Carbon atom 2 has 2 α -, 2 β -, and 1 γ carbon atoms. Carbon atom 2 is a 2° carbon with a 3° carbon attached [$2^\circ(3^\circ) = -2.5$]

$$\delta_2 = -2.5 + (9.1 \times 2) + (9.4 \times 2) + (-2.5 \times 1) + (-2.5 \times 1) = 29.5$$

Carbon atom 3 has 3 α - and 2 β - carbon atoms, and it is a 3° atom with two 2° atoms attached [$3^\circ(2^\circ) = -3.7$]. Thus $\delta_3 = -2.5 + (9.1 \times 3) + (9.4 \times 2) + (-3.7 \times 2) = + 36.2$

Carbon atom 6 has, 1 α -, 2 β -, and 2 γ carbon atoms, and it is a 1° atom with a 3° atom attached [$1^\circ(3^\circ) = -1.1$]. Thus, $\delta_6 = -2.5 + (9.1 \times 1) + (9.4 \times 2) + (-2.5 \times 2) + (-1.1 \times 1) = + 19.3$

The agreement for such calculations is very good. It is essential that the reference compounds used for such additivity calculations be structurally similar to the compound of interest.

Table 4.1: The ^{13}C shift parameters in some linear and branched hydrocarbons

^{13}C Atoms	Shift (ppm) (A)
α	+9.1
β	+9.4
γ	-2.5
δ	+0.3
ϵ	+0.1
1° (3°) ^a	-1.1
1° (4°) ^a	-3.4
2° (3°) ^a	-2.5
2° (4°)	-7.2
3° (2°)	-3.7
3° (3°)	-9.5
4° (1°)	-1.5
4° (2°)	-8.4

^a The notations 1° (3°) and 1° (4°) denote a CH₃ group bound to a R₂CH group and to a R₃C group, respectively. The notation 2° (3°) denotes a RCH₂ group bound to a R₂CH group, and so on.

Table 4.2 lists the shifts in some linear and branched alkanes.

Table 4.2: The ^{13}C Shifts for some Linear and Branched chian Alkanes (ppm from TMS).

Compound	C-1	C-2	C-3	C-4	C-5
Methane	-2.3				
Ethane	5.7				
Propane	15.8	16.3	15.8		
Butane	13.4	25.2	25.2		
Pentane	13.9	22.8	34.7	22.8	13.9
Hexane	14.1	23.1	32.2	32.2	23.1
Heptane	14.1	23.2	32.6	29.7	32.6
Octane	14.2	23.2	32.6	29.9	29.9
Nonane	14.2	23.3	32.6	30.0	30.3
Decane	14.2	-23.2	32.6	31.1	30.5
Isobutane	24.5	25.4			
Isopentane	22.2	31.1	32.0	11.7	
Isohexane	22.7	28.0	42.0	20.9	14.3
Neopentane	31.7	28.1			
2,2-Dimethylbutane	29.1	30.6	36.9	8.9	
3-Methylpentane	11.5	29.5	36.9	(18.8, 3CH ₃)	
2,3-Dimethylbutane	19.5	34.3			
2,2,3-Trimethyl butane	27.4	33.1	38.3	16.1	
2,3-Dimethylpentane	7.0	25.3	36.3	(14.6, 3-CH ₃)	

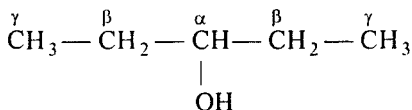
Table 4.3: Incremental Substituent Effects (ppm) on Replacement of H by Y in Alkanes. Y is Terminal or Internal^a (+ downfield, -upfield)

Y	Terminal		Internal		γ
	α	β	β	α	
CH ₃	+9	+6	+10	+8	-2
CH=CH ₂	+20		+6		-0.5
C≡CH	+4.5		+5.5		-3.5
COOH	+21	+16	+3	+2	-2
COO ⁻	+25	+20	+5	+3	-2
COOR	+20	+17	+3	+2	-2
COCl	+33	+28		+2	
CONH ₂	+22		+2.5		-0.5
COR	+30	+24	+1	+1	-2
CHO	+31		0		-2
Phenyl	+23	+17	+9	+7	-2
OH	+48	+41	+10	+8	-5
OR	+58	+51	+8	+5	-4
OCOR	+51	+45	+6	+5	-3
NH ₂	+29	+24	+11	+10	-5
NH ₃ ⁺	+26	+24	+8	+6	-5
NHR	+37	+31	+8	+6	-4
NR ₂	+42				-3
NR ₃ ⁺	+31		+5		-7
NO ₂	+63	+57	+4	+4	
CN	+4	+1	+3	+3	-3
SH	+11	+11	+12	+11	-4
SR	+20		+7		-3
F	+68	+63	+9	+6	-4
Cl	+31	+32	+11	+10	-4
Br	+20	+25	+11	+10	-3
I	-6	+4	+11	+12	-1

a Add these increments to the shift values of the appropriate carbon atom in Table 4.2 or to the shift value calculated from Table 4.1.

From Table 4.3, the approximate shifts for the carbon atoms of, for example, 3-pentanol, may be calculated from the values for pentane in Table 4.2; that

is, the increment for the functional group in Table 4.3 is added to the appropriate value in Table 4.2 as follows:



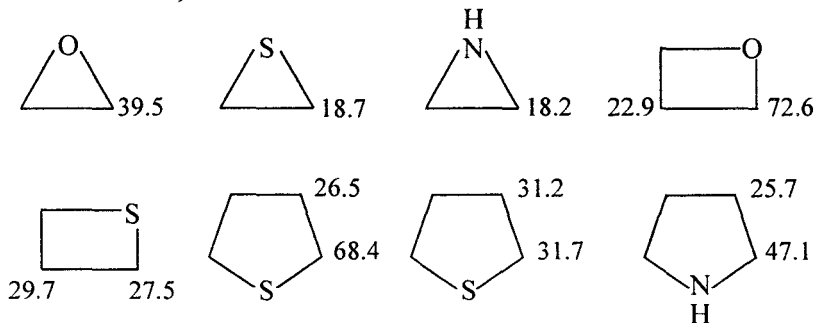
	Calculated	Found
C α	34.7 + 41 = 75.8	73.8
C β	22.8 + 8 = 30.8	30.0
C γ	13.9 - 5 = 8.9	10.1

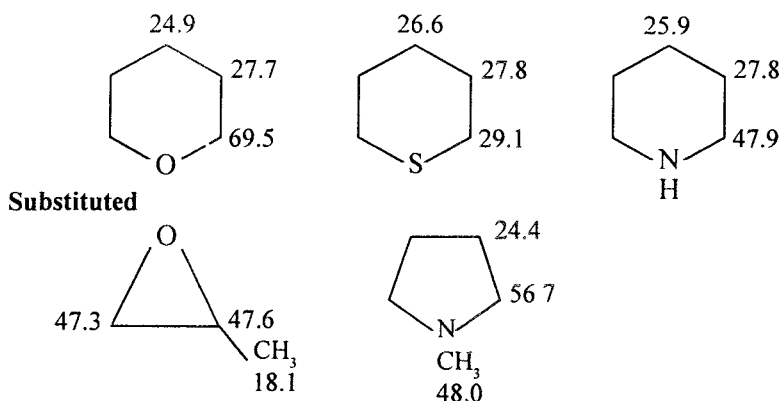
The chemical shifts of the CH₂ groups in monocyclic alkanes are given in Table 4.4. Each ring skeleton has its own set of shift parameters. Rough estimates for substituted rings can be made with the substitution increments in Table 4.3. Table 4.5 presents chemical shifts for several saturated heterocyclics.

Table 4.4: Chemical shifts of Cycloalkanes (ppm from TMS)

C ₃ H ₆	-2.9
C ₄ H ₈	22.4
C ₅ H ₁₀	25.6
C ₆ H ₁₂	26.9
C ₇ H ₁₄	28.4
C ₈ H ₁₆	26.9
C ₉ H ₁₈	26.1
C ₁₀ H ₂₀	25.3

Table 4.5: Chemical shifts for saturated Heterocyclics (ppm from TMS, neat) Unsubstituted



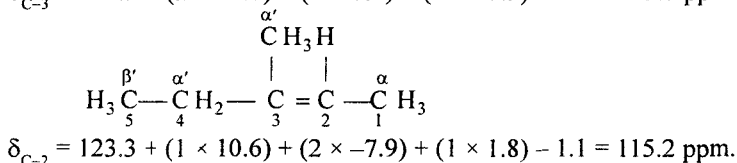
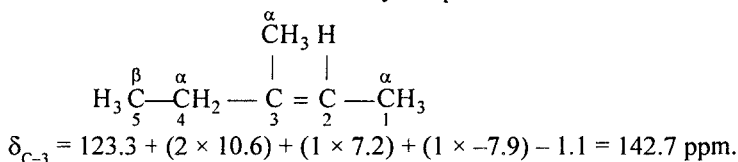


4.2 Alkenes and Alkynes

The sp^2 carbon atoms of alkenes substituted only by alkyl groups, absorb in the range of about 110–150 ppm downfield from TMS. The double bond has a rather small effect on the shift of the sp^3 carbon in the molecule. Calculation of approximate shifts can be made from the following parameters where (α , β , and γ represent substituents on the same end of the double bond as the alkene carbon of interest, and (α' , β' , and γ' represent substituents on the far side.

α	+10.6
β	+7.2
γ	-1.5
α'	-7.9
β'	-1.8
γ'	-1.5
Z (cis) correction	-1.1

These parameters are added to 123.3 ppm, the shift for ethylene. We can calculate the values for *cis*-3-methyl-2-pentene as follows:



The measured values are C-3 = 137.2 and C-2 = 116.8. The agreement is fair. The allylic carbon of a (Z) alkene is usually at lower field from that of

an (E) alkene by about 4–6 ppm. Alkene carbon atoms in polyenes are treated as though they were alkane carbon substituents on one of the double bonds. Thus in calculating the shift of C-2 in 1,4-pentadiene, C-4 is treated like a β-sp³ carbon atom.

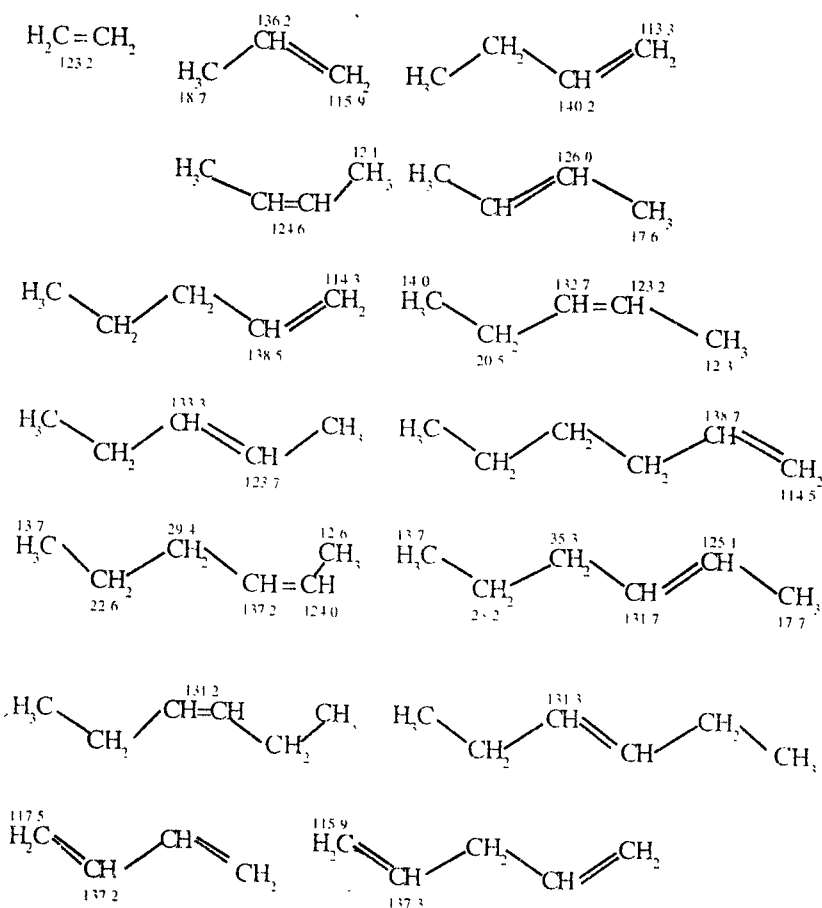
Representative alkenes are presented in Table 4.6.

There are no simple rules to handle polar substituents on an alkene carbon.

Shifts for several substituted alkenes are presented in Table 4.7.

The central carbon atom (=C=) of alkyl substituted allenes absorbs far downfield in the range of about 200–215 ppm, whereas the terminal atoms (C=C=C) absorb upfield in the range of about 75–97 ppm.

Table 4.6: Alkene and Cycloalkene Chemical shifts (ppm from TMS)



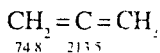
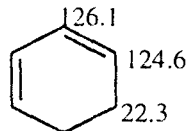
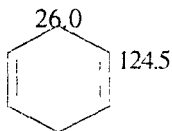
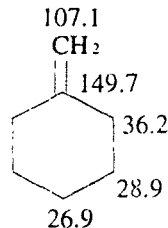
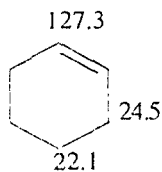
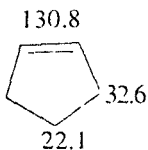
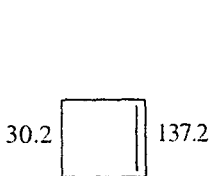
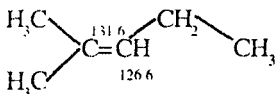
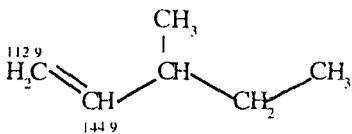
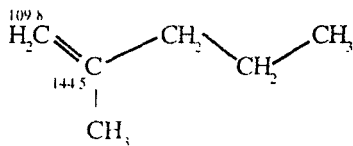
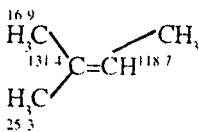
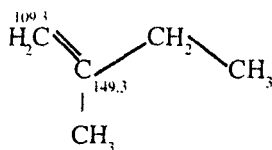
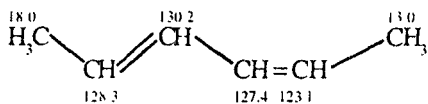
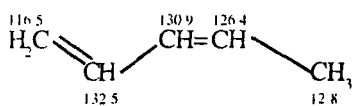
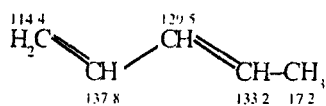
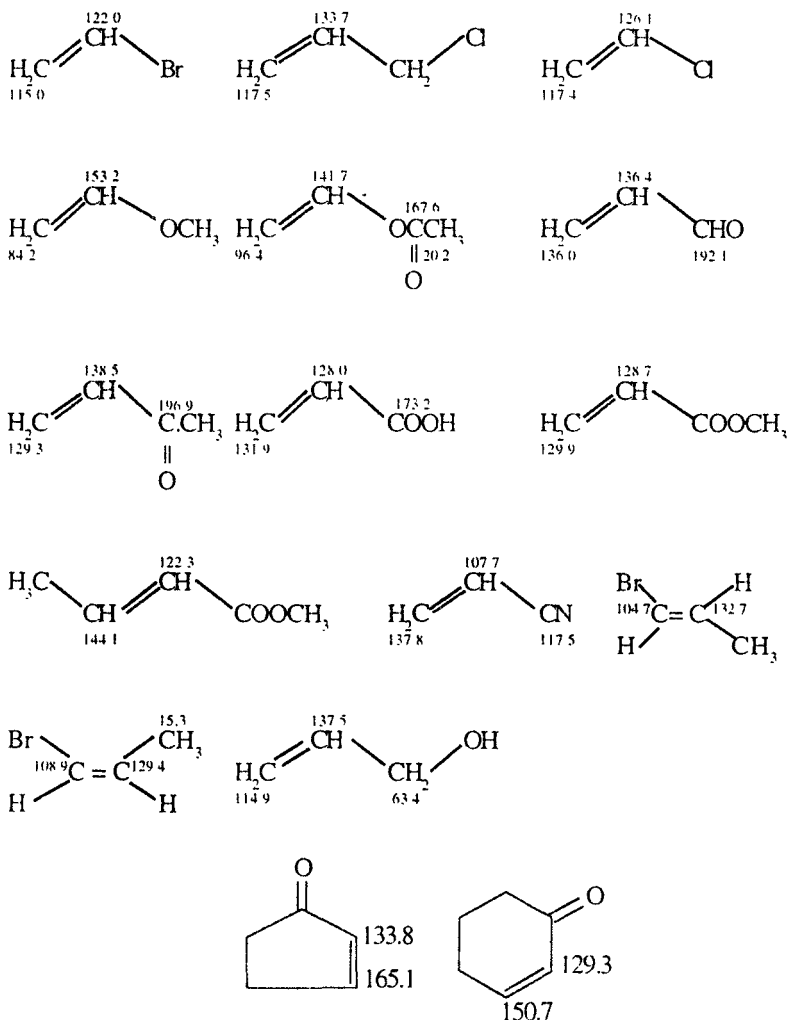


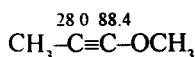
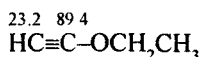
Table 4.7: Chemical Shifts of substituted Alkenes (ppm from TMS)



The sp carbon atoms of alkynes substituted only by alkyl groups absorb in the range of approximately 65–90 ppm (Table 4.8). The triple bond shifts the sp^3 carbon atoms directly attached about 5–15 ppm upfield relative to the corresponding alkane. The terminal $\equiv\text{CH}$ absorbs upfield from the internal $\equiv\text{CR}$. Alkyne carbon atoms with a polar group directly attached absorb from about 20–95 ppm.

Table 4.8: Alkyne Chemical Shifts (ppm)

Compound	C-1	C-2	C-3	C-4	C-5	C-6
1-Butyne	67.0	84.7				
2-Butyne		73.6				
1-Hexyne	67.4	82.8	17.4	29.9	21.2	12.9
2-Hexyne	1.7	73.7	76.9	19.6	21.6	12.1
3-Hexyne	14.4	12.0	79.9			



4.3: Aromatic Compounds

Benzene carbon atoms absorb at 128.5 ppm, neat or as a solution in CDCl_3 or CCl_4 . Substituents shift the attached aromatic carbon atom as much as ± 35 ppm.

Fused ring absorptions are as follows:

Naphthalene: C-1, 128.1; C-2, 125.9; C-4a, 133.7

Anthracene: C-1, 130.1; C-2, 125.4; C-4a, 132.2; C-9, 132.6

Phenanthrene: C-1, 128.3; C-2, 126.3; C-3, 126.3; C-4, 122.2; C-4a, 131.9*;
C-9, 126.6; C-10a, 130.1*.

Incremental shifts from benzene for the aromatic carbon atoms of representative monosubstituted benzene rings (and shifts from TMS of carbon containing substituents) are given in Table 5.9.

*Assignment uncertain.

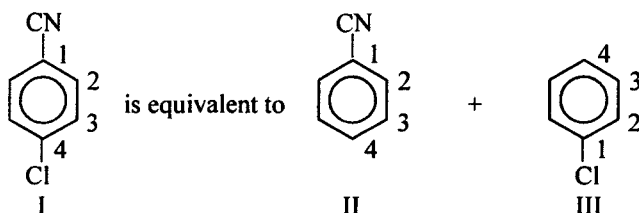
Table 4.9: Incremental shifts of the Aromatic Carbon Atoms of Monosubstituted Benzenes (ppm from Benzene at 128.5 ppm, +downfield, -upfield). Carbon Atom of substituents in parts per million from TMS

Substituent	C-1 (Attachment)	C-2	C-3	C-4	C ¹ of substituents (ppm from TMS)
H	0.0	0.0	0.0	0.0	
CH_3	9.3	+0.7	-0.1	-2.9	21.3
CH_2CH_3	+15.6	-0.5	0.0	-2.6	29.2(CH_2), 15.8(CH_3)
$\text{CH}(\text{CH}_3)_2$	+20.1	-2.0	0.0	-2.5	34.4(CH), 24.1(CH_3)
$\text{C}(\text{CH}_3)_3$	+22.2	-3.4	-0.4	-3.1	34.5(C), 31.4(CH_3)
$\text{CH}=\text{CH}_2$	+9.1	-2.4	+0.2	-0.5	137.1(CH), 113.2(CH_2)
$\text{C}\equiv\text{CH}$	-5.8	+6.9	+0.1	+0.4	84.0(C), 77.8(CH)
C_6H_5	+12.1	-1.8	-0.1	-1.6	
CH_2OH	+13.3	-0.8	-0.6	-0.4	64.5

$\text{CH}_2\text{OC}-\text{CH}_3$ \parallel O	+7.7	~ 0.0	~ 0.0	~ 0.0	20.7(CH_3), 66.1(CH_2), 170.5 (C=O)
OH	+26.6	-12.7	+1.6	-7.3	
OCH_3	+31.4	-14.4	+1.0	-7.7	54.1
OC_6H_5	+29.0	-9.4	+1.6	-5.3	
\parallel O OCCH_3	+22.4	-7.1	-0.4	-3.2	23.9(CH_3), 169.7 (C=O)
\parallel O CH	+8.2	+1.2	+0.6	+5.8	192.0
\parallel O CCH $_3$	+7.8	-0.4	-0.4	+2.8	24.6(CH_3), 195.7 (C=O)
\parallel O CC $_6\text{H}_5$	+9.1	+1.5	-0.2	+3.8	196.4 (C=O)
\parallel O CCF $_3$	-5.6	+1.8	+0.7	+6.7	
\parallel O COH	+2.9	+1.3	+0.4	+4.3	168.0
\parallel O COCH $_3$	+2.0	+1.2	-0.1	+4.8	51.0(CH_3), 166.8 (C=O)
\parallel O CCI	+4.6	+2.9	+0.6	+7.0	168.5
$\text{C}\equiv\text{N}$	-16.0	+3.6	+0.6	+4.3	119.5
NH_2	+19.2	-12.4	+1.3	-9.5	
$\text{N}(\text{CH}_3)_2$	+22.4	-15.7	+0.8	-11.8	40.3
\parallel O NHCCH $_3$	+11.1	-9.9	+0.2	-5.6	
NO_2	+19.6	-5.3	+0.9	+6.0	
$\text{N}=\text{C}=\text{O}$	+5.7	-3.6	+1.2	-2.8	129.5
F	+35.1	-14.3	+0.9	-4.5	
Cl	+6.4	+0.2	+1.0	-2.0	
Br	-5.4	+3.4	+2.2	-1.0	
I	-32.2	+9.9	+2.6	-7.3	
CF $_3$	+2.6	-3.1	+0.4	+3.4	
SH	+2.3	+0.6	+0.2	-3.3	
SCH $_3$	+10.2	-1.8	+0.4	-3.6	15.9

SO ₂ NH ₂	+15.3	-2.9	+0.4	+3.3
Si(CH ₃) ₃	+13.4	+4.4	-1.1	-1.1

Shifts from benzene for polysubstituted benzene ring carbon atoms can be approximated by applying the principle of substituent additivity. For example, the shift from benzene for C-2. of the disubstituted compound 4-chlorobenzonitrile is calculated by adding the effect for an ortho CN group (+3.6) to that for a meta Cl group (+1.3):



CAtom	Calculated	Observed	CAtom	Observed	CAtom	Observed
1	-18.0	-16.6	1	-16.0	4	-2.0
2	+4.6	+5.1	2	+3.6	3	+1.0
3	+0.8	+1.3	3	+0.6	2	+0.2
4	+10.7	+10.8	4	+4.3	1	+6.4

Table 4.10: Shift for Carbon Atoms of Heteroaromatics (neat, ppm from TMS)

Compound	C-2	C-3	C-4	C-5	C-6	Substituent
Furan	142.7	109.6				
2-Methyl furan	152.2	106.2	110.9	141.2		13.4
Furan-2-Carboxaldehyde	153.3	121.7	112.9	148.5		178.2
Methyl 2-furoate	144.8	117.9	111.9	146.4		159.1 (C=O), 51.8 (CH ₃)
Pyrrole	118.4	108.0				
2-Methyl pyrrole	127.2	105.9	108.1	116.7		12.4
Pyrrole-2-						
Carboxaldehyde	134.0	123.0	112.0	129.0		
Thiophene	124.4	126.2				
2-Methylthiophene	139.0	124.7	126.4	122.6		14.8
Thiophene-2-						
Carboxaldehyde	143.3	136.4	128.1	134.6		182.8
Thiazole	152.2		142.4	118.5		
Imidazole	136.2		122.3	122.3		
Pyrazole		134.3	105.2			
1-Methylpyrazole		139.2	105.7	128.7		38.1
Pyridine	150.2	123.9	135.9			
Pyrimidine	159.5		157.4	122.1	157.4	

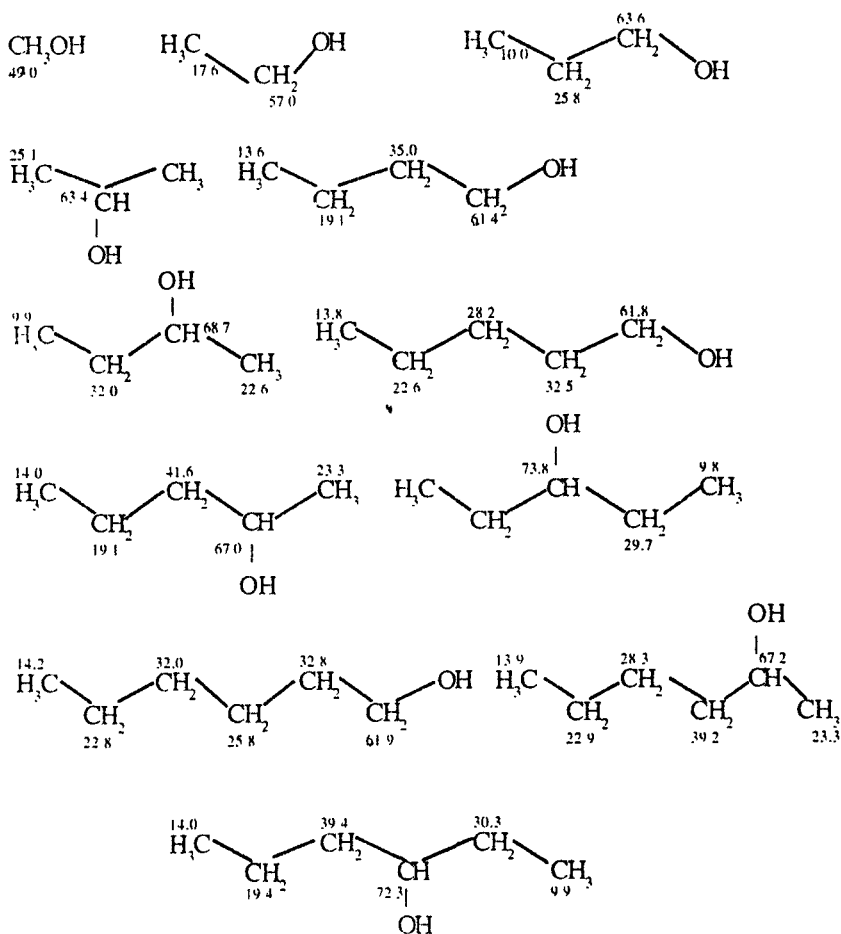
Pyrazine	145.6				
2-Methylpyrazine	154.0	141.8 ^a	143.8 ^a	144.7 ^a	21.6
Pyridazine		152.8	127.6		

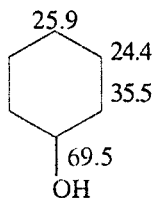
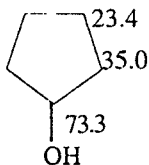
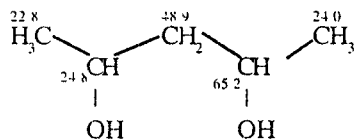
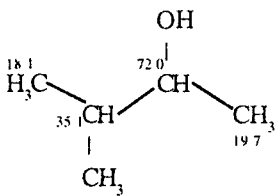
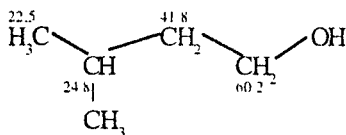
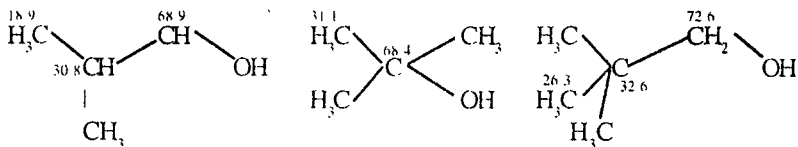
^a Assignment not certain

4.4: Alcohols

Substitution of H in an alkane by an OH group causes down field shifts of 35–52 ppm for C-1, 5–12 ppm for C-2, and upfield shift of about 0–6 ppm for C-3. Shifts for several acyclic and alicyclic alcohols are given in Table 4.11.

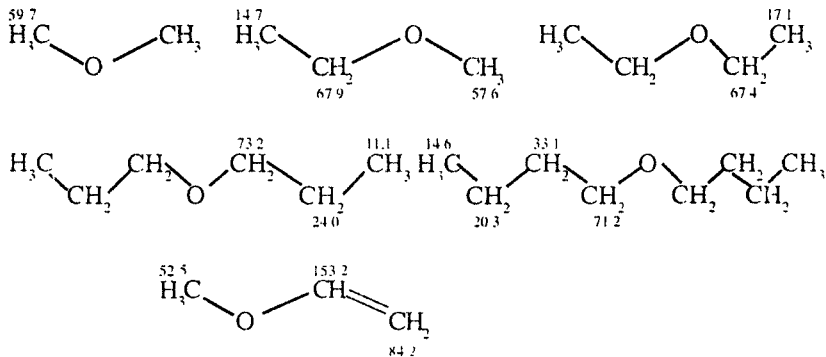
Table 4.11: Chemical shifts of Alcohols (neat, ppm from TMS)

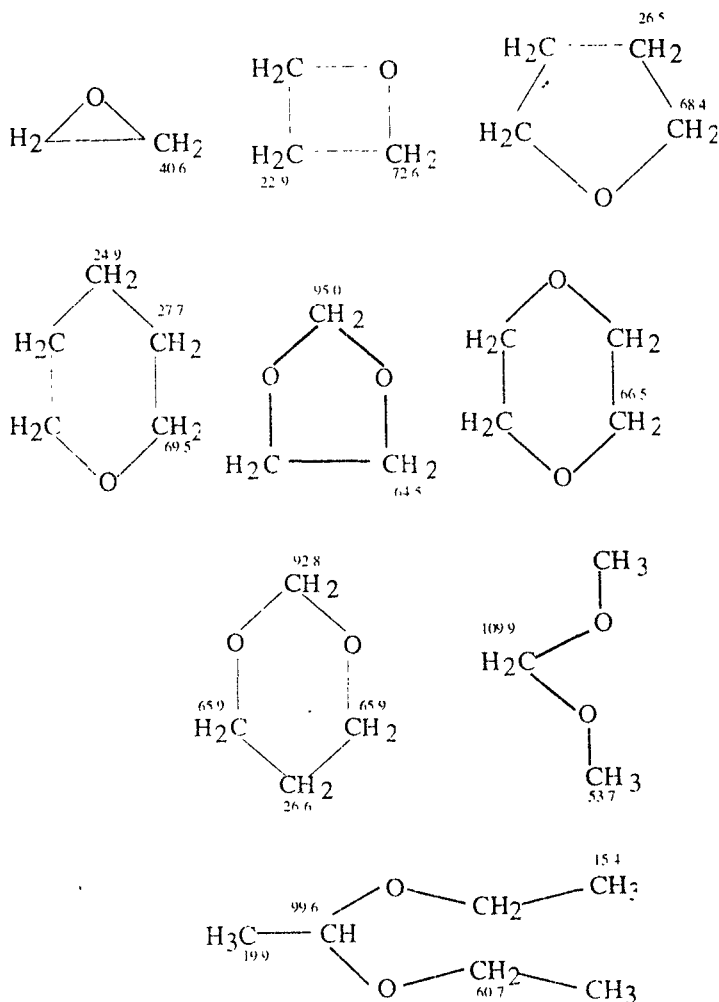




4.5 Ethers, Acetals, and Epoxides :

Table 4.12 Chemical shifts of Ethers, Acetals, and Epoxides (ppm from Tms)





4.6: Halides

Table 4.13: Shift Positions for Alkyl Halides (neat, ppm from TMS)

Compound	C-1	C-2	C-3
CH_4	-2.3		
CH_3F	75.4		
CH_3Cl	24.9		
CH_2Cl_2	54.0		
CHCl_3	77.5		
CCl_4	96.5		

CH_3Br	10.0		
CH_2Br_2	21.4		
CHBr_3	12.1		
CBr_4	-28.5		
CH_3I	-20.7		
CH_2I_2	-54.0		
CHI_3	-139.9		
CI_4	-292.5		
$\text{CH}_3\text{CH}_2\text{F}$	79.3	14.6	
$\text{CH}_3\text{CH}_2\text{Cl}$	39.9	18.7	
$\text{CH}_3\text{CH}_2\text{Br}$	28.3	20.3	
$\text{CH}_3\text{CH}_2\text{I}$	-0.2	21.6	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{Cl}$	46.7	26.5	11.5
$\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}$	35.7	26.8	13.2
$\text{CH}_3\text{CH}_2\text{CH}_2\text{I}$	10.0	27.6	16.2

4.7: Amines

An NH_2 group attached to an alkyl chain causes a downfield shift of about 30 ppm at C-1, a downfield shift of about 11 ppm at C-2, and an upfield shift of about 4.0 ppm at C-3. The NH_3^+ group shows a somewhat smaller effect. N-alkylation increases the downfield effect of the NH_2 group at C-1. Shift positions for selected acyclic and alicyclic amines are given in Table 4.14A.

Table 4.14A: Shift positions of Acyclic and Alicyclic Amines (neat, ppm from TMS)

Compound	C-1	C-2	C-3	C-4
CH_3NH_2	26.9			
$\text{CH}_3\text{CH}_2\text{NH}_2$	35.9	17.7		
$\text{CH}_3\text{CH}_2\text{CH}_2\text{NH}_2$	44.9	27.3	11.2	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2$	42.3	36.7	20.4	14.0
$(\text{CH}_3)_3\text{N}$	47.5			
$\text{CH}_3\text{CH}_2\text{N}(\text{CH}_3)_2$	58.2	13.8		
Cyclohexylamine	50.4	36.7	25.7	25.1
N-Methylcyclohexylamine	58.6	33.3	25.1	26.3

(N- CH_3 , 33.5)

4.8: Thiols, Sulfides, and Disulfides

Since the electronegativity of sulfur is considerably less than that of oxygen, sulfur causes a correspondingly smaller chemical shift. Examples of thiols, sulfides, and disulfides are given in Table 4.14 B

Table 4.14B: Shift positions of Thiols, Sulfides, and Disulfides (ppm from TMS)

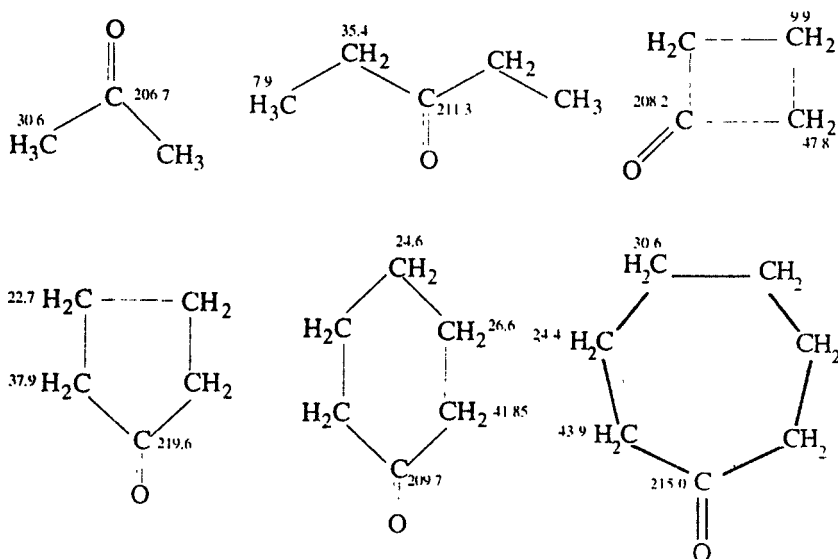
Compounds	C-1	C-2	C-3
CH_3SH	6.5		
$\text{CH}_3\text{CH}_2\text{SH}$	19.8	17.3	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{SH}$	26.4	27.6	12.6
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{SH}$	23.7	35.7	21.0
$(\text{CH}_3)_2\text{S}$	19.3		
$(\text{CH}_3\text{CH}_2)_2\text{S}$	25.5	14.8	
$(\text{CH}_3\text{CH}_2\text{CH}_2)_2\text{S}$	34.3	23.2	13.7
$(\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2)_2\text{S}$	34.1	31.4	22.0
CH_3SSCH_3	22.0		
$(\text{CH}_3\text{CH}_2\text{SSCH}_2\text{CH}_3)$	32.8	14.5	

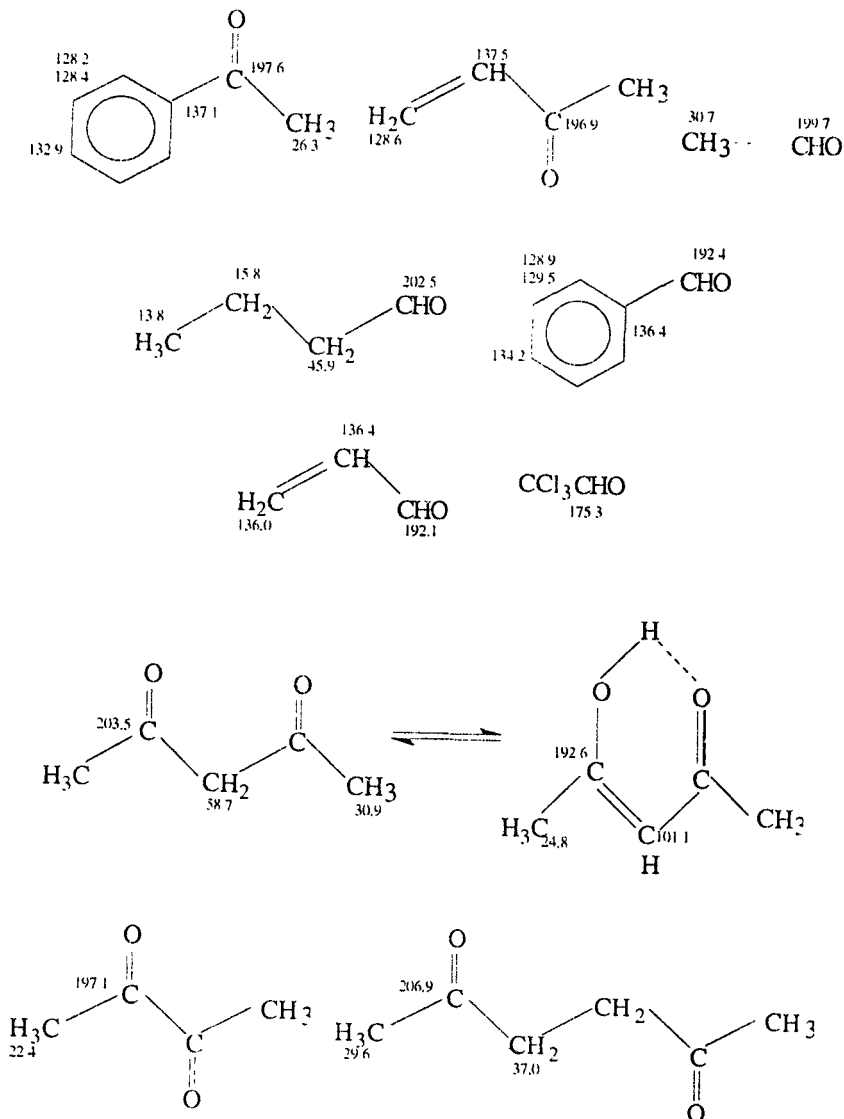
4.9: Functional Groups Containing Carbon

Carbon- ^{13}C NMR spectrometry permits direct observation of carbon containing functional groups. With the exception of $\text{CH}=\text{O}$, the presence of these groups could not be directly ascertained by ^1H NMR.

4.9.1. Ketones and Aldehyde:

Table 4.15 presents chemical shifts of the $\text{C}=\text{O}$ group of some ketones aldehydes. Because of rather large solvent effects, there are differences of several parts per million from different literature sources.

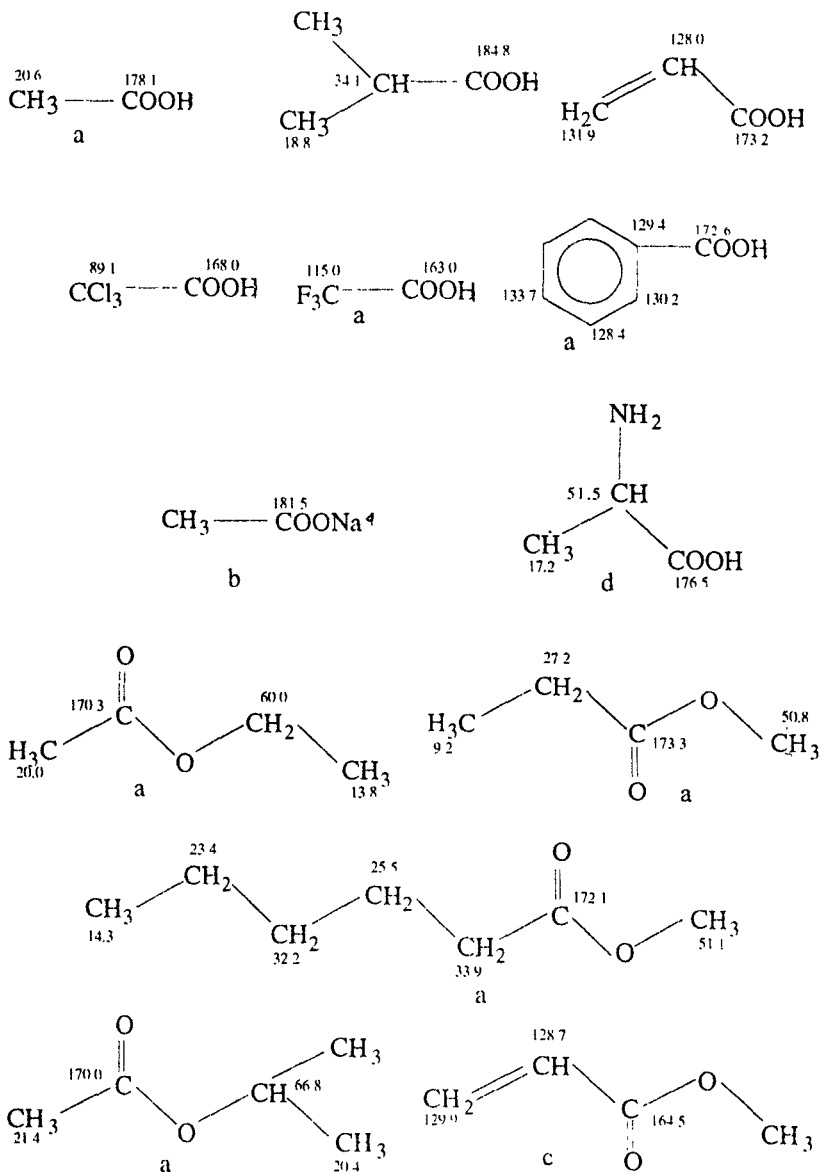
Table 4.15: Shift positions of the $\text{C}=\text{O}$ Group and Other carbon Atoms of Ketones and Aldehydes (ppm from TMS)

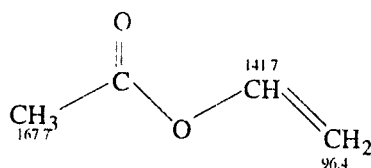


4.9.2. Carboxylic Acids, Ester, Chlorides Anhydrides, Amides and Nitriles:

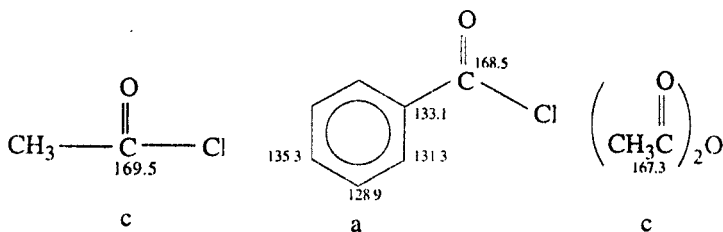
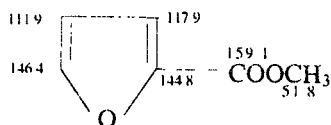
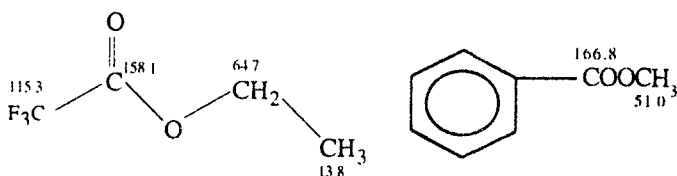
The C=O groups of carboxylic acids and derivatives are in the range of 150–185 ppm. Nitriles absorb in the range of 115–125 ppm.

Table 4.16: Shift Positions for the C=O group and other carbon atoms of carboxylic acids, esters, lactones, chlorides, anhydrides, amides, carbamates, and nitriles (ppm from TMS)





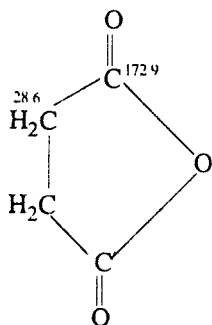
c



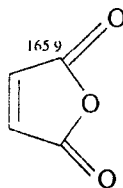
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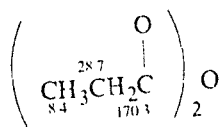
a

c

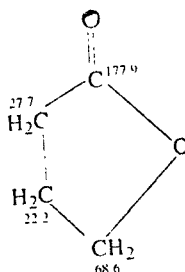


a

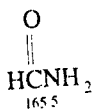




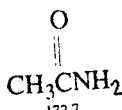
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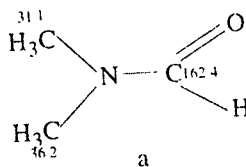
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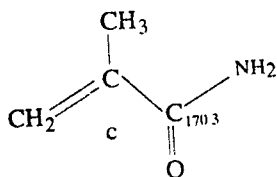
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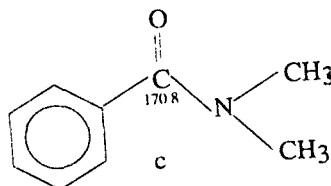
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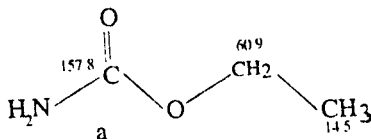
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c



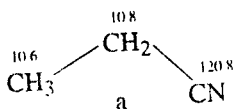
c



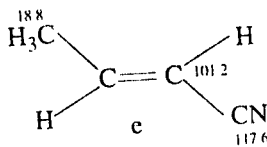
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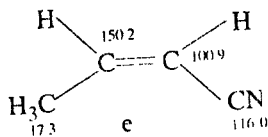
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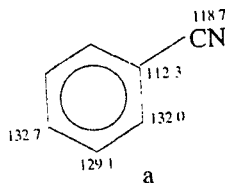
a



e



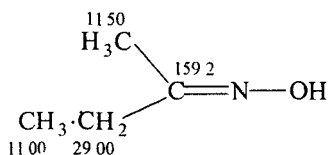
e



a

- In CHCl_3 (~50%)
- Saturated aqueous solution of CH_3COONa
- Neat or saturated solution
- In H_2O
- In DMSO
- In dioxane (~50%)

4.9.3 Oximes : The simple oximes absorb in the range of 145–165 ppm. For example



4.10: Spin Coupling

The ^{13}C – ^{13}C coupling is usually not observed, except in compounds that have been deliberately enriched with ^{13}C , because of the low probability of two adjacent ^{13}C atoms in a molecule. One bond ^{13}C –H coupling ($^1J_{\text{CH}}$) ranges from about 110 to 320 Hz, increasing with increased s character of the ^{13}C –H bond, with substitution on the carbon atom of electron withdrawing groups, and with angular distortion. Appreciable ^{13}C –H coupling also extends over two or more (n) bonds ($^nJ_{\text{CH}}$). Table 4.17 gives some representative ($^1J_{\text{CH}}$) values. Table 4.18 gives some representative ($^2J_{\text{CH}}$) values, which range from about –5 to 60 Hz.

Table 4.17: Some ($^1J_{\text{CH}}$) Values

Compound	J(Hz)
SP^3	
CH_3CH_3	124.9
$\text{CH}_3\text{CH}_2\text{CH}_3$	119.2
$(\text{CH}_3)_3\text{CH}$	114.2
CH_3NH_2	133.0
CH_3OH	141.0
CH_3Cl	150.0
CH_2Cl_2	178.0
CHCl_3	209.0

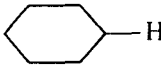
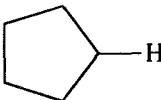
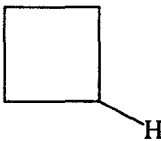
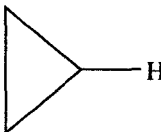
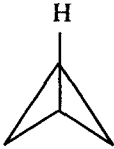
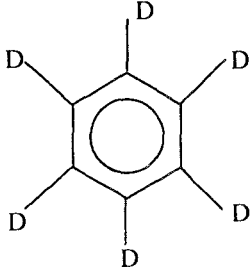
	123.0
	128.0
	134.0
	161.0
	205.0
sp^2	
$\text{CH}_2=\text{CH}_2$	156.2
$\text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2$	148.4
$\text{CH}_3\text{CH}=\text{O}$	172.4
$\text{NH}_2\text{CH}=\text{O}$	188.3
C_6H_6	159.0
sp	
$\text{CH}\equiv\text{CH}$	249.0
$\text{C}_6\text{H}_5\text{C}\equiv\text{CH}$	251.0
$\text{HC}\equiv\text{N}$	269.0

Table 4.18: Some ($^2J_{\text{CH}}$) Values

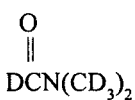
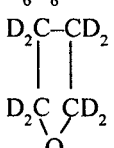
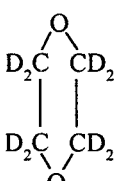
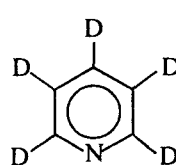
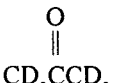
Compound	J(HZ)
sp^3	
CH_3CH_3	-4.5
CH_3CCl_3	5.9

$\underline{\text{C}}\text{H}_2\underline{\text{C}}\text{H}=\text{O}$	26.7
sp^2	
$\underline{\text{C}}\text{H}_2=\underline{\text{C}}\text{H}_2$	-2.4
$(\underline{\text{C}}\text{H}_3)_2\underline{\text{C}}=\text{O}$	5.5
$\text{CH}_2=\underline{\text{C}}\text{H}\underline{\text{C}}\text{H}=\text{O}$	26.9
C_6H_6	1.0
s p	
$\underline{\text{C}}\text{H}\equiv\underline{\text{C}}\text{H}$	49.3
$\text{C}_6\text{H}_5\underline{\text{O}}\underline{\text{C}}\equiv\underline{\text{C}}\text{H}$	61.0

Table 4.19: Coupling Constants for ^{31}P , ^{19}F , and D coupled to ^{13}C .

Compound	$^1\text{J}(\text{HZ})$	$^2\text{J}(\text{HZ})$	$^3\text{J}(\text{HZ})$
CH_3CF_3	271		
CF_2H_2	235		
$\text{CF}_3\text{CO}_2\text{H}$	284	43.7	
$\text{C}_6\text{H}_5\text{F}$	245	21.0	
$(\text{CH}_3\text{CH}_2)_3\text{P}$	5.4	10.0	
$(\text{CH}_3\text{CH}_2)_4\text{P}^+\text{Br}^-$	49	4.3	
$(\text{C}_6\text{H}_5)_3\text{P}^+\text{CH}_3\text{I}$	88(CH_3 52)	10.9	
$\text{CH}_3\text{CH}_2\text{P}(\text{OCH}_2\text{CH}_3)_2$	143	7.1(j_{COR} 6.9)	J_{CCOR} 6-2
$\begin{array}{c} \text{O} \\ \parallel \\ \text{C} \end{array}$			
CDCl_3	31.5		
CD_3CCD_3	19.5		
$\begin{array}{c} \text{O} \\ \parallel \\ \text{C} \end{array}$			
$(\text{CD}_3)_2\text{SO}$	22.0		
	25.5		

4.11: The ^{13}C Chemical Shifts, Couplings, and Multiplicities of Common NMR Solvents

Structure	Name	$\delta(\text{ppm})$	JC-D(HZ)	Multiplicity ^a
CDCl_3	Chloroform-d,	77.0	32	Triplet
CD_3OD	Methanol-d ₄	49.0	21.5	Septet
CD_3SOCD_3	DMSO-D ₆	39.7	21	Septet
	DMF-d ₇	30.1	21	Septet
		35.2	21	Septet
		167.7	30	Triplet
C_6D_6	Benzene-d ₆	128.0	24	Triplet
	THF-d ₈	25.2	20.5	Quintet
		67.4	22	Quintet
	Dioxane-d ₈	66.5	22	Quintet
	Pyridine-d ₅	123.5 (C-3,5)	25	Triplet
		135.5 (C-4)	24.5	Triplet
		149.2 (C-2,6)	27.5	Triplet
	Acetone-d ₆	29.8(methyl)	20	Septet
		206.5 (carbonyl)	<1	Septet ^b
CD_3CN	Acetonitrile-d ₃	1.3(methyl)	32	Septet
		118.2(CN)	<1	Septet ^b
CD_3NO_2	Nitromethan-d ₃	60.5	23.5	Septet

CD ₃ CD ₂ OD	Ethanol-d ₆	15.8(C-2)	19.5	Septet
		55.4(C-1)	22	Quintet
(CD ₃ CD ₂) ₂ O	Ether-d ₁₀	13.4 (C-2)	19	Septet
		64.3(C-1)	21	Quintet
[(CD ₃) ₂ N] ₃ P=O	HMPA-d ₁₈	35.8	21	Septet
CD ₃ CO ₂ D	Acetic acid-d ₄	20.0(C-2)	20	Septet
		178.4(C-1)	<1	Septet ^b
CD ₂ Cl ₂	Dichloromethane-d ₂ (Methylene chloride-d ₂)	53.1	29	Quintet

^a Triplet intensities = 1:1:1, quintet = 1:2:3:2:1, septet = 1:3:6:7:6:3:1.

^b Unresolved, long. range coupling.

4.12: The ¹³C Correlation Table for Chemical Classes

R = H or alkyl substituents

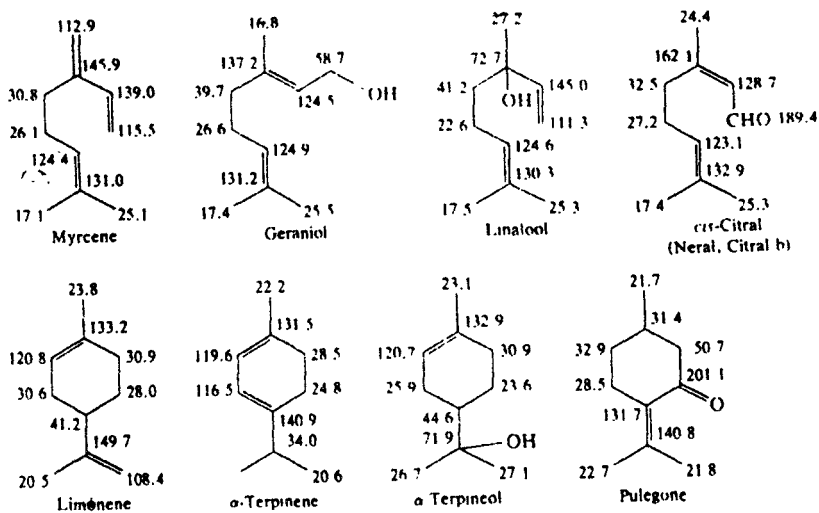
Y = Polar substituents

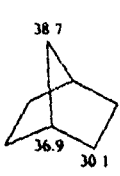
Types and group	δ(ppm)
Acyclic hydrocarbons	
-CH ₃	8-30
-CH ₂	14-55
-CH	24-59
-C-	30-40
Aticyclic hydrocarbons	
C ₃ H ₆	15-19
C ₄ H ₈ to C ₁₀ H ₂₀	21-29
Alkenes	
H ₂ C = C-R	102-121 (H ₂ C=)
	109-150 (=C-R)
H ₂ C=C-Y	80-170
C=C-C=C-R	109-151

Allenes	
$\text{C}=\text{C}=\text{C}$	70–97 ($=\text{C}$) 200–214 ($=\text{C}=\text{C}$)
Alkynes	
$\text{C}\equiv\text{C}-\text{R}$	63–73 ($\text{HC}\equiv$) 71–89 ($\equiv\text{C}-\text{R}$)
$\text{C}\equiv\text{C}-\text{Y}$	20–94
Aromatics	
$\text{Ar}-\text{R}$	120–150
$\text{Ar}-\text{Y}$	94–158
Heteroaromatics	100–166
Alcohols $\text{C}-\text{OH}$	44–86
Ethers $\text{C}-\text{O}-\text{C}$	54–86
Acetals, Ketals $\text{O}-\text{C}-\text{O}$	8–12
Halides	
$\text{C}-\text{F}_{1-3}$	72–134
$\text{C}-\text{Cl}_{1-4}$	20–98
$\text{C}-\text{Br}_{1-4}$	-28.5–+33
$\text{C}-\text{I}_{1-4}$	-292.5–+42
Amines $\text{C}-\text{NR}_2$	20–70
Nitro $\text{C}-\text{NO}_2$	60–78
Mercaptans, Sulfides $\text{C}-\text{S}-\text{R}$	5.5–46
Sulfoxides, Sulfones	
$\text{C}-\text{SO}-\text{R}$, $\text{C}-\text{SO}_2-\text{R}$	36–54
Aldehydes, Sat. $\text{R}-\text{CHO}$	197–220
Aldehydes, α , β -unsat. $\text{R}-\text{C}=\text{C}-\text{CH}=\text{O}$	176–194
Ketones, Sat. $\text{R}_2\text{C}=\text{O}$	195–220
Ketones, α , β unsat.	
$\text{R}-\text{C}=\text{C}-\text{C}=\text{O}$	182–212
Carboxylic acids, sat.	
$\text{R}-\text{COOH}$	166–186
Salts $\text{RCOO}-$	174–194
Carboxylic acids α , β -unsat.	

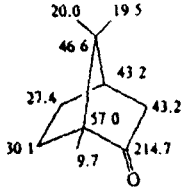
R-C=C-COOH	159-174
Esters, sat. R-COOR ¹	158-177
Esters, α , β - unsat.	
R-C=C-COOR ¹	153-172
Anhydrides (RCO) ₂ O	148-174
Amides RCONH ₂	150-177
Nitriles RC \equiv N	108-124
Oximes R ₂ C=NOH	144-166
Carbamates	
R ₂ NCOOR ¹	151-160
Isocyanates	
R-N=C=O	111-134
Cyanates R-O-C \equiv N	104-120
Isothiocyanates	
R-N=C=S	116-141
Thiocyanates	
R-S-C \equiv N	98-118

¹³C NMR data for several natural products (δ)

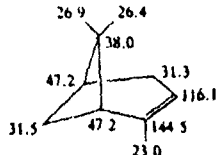




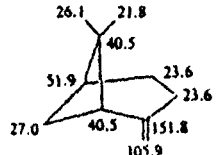
Norbornane



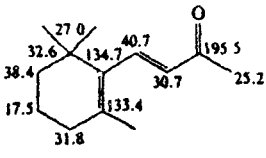
Camphor



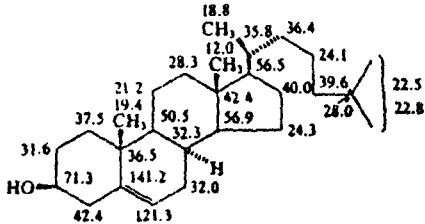
α -Pinene



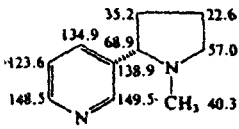
β -Pinene



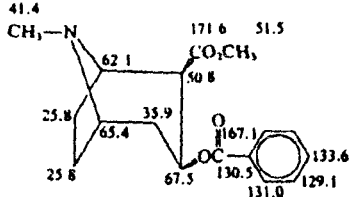
β -Ionone



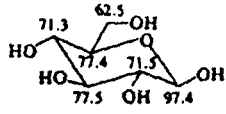
Cholesterol



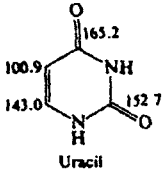
Nicotine



Cocaine



β -D-Glucose



Uracil



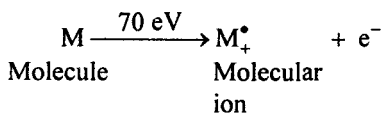
5

Mass Spectrometry

A mass spectrum is a presentation of the masses of the positively charged fragments versus their relative concentrations.

The commonest method of presentation is either a bar graph or a percentage table.

Mass spectra are routinely obtained at an electron beam energy of 70eV. The simplest event that occurs is the removal of a single electron from the molecule in the gas phase by an electron of the electron beam to form the molecular ion, which is a radical cation (M_+^{\bullet}). The symbol $_+^{\bullet}$ indicates that the molecule has lost an electron, it has unpaired electron and is positively charged.



If some of the molecular (parent) ions remain intact long enough to reach the detector, we see a molecular ion peak. It is important to recognize the molecular ion peak because this gives the molecular weight of the compound. The molecular ion peak is usually the peak of highest mass number except for the isotope peaks.

The molecular ion in turn produces a series of fragment ions.

The most intense peak in the spectrum called the base peak is assigned

a value of 100%, and the intensities of the other peaks, including the molecular ion peak, are reported as percentage of the base peak. Of course, the molecular ion peak may sometimes be the base peak.

The molecular ion in turn produces a series of fragment ions as shown for benzamide:

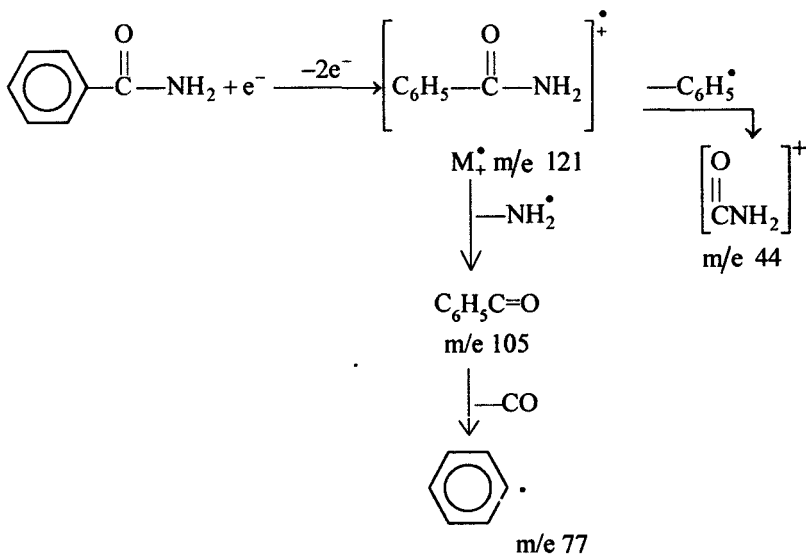


Table 5.1: Exact Masses of Isotopes

Element	Atomic Weight	Nuclide	Mass
Hydrogen	1.00794	^1H	1.00783
		$\text{D}(^2\text{H})$	2.01410
Carbon	12.01115	^{12}C	12.00000 (std)
		^{13}C	13.00336
Nitrogen	14.0067	^{14}N	14.0031
		^{15}N	15.0001
Oxygen	15.9994	^{16}O	15.9949
		^{17}O	16.9991
		^{18}O	17.9992
Fluorine	18.9984	^{19}F	18.9984

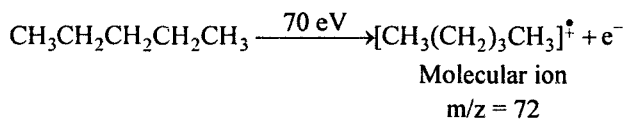
Silicon	28.0855	²⁸ Si	27.9769
		²⁹ Si	28.9765
		³⁰ Si	29.9738
Phosphorus	30.9738	³¹ P	30.9738
Sulfur	32.066	³² S	31.9721
		³³ S	32.9715
		³⁴ S	33.9679
Chlorine	35.4527	³⁵ Cl	34.9689
		³⁷ Cl	36.9659
Bromine	79.904	⁷⁹ Br	78.9183
		⁸¹ Br	80.9163
Iodine	126.9045	¹²⁷ I	126.9045

Table 5.2: Relative isotope Abundances of Common Elements

Elements	Isotope	Relative Abundance	Isotope	Relative Abundance	Isotope	Relative Abundance
Carbon	¹² C	100	¹³ C	1.11		
Hydrogen	¹ H	100	² H	0.016		
Nitrogen	¹⁴ N	100	¹⁵ N	0.38		
Oxygen	¹⁶ O	100	¹⁷ O	0.04	¹⁸ O	0.20
Fluorine	¹⁹ F	100				
Silicon	²⁸ Si	100	²⁹ Si	5.10	³⁰ Si	3.35
Phosphorus	³¹ P	100				
Sulfur	³² S	100	³³ S	0.78	³⁴ S	4.40
Chlorine	³⁵ Cl	100			³⁷ Cl	32.5
Bromine	⁷⁹ Br	100			⁸¹ Br	98.0
Iodine	¹²⁷ I	100				

Peaks attributable to isotopes can help identify the compound responsible for a mass spectrum.

For example



Although the molecular ion of pentane have m/z value of 72, its mass spectrum shows a very small peak at $m/z = 73$. This is called an M+1 peak because the ion responsible for this peak is one unit heavier than the molecular ion. The M+1 peak occurs because there are two naturally occurring isotopes of carbon : 98.89% of natural carbon ^{12}C and 1.11% is ^{13}C . The M+1 fragment results from molecular ions that contain one ^{13}C instead of a ^{12}C .

Above table shows that the M+1 peak can be used to determine the number of carbon atoms in a compound because the contributions to the M+1 peak by isotopes of H, O and the halogens are very small.

Presence of an isotopic peak at $(M^+ + 2)$ indicates the presence of four elements O, S, Br, Cl.

The presence of a large M+2 peak is evidence of a compound containing either chlorine or bromine, because each of these elements has a high percentage of a naturally occurring isotope two unit heavier than the most abundant isotope.

If the M+2 peak is one-third the height of the molecular ion peak, the compound contains a chlorine atom because the natural abundance of ^{37}Cl is one-third that of the ^{35}Cl .

If the M and M+2 peaks are of about the same height, the compound contains a bromine atom because the natural abundances of ^{79}Br and ^{81}Br are of about the same.

Recognition of the Molecular ion Peak

Many peaks can be ruled out as possible molecular ions simply on grounds of reasonable structure requirements. The nitrogen rule is often helpful. It states that a molecule of even-numbered molecular weight must contain either no nitrogen or an even number of nitrogen atoms; an odd-numbered molecular weight requires an odd number of nitrogen atoms. (for the nitrogen rule to hold, only unit atomic masses i.e., integers are used in calculating the formula masses)

This rule holds for all compounds containing carbon, hydrogen, oxygen, nitrogen, sulfur, and the halogens, as well as many of the less usual atoms such as phosphorus, boron, silicon, arsenic, and the alkaline earths.

The intensity of the molecular ion peak depends on the stability of the molecular ion. The most stable molecular ions are those of purely aromatic systems.

In general the following group of compounds will, in order of decreasing ability, give prominent molecular ion peaks: aromatic compounds > conjugated alkenes > cyclic compounds > organic sulfides > short, normal alkanes > mercaptans.

Recognisable molecular ions are usually produced for these compounds in order of decreasing ability:

ketones > amines > esters > ethers > carboxylic acids ~ aldehydes ~ amides ~ halides.

The molecular ion is frequently not detectable in aliphatic alcohols, nitrites, nitrates, nitro compounds, nitriles and in highly branched compounds.

The presence of an M-15 peak (loss of CH_3), or an M-18 peak (loss of H_2O), or an M-31 peak (loss of OCH_3 from methyl esters) and so on, is taken as confirmation of a molecular ion peak. An M-1 peak is common and occasionally an M-2 peak (loss of H_2 by either fragmentation or thermolysis) or even a rare M-3 peak (from alcohols) is reasonable. Peaks in the range of M-3 to M-14, however, indicate that contaminants may be present or that the presumed molecular ion peak is actually a fragment ion peak.

Losses of fragments of masses 19-25 are also unlikely (except for loss of $\text{F} = 19$ or $\text{HF} = 20$ from fluorinated compounds) loss of 16(O), 17(OH), or 18(H_2O) are likely only if an oxygen atom is in the molecule.

Summary of Fragmentation Processes

(1) Hydro carbons:

(a) Alkanes:

- * Straight chain alkanes show low intensity molecular ion peaks. The intensities of these peaks decrease with increasing chain length.
- * Since straight chain alkanes rarely eliminate methyl groups ($-\text{CH}_3$)

peaks corresponding to (M-15) are absent, or are of low intensity, in the spectra of long chain paraffins.

- * Elimination of $-C_2H_5$, $-C_3H_7$, from the molecular ion gives peaks at masses C_nH_{2n+1} ($m/e = 29, 43, 57, 71$ and 85). These peaks are most intense in the C_2 to C_5 range. The peaks at 43 or 57 are usually the base peaks, due to the remarkable stabilities of the propyl ion ($-C_3H_7^+$) and the butyl ion ($-C_4H_9^+$).

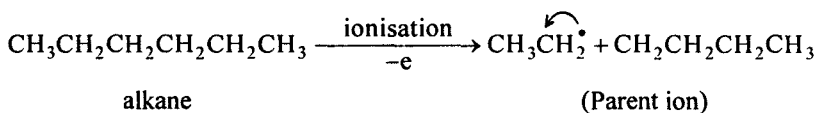
The intensities of other peaks 14 mass units ($-CH_2$) apart (71, 85, etc.) decrease with the increasing weight of the fragment. These peaks 14 units apart appear as clusters because each prominent peak is accompanied by a smaller peak one unit higher due to ^{13}C and a few small peaks one and two units lower, due to the loss of hydrogen atoms.

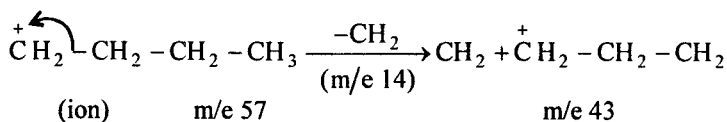
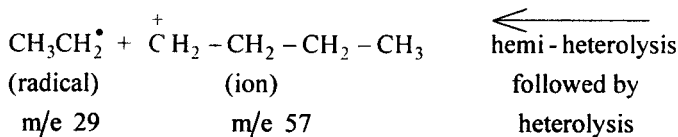
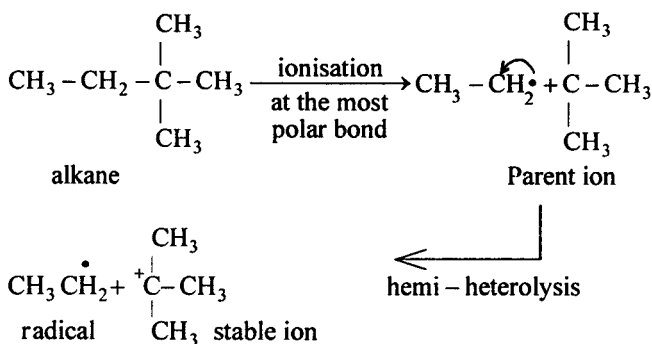
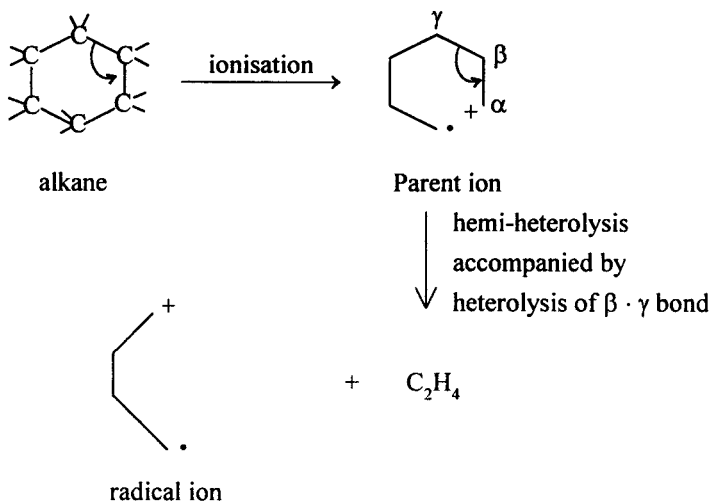
- * In branched alkanes, there is a tendency for the bonds to rupture at the branches resulting in the formation of relatively stable secondary and tertiary carbonium ions.
- * Molecular ion peaks are more abundant in cycloparaffins than in straight chain paraffins containing the same number of carbon atoms, although the cyclic compounds tend to lose their side chains.

If the ring undergoes fragmentation, it loses two carbon atoms simultaneously, thus producing an abundance of $^+C_2H_4$ (m/e 28), $^+C_2H_5$ (m/e 29), and M-28, M-29 ions in the spectrum. Due to this tendency to lose ethylene C_2H_4 and other even-mass number fragments, the percentage of fragments having even mass number are usually higher in the spectra of cycloparaffins than in those of acyclic hydrocarbons.

Mechanisms for fragmentations of different types of alkanes are believed to be as follows:

(i) Straight chain alkanes



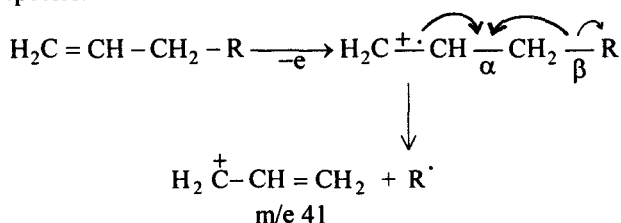
**(ii) Branched chain alkanes****(iii) Cycloalkanes**

(b) Alkenes

- * Alkenes readily produce molecular ions by losing a π -electron.

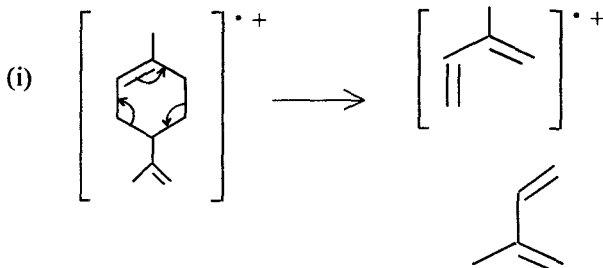
As in alkanes, so in alkenes, the intensity of the M peak decreases with increasing molecular weight.

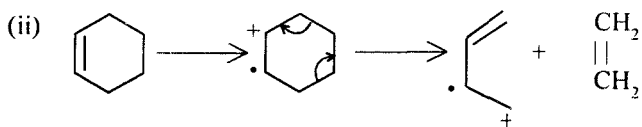
- * The most intense peak (usually the base peak) in the spectra of olefins is due to the stable, charged species produced by allylic cleavage, that is, by the rupture of the C-C bond β to the double bond. The fragment carrying the double bond is usually the charged species.



The natural outcome of allylic cleavage is a series of fragments at masses 41, 55, 69, 83, etc., with the general formula $\text{C}_n\text{H}_{2n-1}$ (allyl carbonium ions)

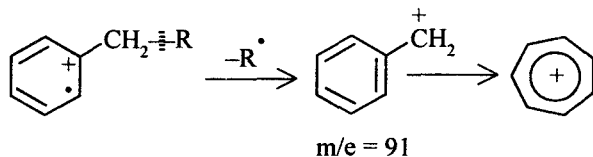
- * McLafferty rearrangements are also common in these ions. These rearrangements produce ions of the general formula $\text{C}_n\text{H}_{2n}^{\cdot+}$.
- * Cyclic alkenes usually show a distinct molecular ion peak. A unique mode of cleavage is the retro-Diels-Alder reaction shown by limonene:



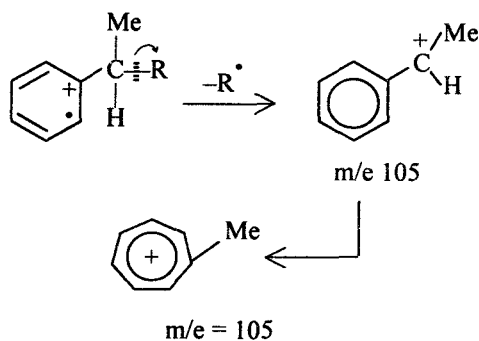


(c) Aromatic hydro carbons

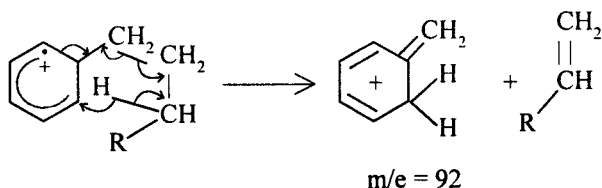
- * An aromatic ring in a molecule stabilises the molecular ion peak, which is usually sufficiently large that accurate intensity measurements can be made on the M+1 and M+2 peaks.
- * In alkyl benzenes the most probable cleavage is at the bond β to the ring. This gives rise to a base peak at m/e 91 due to the formation of tropyllium ion.



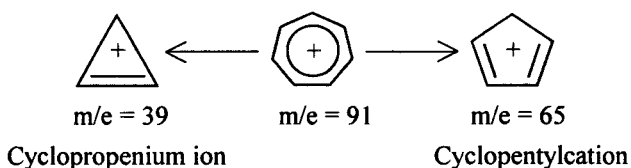
However, in compounds containing substituents on the α -carbon atom, the base peak may have masses higher than 91 by increments of 14, representing substituted tropyllium ions



A strong peak at $m/e = 92$ is observed in the case of many compounds containing a propyl or longer side chain. This peak is due to the ${}^+C_7H_8$ ion produced by the McLafferty rearrangement.



Fragmentation of a tropyllium ion into a cyclopentyl cation, ${}^+C_5H_5$, and a cyclopropenium ion ${}^+C_3H_3$, results in significant peaks at $m/e = 65$



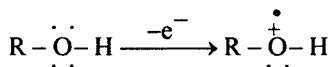
A characteristic cluster of ions resulting from an α cleavage and hydrogen migration in monoalkylbenzenes appears at m/e 77 ($C_6H_5^+$), 78 ($C_6H_6^+$) and 79 ($C_6H_7^+$).

(2) Hydroxy compounds

(a) Alcohols:

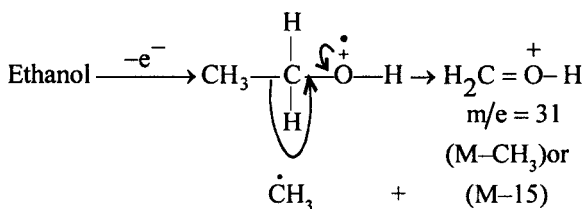
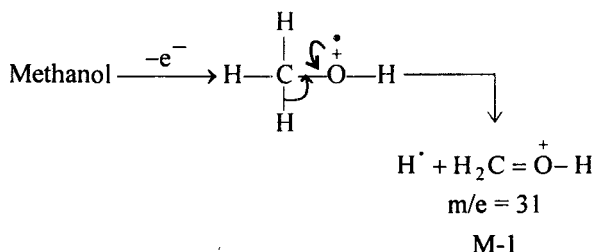
- * In the spectra of alcohols, the molecular ion peak M is usually either very small or totally absent. It is somewhat more abundant in the spectra of secondary than in those of primary and tertiary alcohols.

The odd-electron molecular ion is produced initially by the removal of an n -electron from oxygen:



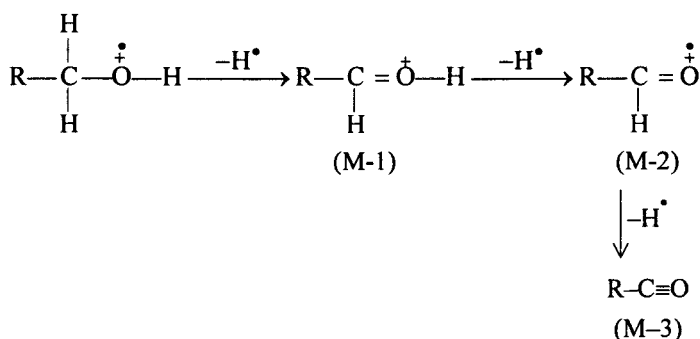
The odd-electron molecular ion readily decomposes into stable products.

One such decomposition involves energetically favoured α -cleavage. This cleavage leads to more stable, even-electron, oxonium ions.

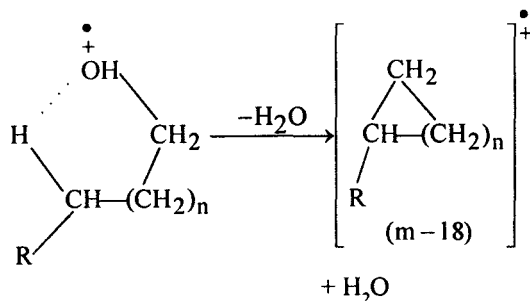


Although ethanol shows an M-1 peak at $m/e = 45$ by α -elimination of a hydrogen radical, the M-15 peak is more intense because α -elimination of a larger substituent is always favoured.

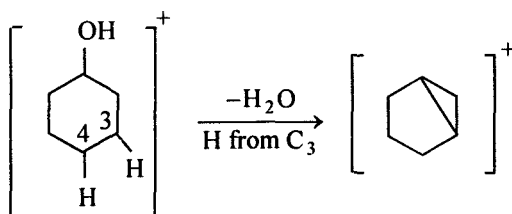
- * In the spectra of primary alcohols, in addition to the M-1 peak, very low intensity M-2 and M-3 peaks are also observed.



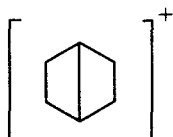
- * All primary alcohols (except methanol) and high molecular-weight secondary and tertiary alcohols display peaks at M-18 due to the loss of H₂O through a cyclic mechanism.



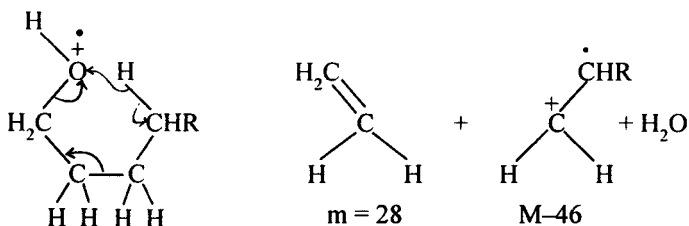
- * In cyclic alcohols, the principal dehydration process involves loss of a hydroxyl group together with a hydrogen atom from either C₃ or C₄ to produce bicyclo ions.



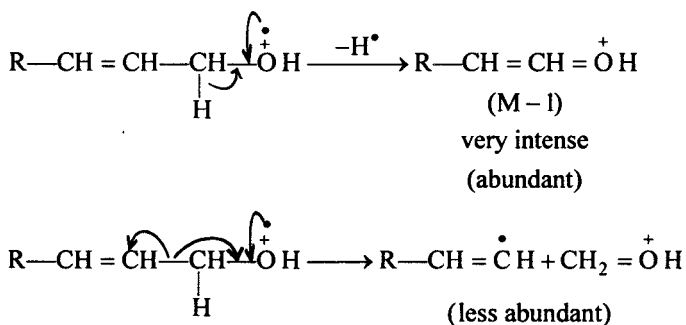
\downarrow $-\text{H}_2\text{O}, \text{H from C}_4$
 when cyclohexanol is
 in the boat form



- * Butanol & longer-chain primary alcohols often suffer double elimination. That is, they lose one molecule of water and one of ethylene simultaneously through a six-numbered cyclic mechanism, thus displaying an M-46 peak

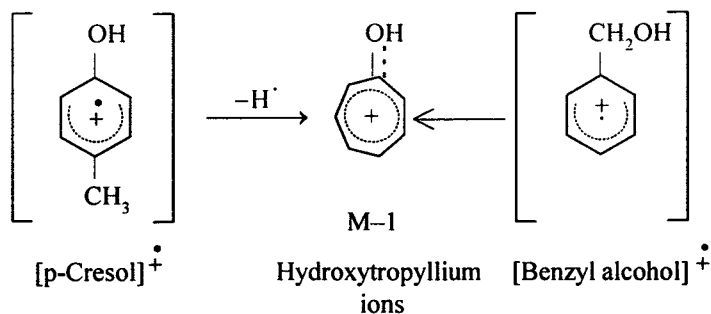


- * The most probable site of cleavage, resulting in a very intense peak, is the bond β to the oxygen atom in alcohols. This cleavage gives a strong peak at $m/e = 31$ $(\text{CH}_2\text{OH})^+$ in the spectra of primary alcohols, while secondary and tertiary alcohols display analogous peaks at $m/e = 45$ $(\text{MeCHOH})^+$ and $m/e = 59$ $[(\text{CH}_3)_2\text{COH}]^+$.
- * Unsaturated alcohols generally behave like their saturated analogs. However, the stability of the allyl system decreases the probability of cleavage adjacent to the double bond.

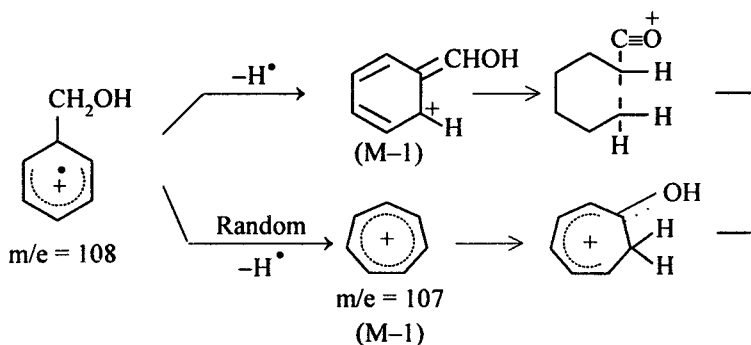
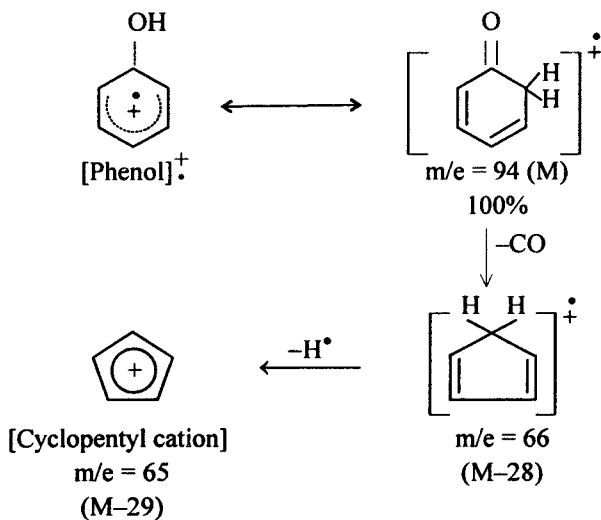


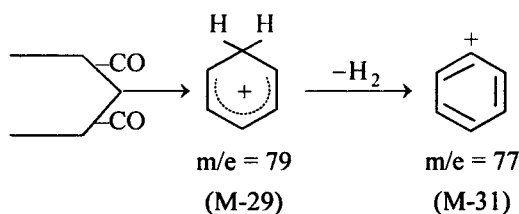
(b) Phenols and other aromatic alcohols:

- * As in all aromatic compounds, the molecular-ion peak M in phenol and aromatic alcohols is strong. In phenols it forms the base peak.
- * The $M-1$ peak due to the loss of hydrogen is small in phenol, but is very strong in cresols and benzyl alcohols. The production of $M-1$ ions is due to the random abstraction of hydrogen bonded to any of the carbon atoms to produce a resonance-stabilised. π complex system such as hydroxy tropyllium ions.



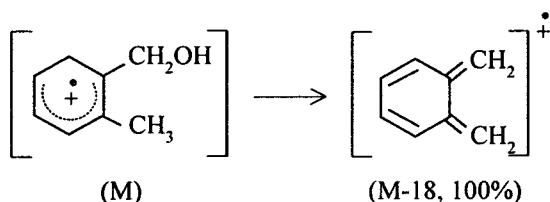
- * The most important fragmentation in phenols and benzyl alcohols is due to the loss of CO and CHO giving peaks corresponding to M-28 and M-29, respectively.





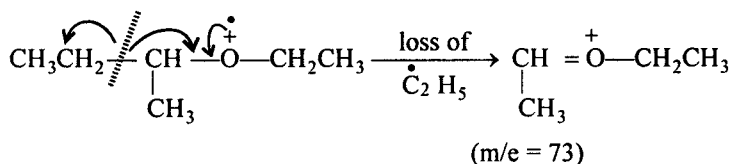
- * Methyl-substituted phenols (Cresols), other hydroxybenzenes (catechol, resorcinol, hydroquinone) and methyl-substituted benzyl alcohols display M-18 peaks due to loss of water.

The dehydration is more pronounced if the substituents are ortho to each other.



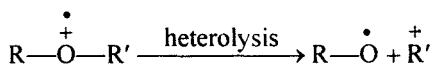
Ethers:

A molecular ion of ether is formed by the removal of one of the nonbonded electrons on oxygen, and, just as with alcohols, the molecular ions of ethers are unstable and readily undergo α -cleavage. (cleavage of a bond β to oxygen).



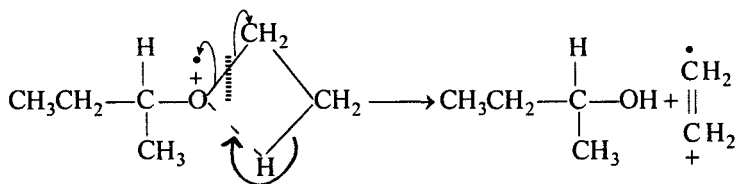
This type of cleavage usually accounts for the base peak and some strong peaks at 45, 59, 73 etc.

- * In ethers, unlike the case of alcohols, cleavage of bonds α to oxygen can also occur.



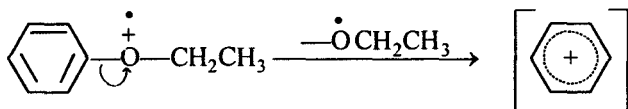
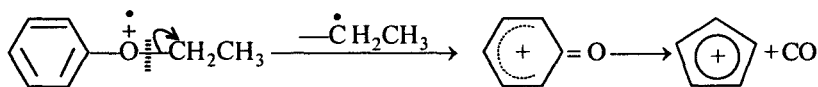
In such a cleavage, the alkyl portion carries the charge and accounts for hydrocarbon peaks at $m/e = 29, 43, 57, 71$ etc.

- * Homolytic fission of bonds α to oxygen may often be accompanied by rearrangement of one hydrogen atom to eliminate an olefin.

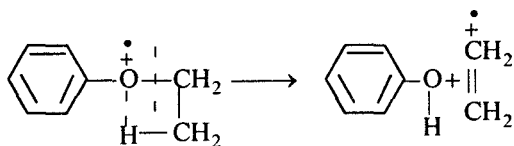


- * Aromatic ethers display a somewhat stronger M peak, and show a fragmentation behaviour similar to that of aliphatic ethers.

- (i) Cleavage of bonds α to oxygen can be homolytic or heterolytic.



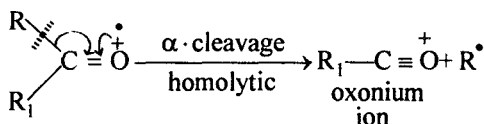
- (ii) Cleavage of bond α to oxygen with rearrangement of hydrogen to eliminate an alkene.



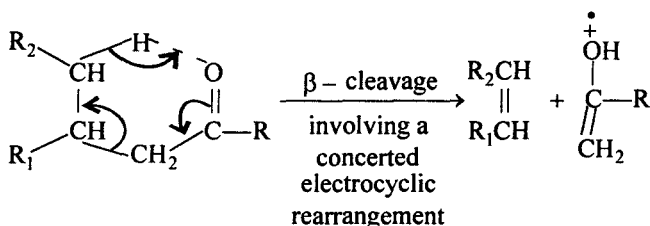
Aldehydes and Ketones:

Organic carbonyl compounds, like other oxygen containing compounds, undergo the loss of one of the lone-pair electrons of the oxygen atom.

The molecular ion thus produced can undergo fragmentation either through the more favourable α -cleavage or, if a concerted migration of γ hydrogen to oxygen is possible, through β -cleavage.

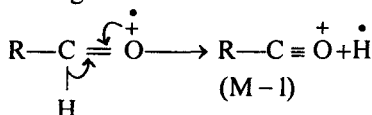


When a γ hydrogen is available for migration, β -cleavage results in the formation of an olefin and a charged enol through the McLafferty rearrangement.

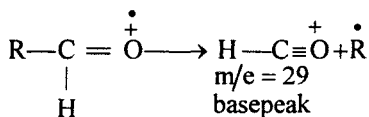


(a) Aldehydes:

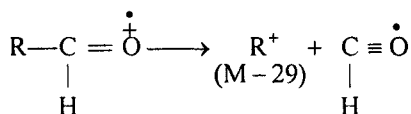
- * Aliphatic as well as aromatic aldehydes display molecular-ion peaks. The M peak is prominent in aromatic aldehydes, whereas the intensity of the M peak in aliphatic aldehydes decreases rapidly in compounds containing more than four carbon atoms.
- * In aldehydes, the M-1 peak is usually as intense as the M peak. The peak results from the loss of hydrogen through homolytic α -cleavage.



- * In lower aldehydes (C_1 - C_3), α -cleavage results in the formation of the stable formyl ion ($\text{H}-\text{C} \equiv \overset{+}{\text{O}}$), which forms the base peak.

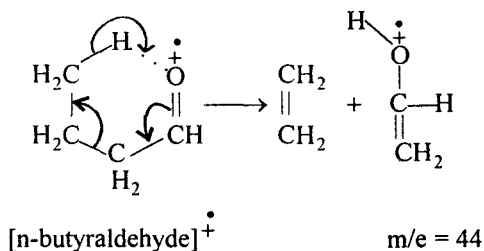


However, with straight chain aldehydes of higher molecular weight, this peak is approximately 40% of the base peak which may be displayed at M-29 due to ions produced through heterolytic cleavage as:



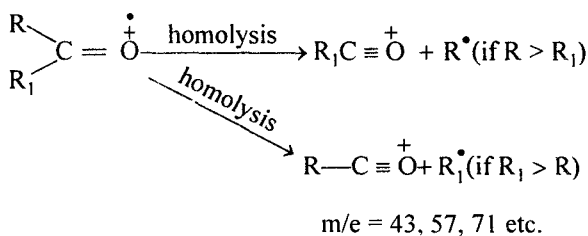
- * The base peak in butyraldehyde and in many higher aliphatic aldehydes results from β -cleavage.

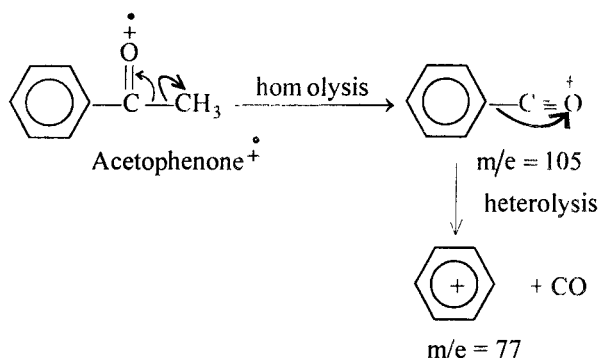
In butyraldehyde this peak is at $m/e = 44$, which must be a peak for a rearranged ion because it has an even mass number. In compounds containing C', H and O', peaks resulting from simple cleavage always appear at odd mass number, but the peaks due to rearranged ion have an even m/e ratio.



(b) Ketones:

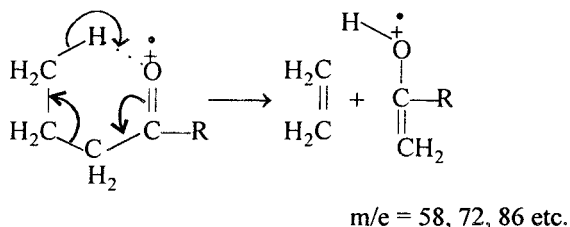
- * The parent-ion peak M in ketones is of significant intensity being greater for the low-molecular weight (upto eight carbons) than for the high-molecular weight ketones.
- * α -cleavage in ketones can produce more stable $\text{R}-\text{C} \equiv \text{O}^+$ ions.



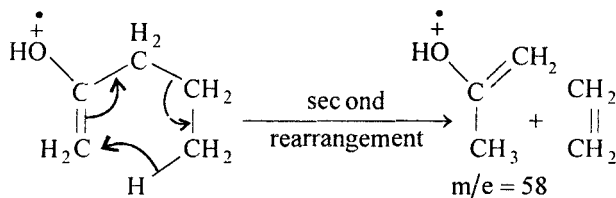


- * McLafferty rearrangements (β -cleavage with migration of γ -hydrogen) are common in ketones containing a chain of three or more carbon atoms attached to the carbonyl group. However, complications arise due to the following facts:

- (a) The mass of the ion produced by the migration of a single hydrogen varies with the number of carbon atoms in the alkyl group (R) which is not involved in the rearrangement.



- (b) If both the alkyl groups in the ketone contain three or more carbons, double rearrangement produces the enolic cation, which can again undergo β -cleavage involving the γ -hydrogen on the second alkyl group.



If the γ -carbon in either of the alkyl groups is substituted, the order of migration of the γ -hydrogen is found to be tertiary > secondary > primary, and the rearrangement preferentially involves the larger alkyl groups.

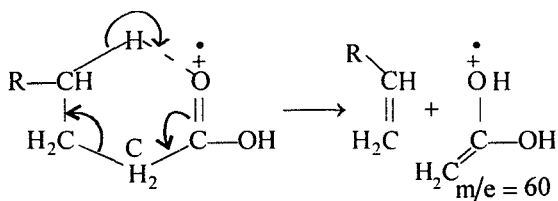
Carboxylic acids and esters

- * Aliphatic monocarboxylic acids and their esters generally display a weak but noticeable molecular-ion peak.

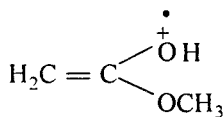
Aromatic monocarboxylic acids and esters, like other aromatic compounds, display a strong M peak.

- * Like other oxy compounds, cleavage of the bond β to carbonyl (β -cleavage), together with the rearrangement of γ -hydrogen (McLafferty rearrangement) is the most important mode of fragmentation of carboxylic acids.

In monocarboxylic acids, this fragmentation produces ions (I) which exhibit a characteristic peak at $m/e = 60$



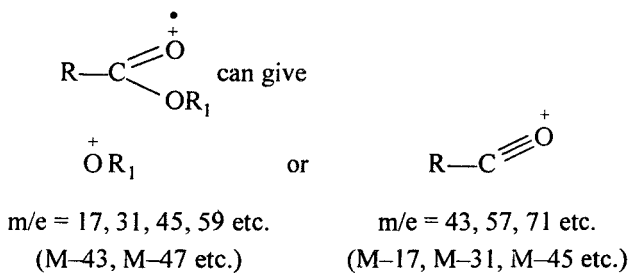
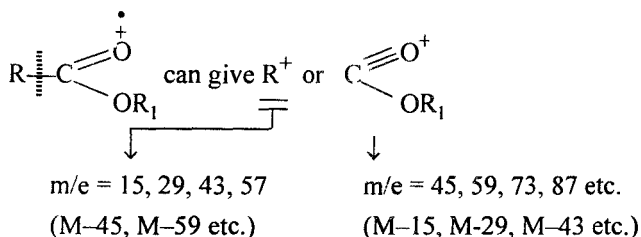
A corresponding β -cleavage peak in methyl esters appears at $m/e = 74$ due to (II).



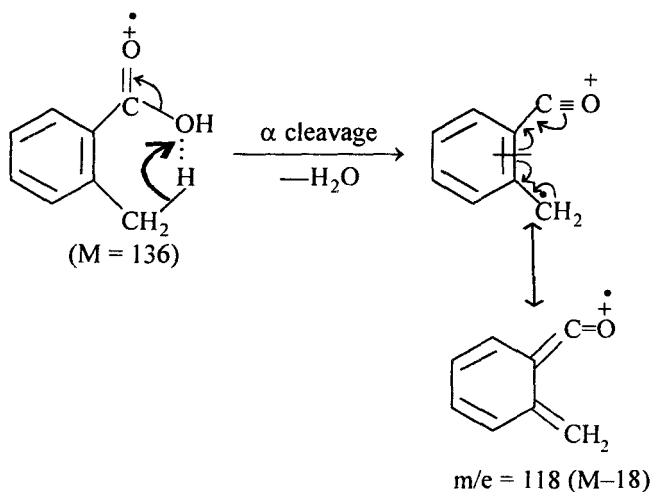
II

Analogous peaks in ethyl and butyl esters appear at 88 and 116, respectively.

- * In acids and esters, a similar cleavage of a bond α to carbonyl can produce four kinds of ions.



- * In aromatic acids containing a methyl group ortho to the carboxyl, elimination of a stable molecule of water produces a peak at M-18. This elimination is so important that in o-toluic acid the M-18 peak is the base peak.

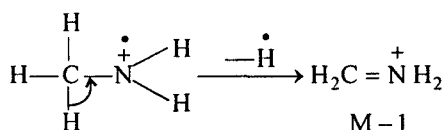


- * Dibasic acids show a peak at $M-90$ due to the loss of both carboxyls through α -cleavage.

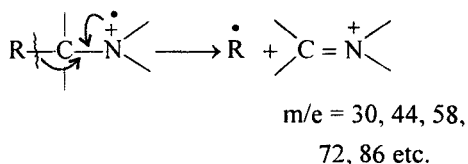
Amines

In amines, as in oxygen containing compounds such as alcohols, ketones, aldehydes, etc., the initial ionisation process occurs through the loss of a nonbonded electron on the hetero atom, nitrogen.

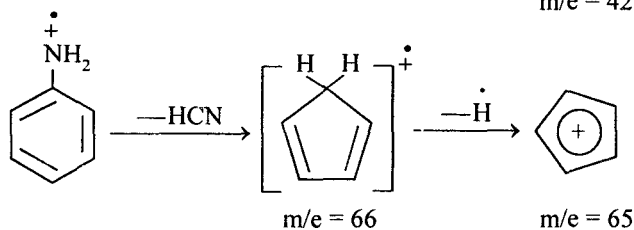
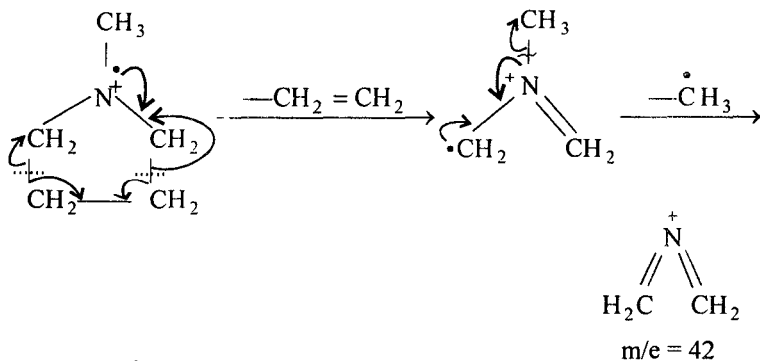
- * The molecular-ion peak M is weak to absent in high-molecular weight aliphatic open-chain amines, but strong in aromatic and cyclic amines.
- * In the case of monoamines, if the molecular-ion peak is present, it appears at an odd mass number in the spectrum. In the case of other nitrogen compounds also, it appears at odd mass number when the compound contains an odd number of nitrogen atoms (the nitrogen rule).
- * A moderate $M-1$ peak is observed in many aromatic and low-molecular-weight aliphatic amines due to the loss of a hydrogen radical.



- * In amines, as in alcohols, the most important fragmentation is that of the bond β to nitrogen. In many amines this fragmentation is responsible for the base peak.

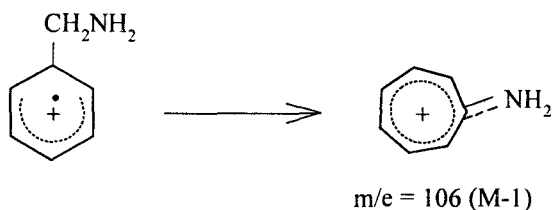


- * In cyclic and aromatic amines, both bonds β to nitrogen can rupture.

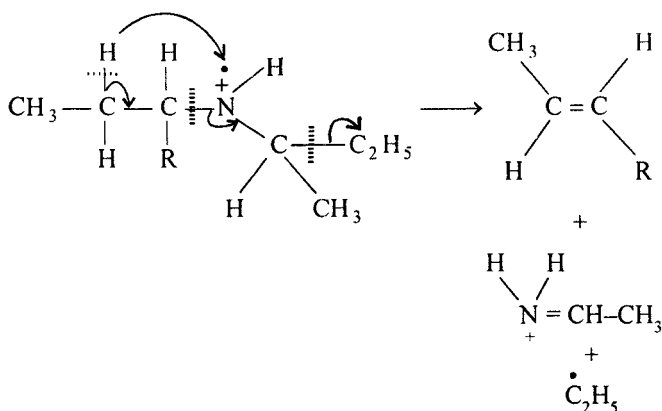


The loss of HCN and H_2CN from aniline is similar to the elimination of CO and CHO from phenol.

- * Like other side-chain aromatic compounds, alkyl anilines undergo β -elimination of the side chain and show a strong peak at $m/e = 106$ to the aminotropylium ion



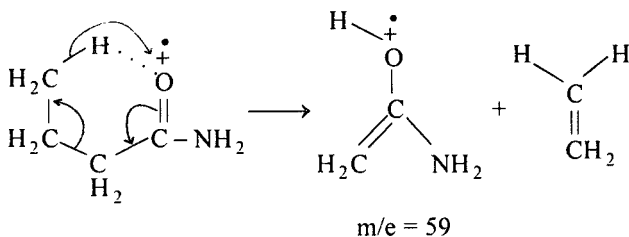
- * If the α -carbon carries substituents, a complicated fragmentation, involving bonds α and β to nitrogen and a migration of β -hydrogen, can take place in secondary and tertiary amines. For example,



Amides

The mass spectroscopic behaviour of amides is generally similar to that of corresponding carboxylic acids.

- * Amides usually display an easily distinguishable molecular-ion peak which, if only one amido group is present, manifests itself at odd mass number in the spectrum.
- * In amides, as in carboxylic acids, cleavage of a carbon-carbon bond β to the carbonyl (β -cleavage) is the most important fragmentation process. In amides which have γ -hydrogen available for migration, the McLafferty rearrangement is equally common. In most primary amides, the resulting ion usually forms the base peak.



- * In the case of long-chain primary amides cleavage of the bond γ to carbonyl can also take place, giving minor peaks at mass 72 (without rearrangement) and 73 (with rearrangement).

- * Strong peaks are also displayed at $m/z = 44$ by primary amides (containing upto four carbon atoms), due to rupture of the bond β to nitrogen (or α to carbonyl). This fragmentation is similar to that observed in amines.

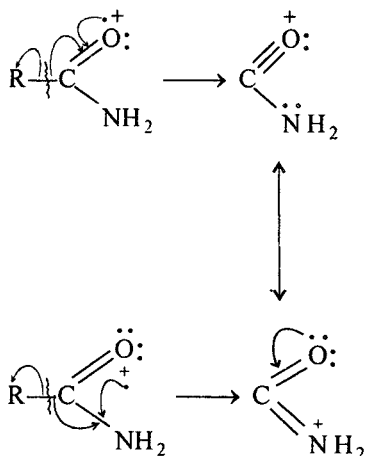


Table 5.3: Masses and Isotopic Abundance Ratios for Various Combinations of Carbon, Hydrogen, Nitrogen and Oxygen^a

FM		FM		FM	
	16		25		
12	O	15.9949	C ₂ H	25.0078	
C	12.0000	H ₂ N	16.0187	26	
13	CH ₄	16.0313	CN	26.0031	
CH	13.0078	17	C ₂ H ₂	26.0157	
14	HO	17.0027	27		
N	14.0031	H ₃ N	17.0266	CHN	27.0109
CH ₂	14.0157	18	C ₂ H ₃	27.0235	
15	H ₂ O	18.0106	28		
HN	15.0109	24	N ₂	28.0062	
CH ₃	15.0235	C ₂	24.0000	CO	27.9949

	FM		FM		FM
CH ₂ N	28.0187	38		H ₂ N ₃	44.0249
C ₂ H ₄	28.0313	C ₂ N	38.0031	CO ₂	43.9898
29		C ₃ H ₂	38.0157	CH ₂ NO	44.0136
HN ₂	29.0266	39		CH ₄ N ₂	44.0375
CHO	29.0027	C ₂ HN	39.0109	C ₂ H ₄ O	44.0262
CH ₃ N	29.0140	C ₃ H ₃	39.0235	C ₂ H ₆ N	44.0501
C ₂ H ₅	29.0391	40		C ₃ H ₈	44.0626
30		CN ₂	40.0062	45	
NO	29.9980	C ₂ O	39.9949	HN ₂ O	45.0089
H ₂ N ₂	30.0218	C ₂ H ₂ N	40.0187	H ₃ N ₃	45.0328
CH ₂ O	30.0106	C ₃ H ₄	40.0313	CHO ₂	44.9976
CH ₄ N	30.0344	41		CH ₃ NO	45.0215
C ₂ H ₆	30.0470	CHN ₂	41.0140	CH ₅ N ₂	45.0453
31		C ₂ HO	41.0027	C ₂ H ₅ O	45.0340
HNO	31.0058	C ₂ H ₃ N	41.0266	C ₂ H ₇ N	45.0579
H ₃ N ₂	31.0297	C ₃ H ₅	41.0391	46	
CH ₃ O	31.0184	42		NO ₂	45.9929
CH ₅ N	31.0422	N ₃	42.0093	H ₂ N ₂ O	46.0167
32		CNO	41.9980	H ₄ N ₃	46.0406
O ₂	31.9898	CH ₂ N ₂	42.0218	CH ₂ O ₂	46.0054
H ₂ NO	32.0136	C ₂ H ₂ O	42.0106	CH ₄ NO	46.0293
H ₄ N ₂	32.0375	C ₂ H ₄ N	42.0344	CH ₆ N ₂	46.0532
CH ₄ O	32.0262	C ₃ H ₆	42.0470	C ₂ H ₆ O	46.0419
33		43		47	
HO ₂	32.9976	HN ₃	43.0171	HNO ₂	47.0007
H ₃ NO	33.0215	CHNO	43.0058	H ₃ N ₂ O	47.0246
34		CH ₃ N ₂	43.0297	H ₅ N ₃	47.0484
H ₂ O ₂	34.0054	C ₂ H ₃ O	43.0184	CH ₃ O ₂	47.0133
36		C ₂ H ₅ N	43.0422	CH ₅ NO	47.0371
C ₃	36.0000	C ₃ H ₇	43.0548	48	
37		44		O ₃	47.9847
C ₃ H	37.0078	N ₂ O	44.0011	H ₂ NO ₂	48.0085

	FM		FM		FM
H ₄ N ₂ O	48.0324	C ₂ HNO	55.0058	C ₂ H ₄ NO	58.0293
CH ₄ O ₂	48.0211	C ₂ H ₃ N ₂	55.0297	C ₂ H ₆ N ₂	58.0532
C ₄	48.0000	C ₃ H ₃ O	55.0184	C ₃ H ₆ O	58.0419
49		C ₃ H ₅ N	55.0422	C ₃ H ₈ N	58.0657
HO ₃	48.9925	C ₄ H ₇	55.0548	C ₄ H ₁₀	58.0783
H ₃ NO ₂	49.0164	56		59	
C ₄ H	49.0078	N ₄	56.0124	HN ₃ O	59.0120
50		CN ₂ O	56.0011	H ₃ N ₄	59.0359
H ₂ O ₃	50.0003	CH ₂ N ₃	56.0249	CHNO ₂	59.0007
C ₃ N	50.0031	C ₂ O ₂	55.9898	CH ₃ N ₂ O	59.0246
C ₄ H ₂	50.0157	C ₂ H ₂ NO	56.0136	CH ₅ N ₃	59.0484
51		C ₂ H ₄ N ₂	56.0375	C ₂ H ₃ O ₂	59.0133
C ₃ HN	51.0109	C ₃ H ₄ O	56.0262	C ₂ H ₅ NO	59.0371
C ₄ H ₃	51.0235	C ₃ H ₆ N	56.0501	C ₂ H ₇ N ₂	59.0610
52		C ₄ H ₈	56.0626	C ₃ H ₇ O	59.0497
C ₂ N ₂	52.0062	57		C ₃ H ₉ N	59.0736
C ₃ O	51.9949	HN ₄	57.0202	60	
C ₃ H ₂ N	52.0187	CHN ₂ O	57.0089	N ₂ O ₂	59.9960
C ₄ H ₄	52.0313	CH ₃ N ₃	57.0328	H ₂ N ₃ O	60.0198
53		C ₂ HO ₂	56.9976	H ₄ N ₄	60.0437
C ₂ HN ₂	53.0140	C ₂ H ₃ NO	57.0215	CO ₃	59.9847
C ₃ HO	53.0027	C ₂ H ₅ N ₂	57.0453	CH ₂ NO ₂	60.0085
C ₃ H ₃ N	53.0266	C ₃ H ₅ O	57.0340	CH ₄ N ₂ O	60.0324
C ₄ H ₅	53.0391	C ₃ H ₇ N	57.0579	CH ₆ N ₃	60.0563
54		C ₄ H ₉	57.0705	C ₂ H ₄ O ₂	60.0211
CN ₃	54.0093	58		C ₂ H ₆ NO	60.0449
C ₂ NO	53.9980	N ₃ O	58.0042	C ₂ H ₈ N ₂	60.0688
C ₂ H ₂ N ₂	54.0218	H ₂ N ₄	58.0280	C ₃ H ₈ O	60.0575
C ₃ H ₂ O	54.0106	CNO ₂	57.9929	C ₅	60.0000
C ₃ H ₄ N	54.0344	CH ₂ N ₂ O	58.0167	61	
C ₄ H ₆	54.0470	CH ₄ N ₃	58.0406	HN ₂ O ₂	61.0038
55		C ₂ H ₂ O ₂	58.0054	H ₃ N ₃ O	61.0277
CHN ₃	55.0171				

	FM		FM		FM
H ₅ N ₄	61.0515	C ₃ N ₂	64.0062	C ₃ H ₄ N ₂	68.0375
CHO ₃	60.9925	C ₄ O	63.9949	C ₄ H ₄ O	68.0262
CH ₃ NO ₂	61.0164	C ₄ H ₂ N	64.0187	C ₄ H ₆ N	68.0501
CH ₅ N ₂ O	61.0402	C ₅ H ₄	64.0313	C ₅ H ₈	68.0626
CH ₇ N ₃	61.0641	65		69	
C ₂ H ₅ O ₂	61.0289	HO ₄	64.9874	CHN ₄	69.0202
C ₂ H ₇ NO	61.0528	H ₃ NO ₃	65.0113	C ₂ HN ₂ O	69.0089
C ₅ H	61.0078	C ₃ HN ₂	65.0140	C ₂ H ₃ N ₃	69.0328
62		C ₄ HO	65.0027	C ₃ HO ₂	68.9976
NO ₃	61.9878	C ₄ H ₃ N	65.0266	C ₃ H ₃ NO	69.0215
H ₂ N ₂ O ₂	62.0016	C ₅ H ₅	65.0391	C ₃ H ₅ N ₂	69.0453
H ₄ N ₃ O	62.0355	66		C ₄ H ₅ O	69.0340
H ₆ N ₄	62.0594	H ₂ O ₄	65.9953	C ₄ H ₇ N	69.0579
CH ₂ O ₃	62.0003	C ₂ N ₃	66.0093	C ₅ H ₉	69.0705
CH ₄ NO ₂	62.0242	C ₃ NO	65.9980	70	
CH ₆ N ₂ O	62.0480	C ₃ H ₂ N ₂	66.0218	CN ₃ O	70.0042
C ₂ H ₆ O ₂	62.0368	C ₄ H ₂ O	66.0106	CH ₂ N ₄	70.0280
C ₄ N	62.0031	C ₄ H ₄ N	66.0344	C ₂ NO ₂	69.9929
C ₅ H ₂	62.0157	C ₅ H ₆	66.0470	C ₂ H ₂ N ₂ O	70.0167
63		67		C ₂ H ₄ N ₃	70.0406
HNO ₃	62.9956	C ₂ HN ₃	67.0171	C ₃ H ₂ O ₂	70.0054
H ₃ N ₂ O ₂	63.0195	C ₃ HNO	67.0058	C ₃ H ₄ NO	70.0293
H ₅ N ₃ O	63.0433	C ₃ H ₃ N ₂	67.0297	C ₃ H ₆ N ₂	70.0532
CH ₃ O ₃	63.0082	C ₄ H ₃ O	67.0184	C ₄ H ₆ O	70.0419
CH ₅ NO ₂	63.0320	C ₄ H ₅ N	67.0422	C ₄ H ₈ N	70.0657
C ₄ HN	63.0109	C ₅ H ₇	67.0548	C ₅ H ₁₀	70.0783
C ₅ H ₃	63.0235	68		71	
64		CN ₄	68.0124	CHN ₃ O	71.0120
O ₄	63.9796	C ₂ N ₂ O	68.0011	CH ₃ N ₄	71.0359
H ₂ NO ₃	64.0034	C ₂ H ₂ N ₃	68.0249	C ₂ HNO ₂	71.0007
H ₄ N ₂ O ₂	64.0273	C ₃ O ₂	67.9598	C ₂ H ₃ N ₂ O	71.0246
CH ₄ O ₃	64.0160	C ₃ H ₂ NO	68.0136	C ₂ H ₅ N ₃	71.0484

	FM		FM		FM
$C_3H_3O_2$	71.0133	C_3H_7NO	73.0528	$C_2H_9N_3$	75.0798
C_3H_5NO	71.0371	$C_3H_9N_2$	73.0767	$C_3H_7O_2$	75.0446
$C_3H_7N_2$	71.0610	C_4H_9O	73.0653	C_3H_9NO	75.0684
C_4H_7O	71.0497	$C_4H_{11}N$	73.0892	C_5HN	75.0109
C_4H_9N	71.0736	C_6H	73.0078	C_6H_3	75.0235
C_5H_{11}	71.0861	74		76	
72		N_3O_2	73.9991	N_2O_3	75.9909
N_4O	72.0073	H_2N_4O	74.0229	$H_2N_3O_2$	76.0147
CN_2O_2	71.9960	CNO_3	73.9878	H_4N_4O	76.0386
CH_2N_3O	72.0198	$CH_2N_2O_2$	74.0116	CO_4	75.9796
CH_4N_4	72.0437	CH_4N_3O	74.0355	CH_2NO_3	76.0034
C_2O_3	71.9847	CH_6N_4	74.0594	$CH_4N_2O_2$	76.0273
$C_2H_2NO_2$	72.0085	$C_2H_2O_3$	74.0003	CH_6N_3O	76.0511
$C_2H_4N_2O$	72.0324	$C_2H_4NO_2$	74.0242	CH_8N_4	76.0750
$C_2H_6N_3$	72.0563	$C_2H_6N_2O$	74.0480	$C_2H_4O_3$	76.0160
$C_3H_4O_2$	72.0211	$C_2H_8N_3$	74.0719	$C_2H_6NO_2$	76.0399
C_3H_6NO	72.0449	$C_3H_6O_2$	74.0368	$C_2H_8N_2O$	76.0637
$C_3H_8N_2$	72.0688	C_3H_8NO	74.0606	$C_3H_8O_2$	76.0524
C_4H_8O	72.0575	$C_3H_{10}N_2$	74.0845	C_4N_2	76.0062
$C_4H_{10}N$	72.0814	$C_4H_{10}O$	74.0732	C_5O	75.9949
C_5H_{12}	72.0939	C_5N	74.0031	C_5H_2N	76.0187
C_6	72.0000	C_6H_2	74.0157	C_6H_4	76.0313
73		75		77	
HN_4O	73.0151	HN_3O_2	75.0069	HN_2O_3	76.9987
CHN_2O_2	73.0038	H_3N_4O	75.0308	$H_3N_3O_2$	77.0226
CH_3N_3O	73.0277	$CHNO_3$	74.9956	H_5N_4O	77.0464
CH_5N_4	73.0515	$CH_3N_2O_2$	75.0195	CHO_4	76.9874
C_2HO_3	72.9925	CH_5N_3O	75.0433	CH_3NO_3	77.0113
$C_2H_3NO_2$	73.0164	CH_7N_4	75.0672	$CH_5N_2O_2$	77.0351
$C_2H_5N_2O$	73.0402	$C_2H_3O_3$	75.0082	CH_7N_3O	77.0590
$C_2H_7N_3$	73.0641	$C_2H_5NO_2$	75.0320	$C_2H_5O_3$	77.0238
$C_3H_5O_2$	73.0289	$C_2H_7N_2O$	75.0559	$C_2H_7NO_2$	77.0477

FM		FM		FM	
C ₄ HN ₂	77.0140	H ₄ N ₂ O ₃	80.0222	C ₅ H ₈ N	82.0657
C ₅ HO	77.0027	CH ₄ O ₄	80.0109	C ₆ H ₁₀	82.0783
C ₅ H ₃ N	77.0266	C ₂ N ₄	80.0124	83	
C ₆ H ₅	77.0391	C ₃ N ₂ O	80.0011	C ₂ HN ₃ O	83.0120
78		C ₃ H ₂ N ₃	80.0249	C ₂ H ₃ N ₄	83.0359
NO ₄	77.9827	C ₄ O ₂	79.9898	C ₃ HNO ₂	83.0007
H ₂ N ₂ O ₃	78.0065	C ₄ H ₂ NO	80.0136	C ₃ H ₃ N ₂ O	83.0246
H ₄ N ₃ O ₂	78.0304	C ₄ H ₄ N ₂	80.0375	C ₃ H ₅ N ₃	83.0484
H ₆ N ₄ O	78.0542	C ₅ H ₄ O	80.0262	C ₄ H ₃ O ₂	83.0133
CH ₂ O ₄	77.9953	C ₅ H ₆ N	80.0501	C ₄ H ₅ NO	83.0371
CH ₄ NO ₃	78.0191	C ₆ H ₈	80.0626	C ₄ H ₇ N ₂	83.0610
C ₂ H ₆ O ₃	78.0317	81		C ₅ H ₇ O	83.0497
CH ₆ N ₂ O ₂	78.0429	H ₃ NO ₄	81.0062	C ₅ H ₉ N	83.0736
C ₃ N ₃	78.0093	C ₂ HN ₄	81.0202	C ₆ H ₁₁	83.0861
C ₄ NO	77.9980	C ₂ HN ₂ O	81.0089	84	
C ₄ H ₂ N ₂	78.0218	C ₃ H ₃ N ₃	81.0328	CN ₄ O	84.0073
C ₅ H ₂ O	78.0106	C ₄ HO ₂	80.9976	C ₂ N ₂ O ₂	83.9960
C ₅ H ₄ N	78.0344	C ₄ H ₃ NO	81.0215	C ₂ H ₂ N ₃ O	84.0198
C ₆ H ₆	78.0740	C ₄ H ₅ N ₂	81.0453	C ₂ H ₄ N ₄	84.0437
79		C ₅ H ₅ O	81.0340	C ₃ O ₃	83.9847
HNO ₄	78.9905	C ₅ H ₇ N	81.0579	C ₃ H ₂ NO ₂	84.0085
H ₃ N ₂ O ₃	79.0144	C ₆ H ₈	81.0705	C ₃ H ₄ N ₂ O	84.0324
H ₅ N ₃ O ₂	79.0382	82		C ₃ H ₆ N ₃	84.0563
CH ₃ O ₄	79.0031	C ₂ N ₃ O	82.0042	C ₄ H ₄ O ₂	84.0211
CH ₅ NO ₃	79.0269	C ₂ H ₂ N ₄	82.0280	C ₄ H ₆ NO	84.0449
C ₃ HN ₃	79.0171	C ₃ NO ₂	81.9929	C ₄ H ₈ N ₂	84.0688
C ₄ HNO	79.0058	C ₃ H ₂ N ₂ O	82.0167	C ₅ H ₈ O	84.0575
C ₄ H ₃ N ₂	79.0297	C ₃ H ₄ N ₃	82.0406	C ₅ H ₁₀ N	84.0814
C ₅ H ₃ O	79.0184	C ₄ H ₂ O ₂	82.0054	C ₆ H ₁₂	84.0939
C ₅ H ₅ N	79.0422	C ₄ H ₄ NO	82.0293	C ₇	84.0000
C ₆ H ₇	79.0548	C ₄ H ₆ N ₂	82.0532	85	
80		C ₅ H ₆ O	82.0419	CHN ₄ O	85.0151
H ₂ NO ₄	79.9983				

	FM		FM		FM
$C_2HN_2O_2$	85.0038	C_7H_2	86.0157	$C_3H_{10}N_3$	88.0876
$C_2H_3N_3O$	85.0277	87		$C_4H_8O_2$	88.0524
$C_2H_5N_4$	85.0515	CHN_3O_2	87.0069	$C_4H_{10}NO$	88.0763
C_3HO_3	84.9925	CH_3N_4O	87.0308	$C_4H_{12}N_2$	88.1001
$C_3H_3NO_2$	85.0164	C_2HNO_3	86.9956	$C_5H_{12}O$	88.0888
$C_3H_5N_2O$	85.0402	$C_2H_3N_2O_2$	87.0195	C_5N_2	88.0662
$C_3H_7N_3$	85.0641	$C_2H_5N_3O$	87.0433	C_6O	87.9949
$C_4H_5O_2$	85.0289	$C_2H_7N_4$	87.0672	C_6H_2N	88.0187
C_4H_7NO	85.0528	$C_3H_3O_3$	87.0082	C_7H_4	88.0313
$C_4H_9N_2$	85.0767	$C_3H_5NO_2$	87.0320	89	
C_5H_9O	85.0653	$C_3H_7N_2O$	87.0559	HN_4O_2	89.0100
$C_5H_{11}N$	85.0892	$C_3H_9N_3$	87.0798	CHN_2O_3	88.9987
C_6H_{13}	85.1018	$C_4H_7O_2$	87.0446	$CH_3N_3O_2$	89.0226
C_7H	85.0078	C_4H_9NO	87.0684	CH_5N_4O	89.0464
86		$C_4H_{11}N_2$	87.0923	C_2HO_4	88.9874
CN_3O_2	85.9991	$C_5H_{11}O$	87.0810	$C_2H_3NO_3$	89.0113
CH_2N_4O	86.0229	$C_5H_{13}N$	87.1049	$C_2H_5N_2O_2$	89.0351
C_2NO_3	85.9878	C_6HN	87.0109	$C_2H_7N_3O$	89.0590
$C_2H_2N_2O_2$	86.0116	C_7H_3	87.0235	$C_2H_9N_4$	89.0829
$C_2H_4N_3O$	86.0355	88		$C_3H_5O_3$	89.0238
$C_2H_6N_4$	86.0594	N_4O_2	88.0022	$C_3H_7NO_2$	89.0477
$C_3H_2O_3$	86.0003	CN_2O_3	87.9909	$C_3H_9N_2O$	89.0715
$C_3H_4NO_2$	86.0242	$CH_2N_3O_2$	88.0147	$C_3H_{11}N_3$	89.0954
$C_3H_6N_2O$	86.0480	CH_4N_4O	88.0386	$C_4H_9O_2$	89.0603
$C_3H_8N_3$	86.0719	C_2O_4	87.9796	$C_4H_{11}NO$	89.0841
$C_4H_6O_2$	86.0368	$C_2H_2NO_3$	88.0034	C_5HN_2	89.0140
C_4H_8NO	86.0606	$C_2H_4N_2O_2$	88.0273	C_6HO	89.0027
$C_4H_{10}N_2$	86.0845	$C_2H_6N_3O$	88.0511	C_6H_3N	89.0266
$C_5H_{10}O$	86.0732	$C_2H_8N_4$	88.0750	C_7H_5	89.0391
$C_5H_{12}N$	86.0970	$C_3H_4O_3$	88.0160	90	
C_6H_{14}	86.1096	$C_3H_6NO_2$	88.0399	N_3O_3	89.9940
C_6N	86.0031	$C_3H_8N_2O$	88.0637	$H_2N_4O_2$	90.0178

FM		FM		FM	
CNO ₄	89.9827	C ₄ HN ₃	91.0171	CH ₅ N ₂ O ₃	93.0300
CH ₂ N ₂ O ₃	90.0065	C ₅ HNO	91.0058	CH ₇ N ₃ O ₂	93.0539
CH ₄ N ₃ O ₂	90.0304	C ₅ H ₃ N ₂	91.0297	C ₂ H ₅ O ₄	93.0187
CH ₆ N ₄ O	90.0542	C ₆ H ₃ O	91.0184	C ₂ H ₇ NO ₃	93.0426
C ₂ H ₂ O ₄	89.9953	C ₆ H ₅ N	91.0422	C ₃ HN ₄	93.0202
C ₂ H ₄ NO ₃	90.0191	C ₇ H ₇	91.0548	C ₄ HN ₂ O	93.0089
C ₂ H ₆ N ₂ O ₂	90.0429	92		C ₄ H ₃ N ₃	93.0328
C ₂ H ₈ N ₃ O	90.0668	N ₂ O ₄	91.9858	C ₅ HO ₂	92.9976
C ₂ H ₁₀ N ₄	90.0907	H ₂ N ₃ O ₃	92.0096	C ₅ H ₃ NO	93.0215
C ₃ H ₆ O ₃	90.0317	H ₄ N ₄ O ₂	92.0335	C ₅ H ₅ N ₂	93.0453
C ₃ H ₈ NO ₂	90.0555	CH ₂ NO ₄	91.9983	C ₆ H ₅ O	93.0340
C ₃ H ₁₀ N ₂ O	90.0794	CH ₄ N ₂ O ₃	92.0222	C ₆ H ₇ N	93.0579
C ₄ H ₁₀ O ₂	90.0681	CH ₆ N ₃ O ₂	92.0460	C ₇ H ₉	93.0705
C ₄ N ₃	90.0093	CH ₈ N ₄ O	92.0699	94	
C ₅ NO	89.9980	C ₂ H ₄ O ₄	92.0109	H ₂ N ₂ O ₄	94.0014
C ₃ H ₂ N ₂	90.0218	C ₂ H ₆ NO ₃	92.0348	H ₄ N ₃ O ₃	94.0253
C ₆ H ₂ O	90.0106	C ₂ H ₈ N ₂ O ₂	92.0586	H ₆ N ₄ O ₂	94.0491
C ₆ H ₄ N	90.0344	C ₃ H ₈ O ₃	92.0473	CH ₄ NO ₄	94.0140
C ₇ H ₆	90.0470	C ₃ N ₄	92.0124	CH ₆ N ₂ O ₃	94.0379
91		C ₄ N ₂ O	92.0011	C ₂ H ₆ O ₄	94.0266
HN ₃ O ₃	91.0018	C ₄ H ₂ N ₃	92.0249	C ₃ N ₃ O	94.0042
H ₃ N ₄ O ₂	91.0257	C ₅ O ₂	91.9898	C ₃ H ₂ N ₄	94.0280
CHNO ₄	90.9905	C ₅ H ₂ NO	92.0136	C ₄ NO ₂	93.9929
CH ₃ N ₂ O ₃	91.0144	C ₅ H ₄ N ₂	92.0375	C ₄ H ₂ N ₂ O	94.0167
CH ₅ N ₃ O ₂	91.0382	C ₆ H ₄ O	92.0262	C ₄ H ₄ N ₃	94.0406
CH ₇ N ₄ O	91.0621	C ₆ H ₆ N	92.0501	C ₅ H ₂ O ₂	94.0054
C ₂ H ₃ O ₄	91.0031	C ₇ H ₈	92.0626	C ₅ H ₄ NO	94.0293
C ₂ H ₅ NO ₃	91.0269	93		C ₅ H ₆ N ₂	94.0532
C ₂ H ₇ N ₂ O ₂	01.0508	HN ₂ O ₄	92.9936	C ₆ H ₆ O	94.0419
C ₂ H ₉ N ₃ O	91.0746	H ₃ N ₃ O ₃	93.0175	C ₆ H ₈ N	94.0657
C ₃ H ₇ O ₃	91.0395	H ₅ N ₄ O ₂	93.0413	C ₇ H ₁₀	94.0783
C ₃ H ₉ NO ₂	91.0634	CH ₃ NO ₄	93.0062	95	
				H ₃ N ₂ O ₄	95.0093

	FM		FM		FM
H ₃ N ₃ O ₃	95.0331	C ₃ HN ₂ O ₂	97.0038	C ₈ H ₂	98.0157
CH ₃ NO ₄	95.0218	C ₃ H ₃ N ₃ O	97.0277	99	
C ₃ HN ₃ O	95.0120	C ₃ H ₅ N ₄	97.0515	C ₂ HN ₃ O ₂	99.0069
C ₃ H ₃ N ₄	95.0359	C ₄ HO ₃	96.9925	C ₂ H ₃ N ₄ O	99.0308
C ₄ HNO ₂	95.0007	C ₄ H ₃ NO ₂	97.0164	C ₃ HNO ₃	98.9956
C ₄ H ₃ N ₂ O	95.0246	C ₄ H ₅ N ₂ O	97.0402	C ₃ H ₃ N ₂ O ₂	99.0195
C ₄ H ₅ N ₃	95.0484	C ₄ H ₇ N ₃	97.0641	C ₃ H ₅ N ₃ O	99.0433
C ₅ H ₃ O ₂	95.0133	C ₅ H ₅ O ₂	97.0289	C ₃ H ₇ N ₄	99.0672
C ₅ H ₅ NO	95.0371	C ₅ H ₇ NO	97.0528	C ₄ H ₃ O ₃	99.0082
C ₅ H ₇ N ₂	95.0610	C ₅ H ₉ N ₂	97.0767	C ₄ H ₅ NO ₂	99.0320
C ₆ H ₇ O	95.0497	C ₆ H ₉ O	97.0653	C ₄ H ₇ N ₂ O	99.0559
C ₆ H ₉ N	95.0736	C ₆ H ₁₁ N	97.0892	C ₄ H ₉ N ₃	99.0798
C ₇ H ₁₁	95.0861	C ₇ H ₁₃	97.1018	C ₅ H ₇ O ₂	99.0446
96		C ₈ H	97.0078	C ₅ H ₉ NO	99.0684
H ₄ N ₂ O ₄	96.0171	98		C ₅ H ₁₁ N ₂	99.0923
C ₂ N ₄ O	96.0073	C ₂ N ₃ O ₂	97.9991	C ₆ H ₁₁ O	99.0810
C ₃ N ₂ O ₂	95.9960	C ₂ H ₂ N ₄ O	98.0229	C ₆ H ₁₃ N	99.1049
C ₃ H ₂ N ₃ O	96.0198	C ₃ NO ₃	97.9878	C ₇ H ₁₅	99.1174
C ₃ H ₄ N ₄	96.0437	C ₃ H ₂ N ₂ O ₂	98.0116	C ₇ HN	99.0109
C ₄ O ₃	95.9847	C ₃ H ₄ N ₃ O	98.0355	C ₈ H ₃	99.0235
C ₄ H ₂ NO ₂	96.0085	C ₃ H ₆ N ₄	98.0594	100	
C ₄ H ₄ N ₂ O	96.0324	C ₄ H ₂ O ₃	98.0003	CN ₄ O ₂	100.0022
C ₄ H ₆ N ₃	96.0563	C ₄ H ₄ NO ₂	98.0242	C ₂ N ₂ O ₃	99.9909
C ₅ H ₄ O ₂	96.0211	C ₄ H ₆ N ₂ O	98.0480	C ₂ H ₂ N ₃ O ₂	100.0147
C ₅ H ₆ NO	96.0449	C ₄ H ₈ N ₃	98.0719	C ₂ H ₄ N ₄ O	100.0386
C ₅ H ₈ N ₂	96.0688	C ₅ H ₆ O ₂	98.0368	C ₃ O ₄	99.9796
C ₆ H ₈ O	96.0575	C ₅ H ₈ NO	98.0606	C ₃ H ₂ NO ₃	100.0034
C ₆ H ₁₀ N	96.0814	C ₅ H ₁₀ N ₂	98.0845	C ₃ H ₄ N ₂ O ₂	100.0273
C ₇ H ₁₂	96.0939	C ₆ H ₁₀ O	98.0732	C ₃ H ₆ N ₃ O	100.0511
C ₈	96.0000	C ₆ H ₁₂ N	98.0970	C ₃ H ₈ N ₄	100.0750
97		C ₇ H ₁₄	98.1096	C ₄ H ₄ O ₃	100.0160
C ₂ HN ₄ O	97.0151	C ₇ N	98.0031	C ₄ H ₆ NO ₂	100.0399

FM		FM		FM	
$C_4H_8N_2O$	100.0637	C_7HO	101.0027	C_2HNO_4	102.9905
$C_4H_{10}N_3$	100.0876	C_7H_3N	101.0266	$C_2H_3N_2O_3$	103.0144
$C_5H_8O_2$	100.0524	C_8H_5	101.0391	$C_2H_5N_3O_2$	103.0382
$C_5H_{10}NO$	100.0763	102		$C_2H_7N_4O$	103.0621
$C_5H_{12}N_2$	100.1001	CN_3O_3	101.9940	$C_3H_3O_4$	103.0031
$C_6H_{12}O$	100.0888	$CH_2N_4O_2$	102.0178	$C_3H_5NO_3$	103.0269
$C_6H_{14}N$	100.1127	C_2NO_4	101.9827	$C_3H_7N_2O_2$	103.0508
C_6N_2	100.0062	$C_2H_2N_2O_3$	102.0065	$C_3H_9N_3O$	103.0746
C_7H_{16}	100.1253	$C_2H_4N_3O_2$	102.0304	$C_3H_{11}N_4$	103.0985
C_7O	99.9949	$C_2H_6N_4O$	102.0542	$C_4H_7O_3$	103.0395
C_7H_2N	100.0187	$C_3H_2O_4$	101.9953	$C_4H_9NO_2$	103.0634
C_8H_4	100.0313	$C_3H_4NO_3$	102.0191	$C_4H_{11}N_2O$	103.0872
101		$C_3H_6N_2O_2$	102.0429	$C_4H_{13}N_3$	103.1111
CHN_4O_2	101.0100	$C_3H_8N_3O$	102.0668	$C_5H_{11}O_2$	103.0759
$C_2HN_2O_3$	100.9987	$C_3H_{10}N_4$	102.0907	$C_5H_{13}NO$	103.0998
$C_2H_3N_3O_2$	101.0226	$C_4H_6O_3$	102.0317	C_5HN_3	103.0171
$C_2H_5N_4O$	101.0464	$C_4H_8NO_2$	102.0555	C_6HNO	103.0058
C_3HO_4	100.9874	$C_4H_{10}N_2O$	102.0794	$C_6H_3N_2$	103.0297
$C_3H_3NO_3$	101.0113	$C_4H_{12}N_3$	102.1032	C_7H_3O	103.0184
$C_3H_5N_2O_2$	101.0351	$C_5H_{10}O_2$	102.0681	C_7H_5N	103.0422
$C_3H_7N_3O$	101.0590	$C_5H_{12}NO$	102.0919	C_8H_7	103.0548
$C_3H_9N_4$	101.0829	$C_5H_{14}N_2$	102.1158	104	
$C_4H_5O_3$	101.0238	C_5N_3	102.0093	CN_2O_4	103.9858
$C_4H_7NO_2$	101.0477	$C_6H_{14}O$	102.1045	$CH_2N_3O_3$	104.0096
$C_4H_9N_2O$	101.0715	C_6NO	101.9980	$CH_4N_4O_2$	104.0335
$C_4H_{11}N_3$	101.0954	$C_6H_2N_2$	102.0218	$C_2H_2NO_4$	103.9983
$C_5H_9O_2$	101.0603	C_7H_2O	102.0106	$C_2H_4N_2O_3$	104.0222
$C_5H_{11}NO$	101.0841	C_7H_4N	102.0344	$C_2H_6N_3O_2$	104.0460
$C_5H_{13}N_2$	101.1080	C_8H_6	102.0470	$C_2H_8N_4O$	104.0699
$C_6H_{13}O$	101.0967	103		$C_3H_4O_4$	104.0109
$C_6H_{15}N$	101.1205	CHN_3O_3	103.0018	$C_3H_6NO_3$	104.0348
C_6HN_2	101.0140	$CH_3N_4O_2$	103.0257	$C_3H_8N_7O_2$	104.0586

FM		FM		FM	
C ₃ H ₁₀ N ₃ O	104.0825	C ₆ HO ₂	104.9976	CH ₇ N ₄ O ₂	107.0570
C ₃ H ₁₂ N ₄	104.1063	C ₆ H ₃ NO	105.0215	C ₂ H ₅ NO ₄	107.0218
C ₄ H ₈ O ₃	104.0473	C ₆ H ₅ N ₂	105.0453	C ₂ H ₇ N ₂ O ₃	107.0457
C ₄ H ₁₀ NO ₂	104.0712	C ₇ H ₅ O	105.0340	C ₂ H ₉ N ₃ O ₂	107.0695
C ₄ H ₁₂ N ₂ O	104.0950	C ₇ H ₇ N	105.0579	C ₃ H ₇ O ₄	107.0344
C ₄ N ₄	104.0124	C ₈ H ₉	105.0705	C ₃ H ₉ NO ₃	107.0583
C ₅ H ₁₂ O ₂	104.0837	106		C ₄ HN ₃ O	107.0120
C ₅ N ₂ O	104.0011	CH ₂ N ₂ O ₄	106.0014	C ₄ H ₃ N ₄	107.0359
C ₅ H ₂ N ₃	104.0249	CH ₄ N ₃ O ₃	106.0253	C ₅ HNO ₂	107.0007
C ₆ O ₂	103.9898	CH ₆ N ₄ O ₂	106.0491	C ₅ H ₃ N ₂ O	107.0246
C ₆ H ₂ NO	104.0136	C ₂ H ₄ NO ₄	106.0140	C ₅ H ₃ N ₃	107.0484
C ₆ H ₄ N ₂	104.0375	C ₂ H ₆ N ₂ O ₃	106.0379	C ₆ H ₃ O ₂	107.0133
C ₇ H ₄ O	104.0262	C ₂ H ₈ N ₃ O ₂	106.0617	C ₆ H ₅ NO	107.0371
C ₇ H ₆ N	104.0501	C ₂ H ₁₀ N ₄ O	106.0856	C ₆ H ₇ N ₂	107.0610
C ₈ H ₈	104.0626	C ₃ H ₆ O ₄	106.0266	C ₇ H ₇ O	107.0497
105		C ₃ H ₈ NO ₃	106.0504	C ₇ H ₉ N	107.0736
CHN ₂ O ₄	104.9936	C ₃ H ₁₀ N ₂ O ₂	106.0743	C ₈ H ₁₁	107.0861
CH ₃ N ₃ O ₃	105.0175	C ₄ H ₁₀ O ₃	106.0630	108	
CH ₅ N ₄ O ₂	105.0413	C ₄ N ₃ O	106.0042	CH ₄ N ₂ O ₄	108.0171
C ₂ H ₃ NO ₄	105.0062	C ₄ H ₂ N ₄	106.0280	CH ₆ N ₃ O ₃	108.0410
C ₂ H ₅ N ₂ O ₃	105.0300	C ₅ NO ₂	105.9929	CH ₈ N ₄ O ₂	108.0648
C ₂ H ₇ N ₃ O ₂	105.0539	C ₅ H ₂ N ₂ O	106.0167	C ₂ H ₆ NO ₄	108.0297
C ₂ H ₉ N ₄ O	105.0777	C ₅ H ₄ N ₃	106.0406	C ₂ H ₈ N ₂ O ₃	108.0535
C ₃ H ₅ O ₄	105.0187	C ₆ H ₂ O ₂	106.0054	C ₃ H ₈ O ₄	108.0422
C ₃ H ₇ NO ₃	105.0426	C ₆ H ₄ NO	106.0293	C ₃ N ₄ O	108.0073
C ₃ H ₉ N ₂ O ₂	105.0664	C ₆ H ₆ N ₂	106.0532	C ₄ N ₂ O ₂	107.9960
C ₃ H ₁₁ N ₃ O	105.0903	C ₇ H ₆ O	106.0419	C ₄ H ₂ N ₃ O	108.0198
C ₄ H ₉ O ₃	105.0552	C ₇ H ₈ N	106.0657	C ₄ H ₄ N ₄	108.0437
C ₄ H ₁₁ NO ₂	105.0790	C ₈ H ₁₀	106.0783	C ₅ O ₃	107.9847
C ₄ HN ₄	105.0202	107		C ₅ H ₂ NO ₂	108.0085
C ₅ HN ₂ O	105.0089	CH ₃ N ₂ O ₄	107.0093	C ₅ H ₄ N ₂ O	108.0324
C ₅ H ₃ N ₃	105.0328	CH ₅ N ₃ O ₃	107.0331	C ₅ H ₆ N ₃	108.0563

FM		FM		FM	
C ₆ H ₄ O ₂	108.0211	C ₄ H ₄ N ₃ O	110.0355	C ₉ H ₃	111.0235
C ₆ H ₆ NO	108.0449	C ₄ H ₆ N ₄	110.0594	112	
C ₆ H ₈ N ₂	108.0688	C ₅ H ₂ O ₃	110.0003	C ₂ N ₄ O ₂	112.0022
C ₇ H ₈ O	108.0575	C ₅ H ₄ NO ₂	110.0242	C ₃ N ₂ O ₃	111.9909
C ₇ H ₁₀ N	108.0814	C ₅ H ₆ N ₂ O	110.0480	C ₃ H ₂ N ₃ O ₂	112.0147
C ₈ H ₁₂	108.0939	C ₅ H ₈ N ₃	110.0719	C ₃ H ₄ N ₄ O	112.0386
C ₉	108.0000	C ₆ H ₆ O ₂	110.0368	C ₄ O ₄	111.9796
109		C ₆ H ₈ NO	110.0606	C ₄ H ₂ NO ₃	112.0034
CH ₅ N ₂ O ₄	109.0249	C ₆ H ₁₀ N ₂	110.0845	C ₄ H ₄ N ₂ O ₂	112.0273
CH ₈ N ₃ O ₃	109.0488	C ₇ H ₁₀ O	110.0732	C ₄ H ₆ N ₃ O	112.0511
C ₂ H ₇ NO ₄	109.0375	C ₇ H ₁₂ N	110.0970	C ₄ H ₈ N ₄	112.0750
C ₃ HN ₄ O	109.0151	C ₈ H ₁₄	110.1096	C ₅ H ₄ O ₃	112.0160
C ₄ HN ₂ O ₂	109.0038	C ₈ N	110.0031	C ₅ H ₆ NO ₂	112.0399
C ₄ H ₃ N ₃ O	109.0277	C ₉ H ₂	110.0157	C ₅ H ₈ N ₂ O	112.0637
C ₄ H ₅ N ₄	109.0515	111		C ₅ H ₁₀ N ₃	112.0876
C ₅ HO ₃	108.9925	C ₃ HN ₃ O ₂	111.0069	C ₆ H ₈ O ₂	112.0524
C ₅ H ₃ NO ₂	109.0164	C ₃ H ₃ N ₄ O	111.0308	C ₆ H ₁₀ NO	112.0763
C ₅ H ₅ N ₂ O	109.0402	C ₄ HNO ₃	110.9956	C ₆ H ₁₂ N ₂	112.1001
C ₅ H ₇ N ₃	109.0641	C ₄ H ₃ N ₂ O ₂	111.0195	C ₇ H ₁₂ O	112.0888
C ₆ H ₅ O ₂	109.0289	C ₄ H ₅ N ₃ O	111.0433	C ₇ H ₁₄ N	112.1127
C ₆ H ₇ NO	109.0528	C ₄ H ₇ N ₄	111.0672	C ₇ N ₂	112.0062
C ₆ H ₉ N ₂	109.0767	C ₅ H ₃ O ₃	111.0082	C ₈ H ₁₆	112.1253
C ₇ H ₉ O	109.0653	C ₅ H ₅ NO ₂	111.0320	C ₈ O	111.9949
C ₇ H ₁₁ N	109.0892	C ₅ H ₇ N ₂ O	111.0559	C ₈ H ₂ N	112.0187
C ₈ H ₁₃	109.1018	C ₅ H ₉ N ₃	111.0798	C ₉ H ₄	112.0313
C ₉ H	109.0078	C ₆ H ₇ O ₂	111.0446	113	
110		C ₆ H ₉ NO	111.0684	C ₂ HN ₄ O ₂	113.0100
CH ₆ N ₂ O ₄	110.0328	C ₆ H ₁₁ N ₂	111.0923	C ₃ HN ₂ O ₃	112.9987
C ₃ N ₃ O ₂	109.9991	C ₇ H ₁₁ O	111.0810	C ₃ H ₃ N ₃ O ₂	113.0226
C ₃ H ₂ N ₄ O	110.0229	C ₇ H ₁₃ N	111.1049	C ₃ H ₅ N ₄ O	113.0464
C ₄ NO ₃	109.9878	C ₈ H ₁₅	111.1174	C ₄ HO ₄	112.9874
C ₄ H ₂ N ₂ O ₂	110.0116	C ₈ HN	111.0109	C ₄ H ₃ NO ₃	113.0113

FM		FM		FM	
$C_4H_5N_2O_2$	113.0351	$C_5H_{12}N_3$	114.1032	C_6HN_3	115.0171
$C_4H_7N_3O$	113.0590	$C_6H_{10}O_2$	114.0681	$C_7H_{15}O$	115.1123
$C_4H_9N_4$	113.0829	$C_6H_{12}NO$	114.0919	$C_7H_{17}N$	115.1362
$C_5H_5O_3$	113.0238	$C_6H_{14}N_2$	114.1158	C_7HNO	115.0058
$C_5H_7NO_2$	113.0477	C_6N_3	114.0093	$C_7H_3N_2$	115.0297
$C_5H_9N_2O$	113.0715	$C_7H_{14}O$	114.1045	C_8H_3O	115.0184
$C_5H_{11}N_3$	113.0954	$C_7H_{16}N$	114.1284	C_8H_5N	115.0422
$C_6H_9O_2$	113.0603	C_7NO	113.9980	C_9H_7	115.0548
$C_6H_{11}NO$	113.0841	$C_7H_2N_2$	114.0218	116	
$C_6H_{13}N_2$	113.1080	C_8H_{18}	114.1409	$C_2N_2O_4$	115.9858
$C_7H_{13}O$	113.0967	C_8H_2O	114.0106	$C_2H_2N_3O_3$	116.0096
$C_7H_{15}N$	113.1205	C_8H_4N	114.0344	$C_2H_4N_4O_2$	116.0335
C_7HN_2	113.0140	C_9H_6	114.0470	$C_3H_2NO_4$	115.9983
C_8H_{17}	113.1331	115		$C_3H_4N_2O_3$	116.0222
C_8HO	113.0027	$C_2HN_3O_3$	115.0018	$C_3H_6N_3O_2$	116.0460
C_8H_3N	113.0266	$C_2H_3N_4O_2$	115.0257	$C_3H_8N_4O$	116.0699
C_9H_5	113.0391	C_3HNO_4	114.9905	$C_4H_4O_4$	116.0109
114		$C_3H_3N_2O_3$	115.0144	$C_4H_6NO_3$	116.0348
$C_2N_3O_3$	113.9940	$C_3H_5N_3O_2$	115.0382	$C_4H_8N_2O_2$	116.0586
$C_2H_2N_4O_2$	114.0178	$C_3H_7N_4O$	115.0621	$C_4H_{10}N_3O$	116.0825
C_3NO_4	113.9827	$C_4H_3O_4$	115.0031	$C_4H_{12}N_4$	116.1063
$C_3H_2N_2O_3$	114.0065	$C_4H_5NO_3$	115.0269	$C_5H_8O_3$	116.0473
$C_3H_4N_3O_2$	114.0304	$C_4H_7N_2O_2$	115.0508	$C_5H_{10}NO_2$	116.0712
$C_3H_6N_4O$	114.0542	$C_4H_9N_3O$	115.0746	$C_5H_{12}N_2O$	116.0950
$C_4H_2O_4$	113.9953	$C_4H_{11}N_4$	115.0985	$C_5H_{14}N_3$	116.1189
$C_4H_4NO_3$	114.0191	$C_5H_7O_3$	115.0395	C_5N_4	116.0124
$C_4H_6N_2O_2$	114.0429	$C_5H_9NO_2$	115.0634	$C_6H_{12}O_2$	116.0837
$C_4H_8N_3O$	114.0668	$C_5H_{11}N_2O$	115.0872	$C_6H_{14}NO$	116.1076
$C_4H_{10}N_4$	114.0907	$C_5H_{13}N_3$	115.1111	$C_6H_{16}N_2$	116.1315
$C_5H_6O_3$	114.0317	$C_6H_{11}O_2$	115.0759	C_6N_2O	116.0011
$C_5H_8NO_2$	114.0555	$C_6H_{13}NO$	115.0998	$C_6H_2N_3$	116.0249
$C_5H_{10}N_2O$	114.0794	$C_6H_{15}N_2$	115.1236	$C_7H_{16}O$	116.1202

FM		FM		FM	
C ₇ O ₂	115.9898	C ₈ H ₇ N	117.0579	C ₂ H ₅ N ₃ O ₃	119.0331
C ₇ H ₂ NO	116.0136	C ₉ H ₉	117.0705	C ₂ H ₇ N ₄ O ₂	119.0570
C ₇ H ₄ N ₂	116.0375	118		C ₃ H ₅ NO ₄	119.0218
C ₈ H ₄ O	116.0262	C ₂ H ₂ N ₂ O ₄	118.0014	C ₃ H ₇ N ₂ O ₃	119.0457
C ₈ H ₆ N	116.0501	C ₂ H ₄ N ₃ O ₃	118.0253	C ₃ H ₉ N ₃ O ₂	119.0695
C ₉ H ₈	116.0626	C ₂ H ₆ N ₄ O ₂	118.0491	C ₃ H ₁₁ N ₄ O	119.0934
117		C ₃ H ₄ NO ₄	118.0140	C ₄ H ₇ O ₄	119.0344
C ₂ HN ₂ O ₄	116.9936	C ₃ H ₆ N ₂ O ₃	118.0379	C ₄ H ₉ NO ₃	119.0583
C ₂ H ₃ N ₃ O ₃	117.0175	C ₃ H ₈ N ₃ O ₂	118.0617	C ₄ H ₁₁ N ₂ O ₂	119.0821
C ₂ H ₅ N ₄ O ₂	117.0413	C ₃ H ₁₀ N ₄ O	118.0856	C ₄ H ₁₃ N ₃ O	119.1060
C ₃ H ₃ NO ₄	117.0062	C ₄ H ₆ O ₄	118.0266	C ₅ H ₁₁ O ₃	119.0708
C ₃ H ₅ N ₂ O ₃	117.0300	C ₄ H ₈ NO ₃	118.0504	C ₅ H ₁₃ NO ₂	119.0947
C ₃ H ₇ N ₃ O ₂	117.0539	C ₄ H ₁₀ N ₂ O ₂	118.0743	C ₅ HN ₃ O	119.0120
C ₃ H ₉ N ₄ O	117.0777	C ₄ H ₁₂ N ₃ O	118.0981	C ₅ H ₃ N ₄	119.0359
C ₄ H ₅ O ₄	117.0187	C ₄ H ₁₄ N ₄	118.1220	C ₆ HNO ₂	119.0007
C ₄ H ₇ NO ₃	117.0426	C ₅ H ₁₀ O ₃	118.0630	C ₆ H ₃ N ₂ O	119.0246
C ₄ H ₉ N ₂ O ₂	117.0664	C ₅ H ₁₂ NO ₂	118.0868	C ₆ H ₅ N ₃	119.0484
C ₄ H ₁₁ N ₃ O	117.0903	C ₅ H ₁₄ N ₂ O	118.1107	C ₇ H ₃ O ₂	119.0133
C ₄ H ₁₃ N ₄	117.1142	C ₅ N ₃ O	118.0042	C ₇ H ₅ NO	119.0371
C ₅ H ₉ O ₃	117.0552	C ₅ H ₂ N ₄	118.0280	C ₇ H ₇ N ₂	119.0610
C ₅ H ₁₁ NO ₂	117.0790	C ₆ H ₁₄ O ₂	118.0994	C ₈ H ₇ O	119.0497
C ₅ H ₁₃ N ₂ O	117.1029	C ₆ NO ₂	117.9929	C ₈ H ₉ N	119.0736
C ₅ H ₁₅ N ₃	117.1267	C ₆ H ₂ N ₂ O	118.0167	C ₉ H ₁₁	119.0861
C ₅ HN ₄	117.0202	C ₆ H ₄ N ₃	118.0406	120	
C ₆ H ₁₃ O ₂	117.0916	C ₇ H ₂ O ₂	118.0054	C ₂ H ₄ N ₂ O ₄	120.0171
C ₆ H ₁₅ NO	117.1154	C ₇ H ₄ NO	118.0293	C ₂ H ₆ N ₃ O ₃	120.0410
C ₆ HN ₂ O	117.0089	C ₇ H ₆ N ₂	118.0532	C ₂ H ₈ N ₄ O ₂	120.0648
C ₆ H ₃ N ₃	117.0328	C ₈ H ₆ O	118.0419	C ₃ H ₆ NO ₄	120.0297
C ₇ HO ₂	116.9976	C ₈ H ₈ N	118.0657	C ₃ H ₈ N ₂ O ₃	120.0535
C ₇ H ₃ NO	117.0215	C ₉ H ₁₀	118.0783	C ₃ H ₁₀ N ₃ O ₂	120.0774
C ₇ H ₅ N ₂	117.0453	119		C ₃ H ₁₂ N ₄ O	120.1012
C ₈ H ₅ O	117.0340	C ₂ H ₃ N ₂ O ₄	119.0093	C ₄ H ₈ O ₄	120.0422

FM		FM		FM	
C ₄ H ₁₀ NO ₃	120.0661	C ₆ H ₃ NO ₂	121.0164	C ₉ H ₁₄	122.1096
C ₄ H ₁₂ N ₂ O ₂	120.0899	C ₆ H ₅ N ₂ O	121.0402	C ₉ N	122.0031
C ₄ N ₄ O	120.0073	C ₆ H ₇ N ₃	121.0641	C ₁₀ H ₂	122.0157
C ₅ H ₁₂ O ₃	120.0786	C ₇ H ₅ O ₂	121.0289	123	
C ₅ N ₂ O ₂	119.9960	C ₇ H ₇ NO	121.0528	C ₂ H ₇ N ₂ O ₄	123.0406
C ₅ H ₂ N ₃ O	120.0198	C ₇ H ₉ N ₂	121.0767	C ₂ H ₉ N ₃ O ₃	123.0644
C ₅ H ₄ N ₄	120.0437	C ₈ H ₉ O	121.0653	C ₃ H ₉ NO ₄	123.0532
C ₆ O ₃	119.9847	C ₈ H ₁₁ N	121.0892	C ₄ HN ₃ O ₂	123.0069
C ₆ H ₂ NO ₂	120.0085	C ₉ H ₁₃	121.1018	C ₄ H ₃ N ₄ O	123.0308
C ₆ H ₄ N ₂ O	120.0324	C ₁₀ H	121.0078	C ₅ HNO ₃	122.9956
C ₆ H ₆ N ₃	120.0563	122		C ₅ H ₃ N ₂ O ₂	123.0195
C ₇ H ₄ O ₂	120.0211	C ₂ H ₆ N ₂ O ₄	122.0328	C ₅ H ₅ N ₃ O	123.0433
C ₇ H ₆ NO	120.0449	C ₂ H ₈ N ₃ O ₃	122.0566	C ₅ H ₇ N ₄	123.0672
C ₇ H ₈ N ₂	120.0688	C ₂ H ₁₀ N ₄ O ₂	122.0805	C ₆ H ₃ O ₃	123.0082
C ₈ H ₈ O	120.0575	C ₃ H ₈ NO ₄	122.0453	C ₆ H ₅ NO ₂	123.0320
C ₈ H ₁₀ N	120.0814	C ₃ H ₁₀ N ₂ O ₃	122.0692	C ₆ H ₇ N ₂ O	123.0559
C ₉ H ₁₂	120.0939	C ₄ H ₁₀ O ₄	122.0579	C ₆ H ₉ N ₃	123.0798
C ₁₀	120.0000	C ₄ N ₃ O ₂	121.9991	C ₇ H ₇ O ₂	123.0446
121	:	C ₄ H ₂ N ₄ O	122.0229	C ₇ H ₉ NO	123.0684
C ₂ H ₅ N ₂ O ₄	121.0249	C ₅ NO ₃	121.9878	C ₇ H ₁₁ N ₂	123.0923
C ₂ H ₇ N ₃ O ₃	121.0488	C ₅ H ₂ N ₂ O ₂	122.0116	C ₈ H ₁₁ O	123.0810
C ₂ H ₉ N ₄ O ₂	121.0726	C ₅ H ₄ N ₃ O	122.0355	C ₈ H ₁₃ N	123.1049
C ₃ H ₇ NO ₄	121.0375	C ₅ H ₆ N ₄	122.0594	C ₉ H ₁₅	123.1174
C ₃ H ₉ N ₂ O ₃	121.0614	C ₆ H ₂ O ₃	122.0003	C ₉ HN	123.0109
C ₃ H ₁₁ N ₃ O ₂	121.0852	C ₆ H ₄ NO ₂	122.0242	C ₁₀ H ₃	123.0235
C ₄ H ₉ O ₄	121.0501	C ₆ H ₆ N ₂ O	122.0480	124	
C ₄ H ₁₁ NO ₃	121.0739	C ₆ H ₈ N ₃	122.0719	C ₂ H ₈ N ₂ O ₄	124.0484
C ₄ HN ₄ O	121.0151	C ₇ H ₆ O ₂	122.0368	C ₃ N ₄ O ₂	124.0022
C ₅ HN ₂ O ₂	121.0038	C ₇ H ₈ NO	122.0606	C ₄ N ₂ O ₃	123.9909
C ₅ H ₃ N ₃ O	121.0277	C ₇ H ₁₀ N ₂	122.0845	C ₄ H ₂ N ₃ O ₂	124.0147
C ₅ H ₅ N ₄	121.0515	C ₈ H ₁₀ O	122.0732	C ₄ H ₄ N ₄ O	124.0386
C ₆ HO ₃	120.9925	C ₈ H ₁₂ N	122.0970	C ₅ O ₄	123.9796

FM		FM		FM	
$C_5H_2NO_3$	124.0034	$C_7H_9O_2$	125.0603	C_8NO	125.9980
$C_5H_4N_2O_2$	124.0273	$C_7H_{11}NO$	125.0841	$C_8H_2N_2$	126.0218
$C_5H_6N_3O$	124.0511	$C_7H_{13}N_2$	125.1080	C_9H_{18}	126.1409
$C_5H_8N_4$	124.0750	$C_8H_{13}O$	125.0967	C_9H_2O	126.0106
$C_6H_4O_3$	124.0160	$C_8H_{15}N$	125.1205	C_9H_4N	126.0344
$C_6H_6NO_2$	124.0399	C_8HN_2	125.0140	$C_{10}H_6$	126.0470
$C_6H_8N_2O$	124.0637	C_9H_{17}	125.1331	127	
$C_6H_{10}N_3$	124.0876	C_9HO	125.0027	$C_3HN_3O_3$	127.0018
$C_7H_8O_2$	124.0524	C_9H_3N	125.0266	$C_3H_3N_4O_2$	127.0257
$C_7H_{10}NO$	124.0763	$C_{10}H_5$	125.0391	C_4HNO_4	126.9905
$C_7H_{12}N_2$	124.1001	126		$C_4H_3N_2O_3$	127.0144
$C_8H_{12}O$	124.0888	$C_3N_3O_3$	125.9940	$C_4H_5N_3O_2$	127.0382
$C_8H_{14}N$	124.1127	$C_3H_2N_4O_2$	126.0178	$C_4H_7N_4O$	127.0621
C_8N_2	124.0062	C_4NO_4	125.9827	$C_5H_3O_4$	127.0031
C_9H_{16}	124.1253	$C_4H_2N_2O_3$	126.0065	$C_5H_5NO_3$	127.0269
C_9O	123.9949	$C_4H_4N_3O_2$	126.0304	$C_5H_7N_2O_2$	127.0508
C_9H_2N	124.0187	$C_4H_6N_4O$	126.0542	$C_5H_9N_3O$	127.0746
$C_{10}H_4$	124.0313	$C_5H_2O_4$	125.9953	$C_5H_{11}N_4$	127.0985
125		$C_5H_4NO_3$	126.0191	$C_6H_7O_3$	127.0395
$C_3HN_4O_2$	125.0100	$C_5H_6N_2O_2$	126.0429	$C_6H_9NO_2$	127.0634
$C_4HN_2O_3$	124.9987	$C_5H_8N_3O$	126.0668	$C_6H_{11}N_2O$	127.0872
$C_4H_3N_3O_2$	125.0226	$C_5H_{10}N_4$	126.0907	$C_6H_{13}N_3$	127.1111
$C_4H_5N_4O$	125.0464	$C_6H_6O_3$	126.0317	$C_7H_{11}O_2$	127.0759
C_5HO_4	124.9874	$C_6H_8NO_2$	126.0555	$C_7H_{13}NO$	127.0998
$C_5H_3NO_3$	125.0113	$C_6H_{10}N_2O$	126.0794	$C_7H_{15}N_2$	127.1236
$C_5H_5N_2O_2$	125.0351	$C_6H_{12}N_3$	126.1032	C_7HN_3	127.0171
$C_5H_7N_3O$	125.0590	$C_7H_{10}O_2$	126.0681	$C_8H_{15}O$	127.1123
$C_5H_9N_4$	125.0829	$C_7H_{12}NO$	126.0919	$C_8H_{17}N$	127.1362
$C_6H_5O_3$	125.0238	$C_7H_{14}N_2$	126.1158	C_8HNO	127.0058
$C_6H_7NO_2$	125.0477	C_7N_3	126.0093	$C_8H_3N_2$	127.0297
$C_6H_9N_2O$	125.0715	$C_8H_{14}O$	126.1045	C_9H_3O	127.0184
$C_6H_{11}N_3$	125.0954	$C_8H_{16}N$	126.1284	C_9H_5N	127.0422

FM		FM		FM	
C_9H_{19}	127.1488	C_9H_6N	128.0501	$C_{10}H_9$	129.0705
$C_{10}H_7$	127.0548	$C_{10}H_9$	128.0626	130	
128		129		$C_3H_2N_2O_4$	130.0014
$C_3N_2O_4$	127.9858	$C_3HN_2O_4$	128.9936	$C_3H_4N_3O_3$	130.0253
$C_3H_2N_3O_3$	128.0096	$C_3H_3N_3O_3$	129.0175	$C_3H_6N_4O_2$	130.0491
$C_3H_4N_4O_2$	128.0335	$C_3H_5N_4O_2$	129.0413	$C_4H_4NO_4$	130.0140
$C_4H_2NO_4$	127.9983	$C_4H_3NO_4$	129.0062	$C_4H_6N_2O_3$	130.0379
$C_4H_4N_2O_3$	128.0222	$C_4H_5N_2O_3$	129.0300	$C_4H_8N_3O_2$	130.0617
$C_4H_6N_3O_2$	128.0460	$C_4H_7N_3O_2$	129.0539	$C_4H_{10}N_4O$	130.0856
$C_4H_8N_4O$	128.0699	$C_4H_9N_4O$	129.0777	$C_5H_6O_4$	130.0266
$C_5H_4O_4$	128.0109	$C_5H_5O_4$	129.0187	$C_5H_8NO_3$	130.0504
$C_5H_6NO_3$	128.0348	$C_5H_7NO_3$	129.0426	$C_5H_{10}N_2O_2$	130.0743
$C_5H_8N_2O_2$	128.0586	$C_5H_9N_2O_2$	129.0664	$C_5H_{12}N_3O$	130.0981
$C_5H_{10}N_3O$	128.0825	$C_5H_{11}N_3O$	129.0903	$C_5H_{14}N_4$	130.1220
$C_5H_{12}N_4$	128.1063	$C_5H_{13}N_4$	129.1142	$C_6H_{10}O_3$	130.0603
$C_6H_8O_3$	128.0473	$C_6H_9O_3$	129.0552	$C_6H_{12}NO_2$	130.0868
$C_6H_{10}NO_2$	128.0712	$C_6H_{11}NO_2$	129.0790	$C_6H_{14}N_2O$	130.1107
$C_6H_{12}N_2O$	128.0950	$C_6H_{13}N_2O$	129.1029	$C_6H_{16}N_3$	130.1346
$C_6H_{14}N_3$	128.1189	$C_6H_{15}N_3$	129.1267	C_6N_3O	130.0042
C_6N_4	128.0124	C_6HN_4	129.0202	$C_6H_2N_4$	130.0280
$C_7H_{12}O_2$	128.0837	$C_7H_{13}O_2$	129.0916	$C_7H_{14}O_2$	130.0994
$C_7H_{14}NO$	128.1076	$C_7H_{15}NO$	129.1154	$C_7H_{16}NO$	130.1233
$C_7H_{16}N_2$	128.1315	$C_7H_{17}N_2$	129.1393	C_7NO_2	129.9929
C_7N_2O	128.0011	C_7HN_2O	129.0089	$C_7H_{18}N_2$	130.1471
$C_7H_2N_3$	128.0249	$C_7H_3N_3$	129.0328	$C_7H_2N_2O$	130.0167
$C_8H_{16}O$	128.1202	$C_8H_{17}O$	129.1280	$C_7H_4N_3$	130.0406
C_8O_2	127.9898	C_8HO_2	128.9976	$C_8H_{18}O$	130.1358
$C_8H_{18}N$	128.1440	$C_8H_{19}N$	129.1519	$C_8H_2O_2$	130.0054
C_8H_2NO	128.0136	C_8H_3NO	129.0215	C_8H_4NO	130.0293
$C_8H_4N_2$	128.0375	$C_8H_5N_2$	129.0453	$C_8H_6N_2$	130.0532
C_9H_{20}	128.1566	C_9H_5O	129.0340	C_9H_6O	130.0419
C_9H_4O	128.0262	C_9H_7N	129.0579	C_9H_8N	130.0657

	FM		FM		FM
$C_{10}H_{10}$	130.0783	$C_3H_6N_3O_3$	132.0410	$C_3H_7N_3O_3$	133.0488
131		$C_3H_8N_4O_2$	132.0648	$C_3H_9N_4O_2$	133.0726
$C_3H_3N_2O_4$	131.0093	$C_4H_6NO_4$	132.0297	$C_4H_7NO_4$	133.0375
$C_3H_5N_3O_3$	131.0331	$C_4H_8N_2O_3$	132.0535	$C_4H_9N_2O_3$	133.0614
$C_3H_7N_4O_2$	131.0570	$C_4H_{10}N_3O_2$	132.0774	$C_4H_{11}N_3O_2$	133.0852
$C_4H_5NO_4$	131.0218	$C_4H_{12}N_4O$	132.1012	$C_4H_{13}N_4O$	133.1091
$C_4H_7N_2O_3$	131.0457	$C_5H_8O_4$	132.0422	$C_5H_9O_4$	133.0501
$C_4H_9N_3O_2$	131.0695	$C_5H_{10}NO_3$	132.0661	$C_5H_{11}NO_3$	133.0739
$C_4H_{11}N_4O$	131.0934	$C_5H_{12}N_2O_2$	132.0899	$C_5H_{13}N_2O_2$	133.0978
$C_5H_7O_4$	131.0344	$C_5H_{14}N_3O$	132.1138	$C_5H_{15}N_3O$	133.1216
$C_5H_9NO_3$	131.0583	$C_5H_{16}N_4$	132.1377	C_5HN_4O	133.0151
$C_5H_{11}N_2O_2$	131.0821	C_5N_4O	132.0073	$C_6H_{13}O_3$	133.0865
$C_5H_{13}N_3O$	131.1060	$C_6H_{12}O_3$	132.0786	$C_6H_{15}NO_2$	133.1103
$C_5H_{15}N_4$	131.1298	$C_6H_{14}NO_2$	132.1025	$C_6HN_2O_2$	133.0038
$C_6H_{11}O_3$	131.0708	$C_6H_{16}N_2O$	132.1264	$C_6H_3N_3O$	133.0277
$C_6H_{13}NO_2$	131.0947	$C_6N_2O_2$	131.9960	$C_6H_5N_4$	133.0515
$C_6H_{15}N_2O$	131.1185	$C_6H_2N_3O$	132.0198	C_7HO_3	132.9925
$C_6H_{17}N_3$	131.1424	$C_6H_4N_4$	132.0437	$C_7H_3NO_2$	133.0164
C_6HN_3O	131.0120	$C_7H_{16}O_2$	132.1151	$C_7H_5N_2O$	133.0402
$C_6H_3N_4$	131.0359	C_7O_3	131.9847	$C_7H_7N_3$	133.0641
$C_7H_{15}O_2$	131.1072	$C_7H_2NO_2$	132.0085	$C_8H_5O_2$	133.0289
$C_7H_{17}NO$	131.1311	$C_7H_4N_2O$	132.0324	C_8H_7NO	133.0528
C_7HNO_2	131.0007	$C_7H_6N_3$	132.0563	$C_8H_9N_2$	133.0767
$C_7H_3N_2O$	131.0246	$C_8H_4O_2$	132.0211	C_9H_9O	133.0653
$C_7H_5N_3$	131.0484	C_8H_6NO	132.0449	$C_9H_{11}N$	133.0892
$C_8H_3O_2$	131.0133	$C_8H_8N_2$	132.0688	$C_{10}H_{13}$	133.1018
C_8H_5NO	131.0371	C_9H_8O	132.0575	$C_{11}H$	133.0078
$C_8H_7N_2$	131.0610	$C_9H_{10}N$	132.0814	134	
C_9H_7O	131.0497	$C_{10}H_{12}$	132.0939	$C_3H_6N_2O_4$	134.0328
C_9H_9N	131.0736	C_{11}	132.0000	$C_3H_8N_3O_3$	134.0566
$C_{10}H_{11}$	131.0861	133		$C_3H_{10}N_4O_2$	134.0805
132		$C_3H_5N_2O_4$	133.0249	$C_4H_8NO_4$	134.0453
$C_3H_4N_2O_4$	132.0171				

FM		FM		FM	
$C_4H_{10}N_2O_3$	134.0692	$C_5H_{11}O_4$	135.0657	$C_6H_2NO_3$	136.0034
$C_4H_{12}N_3O_2$	134.0930	$C_5H_{13}NO_3$	135.0896	$C_6H_2N_2O_2$	136.0273
$C_4H_{14}N_4O$	134.1169	$C_5HN_3O_2$	135.0069	$C_6H_6N_3O$	136.0511
$C_5H_{10}O_4$	134.0579	$C_5H_3N_4O$	135.0308	$C_6H_8N_4$	136.0750
$C_5H_{12}NO_3$	134.0817	C_6HNO_3	134.9956	$C_7H_4O_3$	136.0160
$C_5H_{14}N_2O_2$	134.1056	$C_6H_3N_2O_2$	135.0195	$C_7H_8NO_2$	136.0399
$C_5N_3O_2$	133.9991	$C_6H_5N_3O$	135.0433	$C_7H_8N_2O$	136.0637
$C_5H_2N_4O$	134.0229	$C_6H_7N_4$	135.0672	$C_7H_{10}N_3$	136.0876
$C_6H_{14}O_3$	134.0943	$C_7H_3O_3$	135.0082	$C_8H_8O_2$	136.0524
C_6NO_3	133.9878	$C_7H_5NO_2$	135.0320	$C_8H_{10}NO$	136.0763
$C_6H_2N_2O_2$	134.0116	$C_7H_7N_2O$	135.0559	$C_8H_{12}N_2$	136.1001
$C_6H_4N_3O$	134.0355	$C_7H_9N_3$	135.0798	$C_9H_{12}O$	136.0888
$C_6H_6N_4$	134.0594	$C_8H_7O_2$	135.0446	$C_9H_{14}N$	136.1127
$C_7H_2O_3$	134.0003	C_8H_9NO	135.0684	C_9N_2	136.0062
$C_7H_4NO_2$	134.0242	$C_8H_{11}N_2$	135.0923	$C_{10}H_{16}$	136.1253
$C_7H_6N_2O$	134.0480	$C_9H_{11}O$	135.0810	$C_{10}O$	135.9949
$C_7H_8N_3$	134.0719	$C_9H_{13}N$	135.1049	$C_{10}H_2N$	136.0187
$C_8H_6O_2$	134.0368	$C_{10}H_{15}$	135.1174	$C_{11}H_4$	136.0313
C_8H_8NO	134.0606	$C_{10}HN$	135.0109	137	
$C_8H_{10}N_2$	134.0845	$C_{11}H_3$	135.0235	$C_3H_9N_2O_4$	137.0563
$C_9H_{10}O$	134.0732	136		$C_3H_{11}N_3O_3$	137.0881
$C_9H_{12}N$	134.0970	$C_3H_8N_2O_4$	136.0484	$C_4H_{11}NO_4$	137.0688
$C_{10}H_{14}$	134.1096	$C_3H_{10}N_3O_3$	136.0723	$C_4HN_4O_2$	137.0100
$C_{10}N$	134.0031	$C_3H_{12}N_4O_2$	136.0961	$C_5HN_2O_3$	136.9987
$C_{11}H_2$	134.0157	$C_4H_{10}NO_4$	136.0610	$C_5H_3N_3O_2$	137.0226
135		$C_4H_{12}N_2O_3$	136.0848	$C_5H_5N_4O$	137.0464
$C_3H_7N_2O_4$	135.0406	$C_4N_4O_2$	136.0022	C_6HO_4	136.9874
$C_3H_9N_3O_3$	135.0644	$C_5H_{12}O_4$	136.0735	$C_6H_3NO_3$	137.0113
$C_3H_{11}N_4O_2$	135.0883	$C_5N_2O_3$	135.9909	$C_6H_5N_2O_2$	137.0351
$C_4H_9NO_4$	135.0532	$C_5H_2N_3O_2$	136.0147	$C_6H_7N_3O$	137.0590
$C_4H_{11}N_2O_3$	135.0770	$C_5H_4N_4O$	136.0386	$C_6H_9N_4$	137.0829
$C_4H_{13}N_3O_2$	135.1009	C_6O_4	135.9796	$C_7H_5O_3$	137.0238

	FM		FM		FM
$C_7H_7NO_2$	137.0477	$C_8H_{14}N_2$	138.1158	C_9HNO	139.0058
$C_7H_9N_2O$	137.0715	C_8N_3	138.0093	$C_9H_3N_2$	139.0297
$C_7H_{11}N_3$	137.0954	$C_9H_{14}O$	138.1045	$C_{10}H_{19}$	139.1488
$C_8H_9O_2$	137.0603	$C_9H_{16}N$	138.1284	$C_{10}H_3O$	139.0184
$C_8H_{11}NO$	137.0841	C_9NO	137.9980	$C_{10}H_5N$	139.0422
$C_8H_{13}N_2$	137.1080	$C_9H_2N_2$	138.0218	$C_{11}H_7$	139.0548
$C_9H_{13}O$	137.0967	$C_{10}H_{18}$	138.1409	140	
$C_9H_{15}N$	137.1205	$C_{10}H_2O$	138.0106	$C_4N_2O_4$	139.9858
C_9HN_2	137.0140	$C_{10}H_4N$	138.0344	$C_4H_2N_3O_3$	140.0096
$C_{10}H_{17}$	137.1331	$C_{11}H_6$	138.0470	$C_4H_4N_4O_2$	140.0335
$C_{10}HO$	137.0027	139		$C_5H_2NO_4$	139.9983
$C_{10}H_3N$	137.0266	$C_4HN_3O_3$	139.0018	$C_5H_4N_2O_3$	140.0222
$C_{11}H_5$	137.0391	$C_4H_3N_4O_2$	139.0257	$C_5H_6N_3O_2$	140.0460
138		C_5HNO_4	138.9905	$C_5H_8N_4O$	140.0699
$C_3H_{10}N_2O_4$	138.0641	$C_5H_3N_2O_3$	139.0144	$C_6H_4O_4$	140.0109
$C_4N_3O_3$	137.9940	$C_5H_5N_3O_2$	139.0382	$C_6H_6NO_3$	140.0348
$C_4H_2N_4O_2$	138.0178	$C_5H_7N_4O$	139.0621	$C_6H_8N_2O_2$	140.0586
C_5NO_4	137.9827	$C_6H_3O_4$	139.0031	$C_6H_{10}N_3O$	140.0825
$C_5H_2N_2O_3$	138.0065	$C_6H_5NO_3$	139.0269	$C_6H_{12}N_4$	140.1063
$C_5H_4N_3O_2$	138.0304	$C_6H_7N_2O_2$	139.0508	$C_7H_8O_3$	140.0473
$C_5H_6N_4O$	138.0542	$C_6H_9N_3O$	139.0746	$C_7H_{10}NO_2$	140.0712
$C_6H_2O_4$	137.9953	$C_6H_{11}N_4$	139.0985	$C_7H_{12}N_2O$	140.0950
$C_6H_4NO_3$	138.0191	$C_7H_7O_3$	139.0395	$C_7H_{14}N_3$	140.1189
$C_6H_6N_2O_2$	138.0429	$C_7H_9NO_2$	139.0634	C_7N_4	140.0124
$C_6H_8N_3O$	138.0668	$C_7H_{11}N_2O$	139.0872	$C_8H_{12}O_2$	140.0837
$C_6H_{10}N_4$	138.0907	$C_7H_{13}N_3$	139.1111	$C_8H_{14}NO$	140.1076
$C_7H_6O_3$	138.0317	$C_8H_{11}O_2$	139.0759	$C_8H_{16}N_2$	140.1315
$C_7H_8NO_2$	138.0555	$C_8H_{13}NO$	139.0998	C_8N_2O	140.0011
$C_7H_{10}N_2O$	138.0794	$C_8H_{15}N_2$	139.1236	$C_8H_2N_3$	140.0249
$C_7H_{12}N_3$	138.1032	C_8HN_3	139.0171	$C_9H_{16}O$	140.1202
$C_8H_{10}O_2$	138.0681	$C_9H_{15}O$	139.1123	C_9O_2	139.9898
$C_8H_{12}NO$	138.0919	$C_9H_{17}N$	139.1362	$C_9H_{18}N$	140.1440

FM		FM		FM	
C ₉ H ₂ NO	140.0136	C ₉ H ₃ NO	141.0215	C ₉ H ₂ O ₂	142.0054
C ₉ H ₄ N ₂	140.0375	C ₉ H ₅ N ₂	141.0453	C ₉ H ₂₀ N	142.1597
C ₁₀ H ₂₀	140.1566	C ₁₀ H ₂₁	141.1644	C ₉ H ₄ NO	142.0293
C ₁₀ H ₄ O	140.0262	C ₁₀ H ₅ O	141.0340	C ₉ H ₆ N ₂	142.0532
C ₁₀ H ₆ N	140.0501	C ₁₀ H ₇ N	141.0579	C ₁₀ H ₂₂	142.1722
C ₁₁ H ₈	140.0626	C ₁₁ H ₉	141.0705	C ₁₀ H ₆ O	142.0419
141		142		C ₁₀ H ₈ N	142.0657
C ₄ HN ₂ O ₄	140.9936	C ₄ H ₂ N ₂ O ₄	142.0014	C ₁₁ H ₁₀	142.0783
C ₄ H ₃ N ₃ O ₃	141.0175	C ₄ H ₄ N ₃ O ₃	142.0253	143	
C ₄ H ₅ N ₄ O ₂	141.0413	C ₄ H ₆ N ₄ O ₂	142.0491	C ₄ H ₃ N ₂ O ₄	143.0093
C ₅ H ₃ NO ₄	141.0062	C ₅ H ₄ NO ₄	142.0140	C ₄ H ₅ N ₃ O ₃	143.0331
C ₅ H ₅ N ₂ O ₃	141.0300	C ₅ H ₆ N ₂ O ₃	142.0379	C ₄ H ₇ N ₄ O ₂	143.0570
C ₅ H ₇ N ₃ O ₂	141.0539	C ₅ H ₈ N ₃ O ₂	142.0617	C ₅ H ₅ NO ₄	143.0218
C ₅ H ₉ N ₄ O	141.0777	C ₅ H ₁₀ N ₄ O	142.0856	C ₅ H ₇ N ₂ O ₃	143.0457
C ₆ H ₅ O ₄	141.0187	C ₆ H ₆ O ₄	142.0266	C ₅ H ₉ N ₃ O ₂	143.0695
C ₆ H ₇ NO ₃	141.0426	C ₆ H ₈ NO ₃	142.0504	C ₅ H ₁₁ N ₄ O	143.0934
C ₆ H ₉ N ₂ O ₂	141.0664	C ₆ H ₁₀ N ₂ O ₂	142.0743	C ₆ H ₇ O ₄	143.0344
C ₆ H ₁₁ N ₃ O	141.0903	C ₆ H ₁₂ N ₃ O	142.0981	C ₆ H ₉ NO ₃	143.0583
C ₆ H ₁₃ N ₄	141.1142	C ₆ H ₁₄ N ₄	142.1220	C ₆ H ₁₁ N ₂ O ₂	143.0821
C ₇ H ₉ O ₃	141.0552	C ₇ H ₁₀ O ₃	142.0630	C ₆ H ₁₃ N ₃ O	143.1060
C ₇ H ₁₁ NO ₂	141.0790	C ₇ H ₁₂ NO ₂	142.0868	C ₆ H ₁₅ N ₄	143.1298
C ₇ H ₁₃ N ₂ O	141.1029	C ₇ H ₁₄ N ₂ O	142.1107	C ₇ H ₁₁ O ₃	143.0708
C ₇ H ₁₅ N ₃	141.1267	C ₇ H ₁₆ N ₃	142.1346	C ₇ H ₁₃ NO ₂	143.0947
C ₇ HN ₄	141.0202	C ₇ N ₃ O	142.0042	C ₇ H ₁₅ N ₂ O	143.1185
C ₇ H ₁₃ O ₂	141.0916	C ₇ H ₂ N ₄	142.0280	C ₇ H ₁₇ N ₃	143.1424
C ₈ H ₁₅ NO	141.1154	C ₈ H ₁₄ O ₂	142.0994	C ₇ HN ₃ O	143.0120
C ₈ H ₁₇ N ₂	141.1393	C ₈ H ₁₆ NO	142.1233	C ₇ H ₃ N ₄	143.0359
C ₈ HN ₂ O	141.0089	C ₈ NO ₂	141.9929	C ₈ H ₁₅ O ₂	143.1072
C ₈ H ₃ N ₃	141.0328	C ₈ H ₁₈ N ₂	142.1471	C ₈ H ₁₇ NO	143.1311
C ₉ H ₁₇ O	141.1280	C ₈ H ₂ N ₂ O	142.0167	C ₈ HNO ₂	143.0007
C ₉ HO ₂	140.9976	C ₈ H ₄ N ₃	142.0406	C ₈ H ₁₉ N ₂	143.1549
C ₉ H ₁₉ N	141.1519	C ₉ H ₁₈ O	142.1358	C ₈ H ₃ N ₂ O	143.0246

FM		FM		FM	
$C_8H_5N_3$	143.0484	$C_8H_{18}NO$	144.1389	$C_7H_3N_3O$	145.0277
$C_9H_{19}O$	143.1436	$C_8H_2NO_2$	144.0085	$C_7H_5N_4$	145.0515
$C_9H_3O_2$	143.0133	$C_8H_{20}N_2$	144.1628	$C_8H_{17}O_2$	145.1229
$C_9H_{21}N$	143.1675	$C_8H_4N_2O$	144.0324	C_8HO_3	144.9925
C_9H_5NO	143.0371	$C_8H_6N_3$	144.0563	$C_8H_{19}NO$	145.1467
$C_9H_7N_2$	143.0610	$C_9H_{20}O$	144.1515	$C_8H_3NO_2$	145.0164
$C_{10}H_7O$	143.0497	$C_9H_4O_2$	144.0211	$C_8H_5N_2O$	145.0402
$C_{10}H_9N$	143.0736	C_9H_6NO	144.0449	$C_8H_7N_3$	145.0641
$C_{11}H_{11}$	143.0861	$C_9H_8N_2$	144.0688	$C_9H_5O_2$	145.0289
144		$C_{10}H_8O$	144.0575	C_9H_7NO	145.0528
$C_4H_4N_2O_4$	144.0171	$C_{10}H_{10}N$	144.0814	$C_9H_9N_2$	145.0767
$C_4H_6N_3O_3$	144.0410	$C_{11}H_{12}$	144.0939	$C_{10}H_9O$	145.0653
$C_4H_8N_4O_2$	144.0648	C_{12}	144.0000	$C_{10}H_{11}N$	145.0892
$C_5H_6NO_4$	144.0297	145		$C_{11}H_{13}$	145.1018
$C_5H_8N_2O_3$	144.0535	$C_4H_5N_2O_4$	145.0249	$C_{12}H$	145.0078
$C_5H_{10}N_3O_2$	144.0774	$C_4H_7N_3O_3$	145.0488	146	
$C_5H_{12}N_4O$	144.1012	$C_4H_9N_4O_2$	145.0726	$C_4H_6N_2O_4$	146.0328
$C_6H_8O_4$	144.0422	$C_5H_7NO_4$	145.0375	$C_4H_8N_3O_3$	146.0566
$C_6H_{10}NO_3$	144.0661	$C_5H_9N_2O_3$	145.0614	$C_4H_{10}N_4O_2$	146.0805
$C_6H_{12}N_2O_2$	144.0899	$C_5H_{11}N_3O_2$	145.0852	$C_5H_8NO_4$	146.0453
$C_6H_{14}N_3O$	144.1138	$C_5H_{13}N_4O$	145.1091	$C_5H_{10}N_2O_3$	146.0692
$C_6H_{16}N_4$	144.1377	$C_6H_9O_4$	145.0501	$C_5H_{12}N_3O_2$	146.0930
C_6N_4O	144.0073	$C_6H_{11}NO_3$	145.0739	$C_5H_{14}N_4O$	146.1169
$C_7H_{12}O_3$	144.0786	$C_6H_{13}N_2O_2$	145.0978	$C_6H_{10}O_4$	146.0579
$C_7H_{14}NO_2$	144.1025	$C_6H_{15}N_3O$	145.1216	$C_6H_{12}NO_3$	146.0817
$C_7H_{16}N_2O$	144.1264	$C_6H_{17}N_4$	145.1455	$C_6H_{14}N_2O_2$	146.1056
$C_7N_2O_2$	143.9960	C_6HN_4O	145.0151	$C_6H_{16}N_3O$	146.1295
$C_7H_{18}N_3$	144.1502	$C_7H_{13}O_3$	145.0865	$C_6N_3O_2$	145.9991
$C_7H_2N_3O$	144.0198	$C_7H_{15}NO_2$	145.1103	$C_6H_{18}N_4$	146.1533
$C_7H_4N_4$	144.0437	$C_7H_{17}N_2O$	145.1342	$C_6H_2N_4O$	146.0229
$C_8H_{16}O_2$	144.1151	$C_7HN_2O_2$	145.0038	$C_7H_{14}O_3$	146.0943
C_8O_3	143.9847	$C_7H_{19}N_3$	145.1580	$C_7H_{16}NO_2$	146.1182

FM		FM		FM	
C_7NO_3	145.9878	$C_7H_{15}O_3$	147.1021	$C_6H_4N_4O$	148.0386
$C_7H_{18}N_2O$	146.1420	$C_7H_{17}NO_2$	147.1260	$C_7H_{16}O_3$	148.1100
$C_7H_2N_2O_2$	146.0116	C_7HNO_3	146.9956	C_7O_4	147.9796
$C_7H_4N_3O$	146.0355	$C_7H_3N_2O_2$	147.0195	$C_7H_2NO_3$	148.0034
$C_7H_6N_4$	146.0594	$C_7H_5N_3O$	147.0433	$C_7H_4N_2O_2$	148.0273
$C_8H_{18}O_2$	146.1307	$C_7H_7N_4$	147.0672	$C_7H_6N_3O$	148.0511
$C_8H_2O_3$	146.0003	$C_8H_5O_3$	147.0082	$C_7H_8N_4$	148.0750
$C_8H_4NO_2$	146.0242	$C_8H_5NO_2$	147.0320	$C_8H_4O_3$	148.0160
$C_8H_8N_2O$	146.0480	$C_8H_7N_2O$	147.0559	$C_8H_6NO_2$	148.0399
$C_8H_8N_3$	146.0719	$C_8H_9N_3$	147.0798	$C_8H_8N_2O$	148.0637
$C_9H_6O_2$	146.0368	$C_9H_7O_2$	147.0446	$C_8H_{10}N_3$	148.0876
C_9H_8NO	146.0606	C_9H_9NO	147.0684	$C_9H_8O_2$	148.0524
$C_9H_{10}N_2$	146.0845	$C_9H_{11}N_2$	147.0923	$C_9H_{10}NO$	148.0763
$C_{10}H_{10}O$	146.0732	$C_{10}H_{11}O$	147.0810	$C_9H_{12}N_2$	148.1001
$C_{10}H_{12}N$	146.0970	$C_{10}H_{13}N$	147.1049	$C_{10}H_{12}O$	148.0888
$C_{11}H_{14}$	146.1096	$C_{11}H_{15}$	147.1174	$C_{10}H_{14}N$	148.1127
$C_{11}N$	146.0031	$C_{11}HN$	147.0109	$C_{10}N_2$	148.0062
$C_{12}H_2$	146.0157	$C_{12}H_3$	147.0235	$C_{11}H_{16}$	148.1253
147		148		$C_{11}O$	147.9949
$C_4H_7N_2O_4$	147.0406	$C_4H_8N_2O_4$	148.0484	$C_{11}H_2N$	148.0187
$C_4H_9N_3O_3$	147.0644	$C_4H_{10}N_3O_3$	148.0723	$C_{12}H_4$	148.0313
$C_4H_{11}N_4O_2$	147.0883	$C_4H_{12}N_4O_2$	148.0961	149	
$C_5H_9NO_4$	147.0532	$C_5H_{10}NO_4$	148.0610	$C_4H_9N_2O_4$	149.0563
$C_5H_{11}N_2O_3$	147.0770	$C_5H_{12}N_2O_3$	148.0848	$C_4H_{11}N_3O_3$	149.0801
$C_5H_{13}N_3O_2$	147.1009	$C_5H_{14}N_3O_2$	148.1087	$C_4H_{13}N_4O_2$	149.1040
$C_5H_{15}N_4O$	147.1247	$C_5H_{16}N_4O$	148.1325	$C_5H_{11}NO_4$	149.0688
$C_6H_{11}O_4$	147.0657	$C_5N_4O_2$	148.0022	$C_5H_{13}N_2O_3$	149.0927
$C_6H_{13}NO_3$	147.0896	$C_6H_{12}O_4$	148.0735	$C_5H_{15}N_3O_2$	149.1165
$C_6H_{15}N_2O_2$	147.1134	$C_6H_{14}NO_3$	148.0974	$C_5HN_4O_2$	149.0100
$C_6H_{17}N_3O$	147.1373	$C_6H_{16}N_2O_2$	148.1213	$C_6H_{13}O_4$	149.0814
$C_6HN_3O_2$	147.0069	$C_6N_2O_3$	147.9909	$C_6H_{15}NO_3$	149.1052
$C_6H_3N_4O$	147.0308	$C_6H_2N_3O_2$	148.0147	$C_6HN_2O_3$	148.9987

FM		FM		FM	
$C_6H_3N_3O_2$	149.0226	$C_6H_4N_3O_2$	150.0304	$C_6H_7N_4O$	151.0621
$C_6H_5N_4O$	149.0464	$C_6H_6N_4O$	150.0542	$C_7H_3O_4$	151.0031
C_7HO_4	148.9874	$C_7H_2O_4$	149.9953	$C_7H_5NO_3$	151.0269
$C_7H_3NO_3$	149.0113	$C_7H_4NO_3$	150.0191	$C_7H_7N_2O_2$	151.0508
$C_7H_5N_2O_2$	149.0351	$C_7H_6N_2O_2$	150.0429	$C_7H_9N_3O$	151.0746
$C_7H_7N_3O$	149.0590	$C_7H_8N_3O$	150.0668	$C_7H_{11}N_4$	151.0985
$C_7H_9N_4$	149.0829	$C_7H_{10}N_4$	150.0907	$C_8H_7O_3$	151.0395
$C_8H_5O_3$	149.0238	$C_8H_6O_3$	150.0317	$C_8H_9NO_2$	151.0634
$C_8H_7NO_2$	149.0477	$C_8H_8NO_2$	150.0555	$C_8H_{11}N_2O$	151.0872
$C_8H_9N_2O$	149.0715	$C_8H_{10}N_2O$	150.0794	$C_8H_{13}N_3$	151.1111
$C_8H_{11}N_3$	149.0954	$C_8H_{12}N_3$	150.1032	$C_9H_{11}O_2$	151.0759
$C_9H_9O_2$	149.0603	$C_9H_{10}O_2$	150.0681	$C_9H_{13}NO$	151.0998
$C_9H_{11}NO$	149.0841	$C_9H_{12}NO$	150.0919	$C_9H_{15}N_2$	151.1236
$C_9H_{13}N_2$	149.1080	$C_9H_{14}N_2$	150.1158	C_9HN_3	151.0171
$C_{10}H_{13}O$	149.0967	C_9N_3	150.0093	$C_{10}H_{15}O$	151.1123
$C_{10}H_{15}N$	149.1205	$C_{10}H_{14}O$	150.1045	$C_{10}H_{17}N$	151.1362
$C_{10}HN_2$	149.0140	$C_{10}H_{16}N$	150.1284	$C_{10}HNO$	151.0058
$C_{11}H_{17}$	149.1331	$C_{10}NO$	149.9980	$C_{10}H_3N_2$	151.0297
$C_{11}HO$	149.0027	$C_{10}H_2N_2$	150.0218	$C_{11}H_{19}$	151.1488
$C_{11}H_3N$	149.0266	$C_{11}H_{18}$	150.1409	$C_{11}H_3O$	151.0184
$C_{12}H_5$	149.0391	$C_{11}H_2O$	150.0106	$C_{11}H_5N$	151.0422
150		$C_{11}H_4N$	150.0344	$C_{12}H_7$	151.0548
$C_4H_{10}N_2O_4$	150.0641	$C_{12}H_6$	150.0470	152	
$C_4H_{12}N_3O_3$	150.0879	151		$C_4H_{12}N_2O_4$	152.0797
$C_4H_{14}N_4O_2$	150.1118	$C_4H_{11}N_2O_4$	151.0719	$C_5N_2O_4$	151.9858
$C_5H_{12}NO_4$	150.0766	$C_4H_{13}N_3O_3$	151.0958	$C_5H_2N_3O_3$	152.0096
$C_5H_{14}N_2O_3$	150.1005	$C_5H_{13}NO_4$	151.0845	$C_5H_4N_4O_2$	152.0335
$C_5N_3O_3$	149.9940	$C_5HN_3O_3$	151.0018	$C_6H_2NO_4$	151.9983
$C_5H_2N_4O_2$	150.0178	$C_5H_3N_4O_2$	151.0257	$C_6H_4N_2O_3$	152.0222
$C_6H_{14}O_4$	150.0892	C_6HNO_4	150.9905	$C_6H_6N_3O_2$	152.0460
C_6NO_4	149.9827	$C_6H_3N_2O_3$	151.0144	$C_6H_8N_4O$	152.0699
$C_6H_2N_2O_3$	150.0065	$C_6H_5N_3O_2$	151.0382	$C_7H_4O_4$	152.0109

FM		FM		FM	
$C_7H_6NO_3$	152.0348	$C_7H_7NO_3$	153.0426	$C_7H_8NO_3$	154.0504
$C_7H_8N_2O_2$	152.0586	$C_7H_9N_2O_2$	153.0664	$C_7H_{10}N_2O_2$	154.0743
$C_7H_{10}N_3O$	152.0825	$C_7H_{11}N_3O$	153.0903	$C_7H_{12}N_3O$	154.0981
$C_7H_{12}N_4$	152.1063	$C_7H_{13}N_4$	153.1142	$C_7H_{14}N_4$	154.1220
$C_8H_8O_3$	152.0473	$C_8H_9O_3$	153.0552	$C_8H_{10}O_3$	154.0630
$C_8H_{10}NO_2$	152.0712	$C_8H_{11}NO_2$	153.0790	$C_8H_{12}NO_2$	154.0868
$C_8H_{12}N_2O$	152.0950	$C_8H_{13}N_2O$	153.1029	$C_8H_{14}N_2O$	154.1107
$C_8H_{14}N_3$	152.1189	$C_8H_{15}N_3$	153.1267	$C_8H_{16}N_3$	154.1346
C_8N_4	152.0124	C_8HN_4	153.0202	C_8N_3O	154.0042
$C_9H_{12}O_2$	152.0837	$C_9H_{13}O_2$	153.0916	$C_8H_2N_4$	154.0280
$C_9H_{14}NO$	152.1076	$C_9H_{15}NO$	153.1154	$C_9H_{14}O_2$	154.0994
$C_9H_{16}N_2$	152.1315	$C_9H_{17}N_2$	153.1393	$C_9H_{16}NO$	154.1233
C_9N_2O	152.0011	C_9HN_2O	153.0089	C_9NO_2	153.9929
$C_9H_2N_3$	152.0249	$C_9H_3N_3$	153.0328	$C_9H_{18}N_2$	154.1471
$C_{10}H_{16}O$	152.1202	$C_{10}H_{17}O$	153.1280	$C_9H_2N_2O$	154.0167
$C_{10}O_2$	151.9898	$C_{10}HO_2$	152.9976	$C_9H_4N_3$	154.0406
$C_{10}H_{18}N$	152.1440	$C_{10}H_{19}N$	153.1519	$C_{10}H_{18}O$	154.1358
$C_{10}H_2NO$	152.0136	$C_{10}H_3NO$	153.0215	$C_{10}H_2O_2$	154.0054
$C_{10}H_4N_2$	152.0375	$C_{10}H_5N_2$	153.0453	$C_{10}H_{20}N$	154.1597
$C_{11}H_{20}$	152.1566	$C_{11}H_{21}$	153.1644	$C_{10}H_4NO$	154.0293
$C_{11}H_4O$	152.0262	$C_{11}H_5O$	153.0340	$C_{10}H_6N_2$	154.0532
$C_{11}H_6N$	152.0501	$C_{11}H_7N$	153.0579	$C_{11}H_{22}$	154.1722
$C_{12}H_8$	152.0626	$C_{12}H_9$	153.0705	$C_{11}H_6O$	154.0419
153		154		$C_{11}H_8N$	154.0657
$C_3HN_2O_4$	152.9936	$C_5H_2N_2O_4$	154.0014	$C_{12}H_{10}$	154.0783
$C_5H_3N_3O_3$	153.0175	$C_5H_4N_3O_3$	154.0253	155	
$C_5H_5N_4O_2$	153.0413	$C_5H_6N_4O_2$	154.0491	$C_5H_3N_2O_4$	155.0093
$C_6H_3NO_4$	153.0062	$C_6H_4NO_4$	154.0140	$C_5H_5N_3O_3$	155.0331
$C_6H_5N_2O_3$	153.0300	$C_6H_6N_2O_3$	154.0379	$C_5H_7N_4O_2$	155.0570
$C_6H_7N_3O_2$	153.0539	$C_6H_8N_3O_2$	154.0617	$C_6H_5NO_4$	155.0218
$C_6H_9N_4O$	153.0777	$C_6H_{10}N_4O$	154.0856	$C_6H_7N_2O_3$	155.0457
$C_7H_5O_4$	153.0187	$C_7H_6O_4$	154.0266	$C_6H_9N_3O_2$	155.0695

	FM		FM		FM
$C_6H_{11}N_4O$	155.0934	$C_6H_8N_2O_3$	156.0535	C_{13}	156.0000
$C_7H_7O_4$	155.0344	$C_6H_{10}N_3O_2$	156.0774	157	
$C_7H_9NO_3$	155.0583	$C_6H_{12}N_4O$	156.1012	$C_5H_5N_2O_4$	157.0249
$C_7H_{11}N_2O_2$	155.0821	$C_7H_8O_4$	156.0422	$C_5H_7N_3O_3$	157.0488
$C_7H_{13}N_3O$	155.1060	$C_7H_{10}NO_3$	156.0661	$C_5H_9N_4O_2$	157.0726
$C_7H_{15}N_4$	155.1298	$C_7H_{12}N_2O_2$	156.0899	$C_6H_7NO_4$	157.0375
$C_8H_{11}O_3$	155.0708	$C_7H_{14}N_3O$	156.1138	$C_6H_9N_2O_3$	157.0614
$C_8H_{13}NO_2$	155.0947	$C_7H_{16}N_4$	156.1377	$C_6H_{11}N_3O_2$	157.0852
$C_8H_{15}N_2O$	155.1185	C_7N_4O	156.0073	$C_6H_{13}N_4O$	157.1091
$C_8H_{17}N_3$	155.1424	$C_8H_{12}O_3$	156.0786	$C_7H_9O_4$	157.0501
C_8HN_3O	155.0120	$C_8H_{14}NO_2$	156.1025	$C_7H_{11}NO_3$	157.0739
$C_8H_3N_4$	155.0359	$C_8H_{16}N_2O$	156.1264	$C_7H_{13}N_2O_2$	157.0978
$C_9H_{15}O_2$	155.1072	$C_8N_2O_2$	155.9960	$C_7H_{15}N_3O$	157.1216
$C_9H_{17}NO$	155.1311	$C_8H_{18}N_3$	156.1502	$C_7H_{17}N_4$	157.1455
C_9HNO_2	155.0007	$C_8H_2N_3O$	156.0198	C_7HN_4O	157.0151
$C_9H_{19}N_2$	155.1549	$C_8H_4N_4$	156.0437	$C_8H_{13}O_3$	157.0865
$C_9H_3N_2O$	155.0246	$C_9H_{16}O_2$	156.1151	$C_8H_{15}NO_2$	157.1103
$C_9H_5N_3$	155.0484	C_9O_3	155.9847	$C_8H_{17}N_2O$	157.1342
$C_{10}H_{19}O$	155.1436	$C_9H_{18}NO$	156.1389	$C_8HN_2O_2$	157.0038
$C_{10}H_3O_2$	155.0133	$C_9H_2NO_2$	156.0085	$C_8H_{19}N_3$	157.1580
$C_{10}H_{21}N$	155.1675	$C_9H_{20}N_2$	156.1628	$C_8H_3N_3O$	157.0277
$C_{10}H_5NO$	155.0371	$C_9H_4N_2O$	156.0324	$C_8H_5N_4$	157.0515
$C_{10}H_7N_2$	155.0610	$C_9H_6N_3$	156.0563	$C_9H_{17}O_2$	157.1229
$C_{11}H_{23}$	155.1801	$C_{10}H_{20}O$	156.1515	C_9HO_3	156.9925
$C_{11}H_7O$	155.0497	$C_{10}H_4O_2$	156.0211	$C_9H_{19}NO$	157.1467
$C_{11}H_9N$	155.0736	$C_{10}H_{22}N$	156.1753	$C_9H_3NO_2$	157.0164
$C_{12}H_{11}$	155.0861	$C_{10}H_6NO$	156.0449	$C_9H_{21}N_2$	157.1706
156		$C_{10}H_8N_2$	156.0688	$C_9H_5N_2O$	157.0402
$C_5H_4N_2O_4$	156.0171	$C_{11}H_{24}$	156.1879	$C_9H_7N_3$	157.0641
$C_5H_6N_3O_3$	156.0410	$C_{11}H_8O$	156.0575	$C_{10}H_{21}O$	157.1593
$C_5H_8N_4O_2$	156.0648	$C_{11}H_{10}N$	156.0814	$C_{10}H_5O_2$	157.0289
$C_6H_6NO_4$	156.0297	$C_{12}H_{12}$	156.0939	$C_{10}H_{23}N$	157.1832

FM		FM		FM	
$C_{10}H_7NO$	157.0528	$C_9H_4NO_2$	158.0242	$C_8H_3N_2O_2$	159.0195
$C_{10}H_9N_2$	157.0767	$C_9H_{22}N_2$	158.1784	$C_8H_{21}N_3$	159.1737
$C_{11}H_9O$	157.0653	$C_9H_6N_2O$	158.0480	$C_8H_5N_3O$	159.0433
$C_{11}H_{11}N$	157.0892	$C_9H_8N_3$	158.0719	$C_8H_7N_4$	159.0672
$C_{12}H_{13}$	157.1018	$C_{10}H_{22}O$	158.1671	$C_9H_{19}O_2$	159.1385
$C_{13}H$	157.0078	$C_{10}H_6O_2$	158.0368	$C_9H_3O_3$	159.0082
158		$C_{10}H_8NO$	158.0606	$C_9H_{21}NO$	159.1624
$C_5H_6N_2O_4$	158.0328	$C_{10}H_{10}N_2$	158.0845	$C_9H_5NO_2$	159.0320
$C_5H_8N_3O_3$	158.0566	$C_{11}H_{10}O$	158.0732	$C_9H_7N_2O$	159.0559
$C_5H_{10}N_4O_2$	158.0805	$C_{11}H_{12}N$	158.0970	$C_9H_9N_3$	159.0798
$C_6H_8NO_4$	158.0453	$C_{12}H_{14}$	158.1096	$C_{10}H_7O_2$	159.0446
$C_6H_{10}N_2O_3$	158.0692	$C_{12}N$	158.0031	$C_{10}H_9NO$	159.0684
$C_6H_{12}N_3O_2$	158.0930	$C_{13}H_2$	158.0157	$C_{10}H_{11}N_2$	159.0923
$C_6H_{14}N_4O$	158.1169	159		$C_{11}H_{11}O$	159.0810
$C_7H_{10}O_4$	158.0579	$C_5H_7N_2O_4$	159.0406	$C_{11}H_{13}N$	159.1049
$C_7H_{12}NO_3$	158.0817	$C_5H_9N_3O_3$	159.0644	$C_{12}H_{15}$	159.1174
$C_7H_{14}N_2O_2$	158.1056	$C_5H_{11}N_4O_2$	159.0883	$C_{12}HN$	159.0109
$C_7H_{16}N_3O$	158.1295	$C_6H_9NO_4$	159.0532	$C_{13}H_3$	158.0235
$C_7N_3O_2$	157.9991	$C_6H_{11}N_2O_3$	159.0770	160	
$C_7H_{18}N_4$	158.1533	$C_6H_{13}N_3O_2$	159.1009	$C_5H_8N_2O_4$	160.0484
$C_7H_2N_4O$	158.0229	$C_6H_{15}N_4O$	159.1247	$C_5H_{10}N_3O_3$	160.0723
$C_8H_{14}O_3$	158.0943	$C_7H_{11}O_4$	159.0657	$C_5H_{12}N_4O_2$	160.0961
$C_8H_{16}NO_2$	158.1182	$C_7H_{13}NO_3$	159.0896	$C_6H_{10}NO_4$	160.0610
C_8NO_3	157.9878	$C_7H_{15}N_2O_2$	159.1134	$C_6H_{12}N_2O_3$	160.0848
$C_8H_{18}N_2O$	158.1420	$C_7H_{17}N_3O$	159.1373	$C_6H_{14}N_3O_2$	160.1087
$C_8H_2N_2O_2$	158.0116	$C_7HN_3O_2$	159.0069	$C_6H_{16}N_4O$	160.1325
$C_8H_{20}N_3$	158.1659	$C_7H_{19}N_4$	159.1611	$C_6N_4O_2$	160.0022
$C_8H_4N_3O$	158.0355	$C_7H_3N_4O$	159.0308	$C_7H_{12}O_4$	160.0735
$C_8H_6N_4$	158.0594	$C_8H_{15}O_3$	159.1021	$C_7H_{14}NO_3$	160.0974
$C_9H_{18}O_2$	158.1307	$C_8H_{17}NO_2$	159.1260	$C_7H_{16}N_2O_2$	160.1213
$C_9H_2O_3$	158.0003	C_8HNO_3	158.9956	$C_7N_2O_3$	159.9909
$C_9H_{20}NO$	158.1546	$C_8H_{19}N_2O$	159.1498	$C_7H_{18}N_3O$	160.1451

	FM		FM		FM
$C_7H_2N_3O_2$	160.0147	$C_6H_{15}N_3O_2$	161.1165	$C_5H_{12}N_3O_3$	162.0879
$C_7H_{20}N_4$	160.1690	$C_6H_{17}N_4O$	161.1404	$C_5H_{14}N_4O_2$	162.1118
$C_7H_4N_4O$	160.0386	$C_5HN_4O_2$	161.0100	$C_6H_{12}NO_4$	162.0766
$C_8H_{16}O_3$	160.1100	$C_7H_{13}O_4$	161.0814	$C_6H_{14}N_2O_3$	162.1005
C_8O_4	159.9796	$C_7H_{15}NO_3$	161.1052	$C_6H_{16}N_3O_2$	162.1244
$C_8H_{18}NO_2$	160.1338	$C_7H_{17}N_2O_2$	161.1291	$C_6N_3O_3$	161.9940
$C_8H_2NO_3$	160.0034	$C_7HN_2O_3$	160.9987	$C_6H_{18}N_4O$	162.1482
$C_8H_{20}N_2O$	160.1577	$C_7H_{19}N_3O$	161.1529	$C_6H_2N_4O_2$	162.0178
$C_8H_4N_2O_2$	160.0273	$C_7H_3N_3O_2$	161.0226	$C_7H_{14}O_4$	162.0892
$C_8H_6N_3O$	160.0511	$C_7H_5N_4O$	161.0464	$C_7H_{16}NO_3$	162.1131
$C_8H_8N_4$	160.0750	$C_8H_{17}O_3$	161.1178	C_7NO_4	161.9827
$C_9H_{20}O_2$	160.1464	C_8HO_4	160.9874	$C_7H_{18}N_2O_2$	162.1369
$C_9H_4O_3$	160.0160	$C_8H_{19}NO_2$	161.1416	$C_7H_2N_2O_3$	162.0065
$C_9H_6NO_2$	160.0399	$C_8H_3NO_3$	161.0113	$C_7H_4N_3O_2$	162.0304
$C_9H_8N_2O$	160.0637	$C_8H_5N_2O_2$	161.0351	$C_7H_6N_4O$	162.0542
$C_9H_{10}N_3$	160.0876	$C_8H_7N_3O$	161.0590	$C_8H_{18}O_3$	162.1256
$C_{10}H_8O_2$	160.0524	$C_8H_9N_4$	161.0829	$C_8H_2O_4$	161.9953
$C_{10}H_{10}NO$	160.0763	$C_9H_5O_3$	161.0238	$C_8H_4NO_3$	162.0191
$C_{10}H_{12}N_2$	160.1001	$C_9H_7NO_2$	161.0477	$C_8H_6N_2O_2$	162.0429
$C_{11}H_{12}O$	160.0888	$C_9H_9N_2O$	161.0715	$C_8H_8N_3O$	162.0668
$C_{11}H_{14}N$	160.1127	$C_9H_{11}N_3$	161.0954	$C_8H_{10}N_4$	162.0907
$C_{11}N_2$	160.0062	$C_{10}H_9O_2$	161.0603	$C_9H_6O_3$	162.0317
$C_{12}H_{16}$	160.1253	$C_{10}H_{11}NO$	161.0841	$C_9H_8NO_2$	162.0555
$C_{12}O$	159.9949	$C_{10}H_{13}N_2$	161.1080	$C_9H_{10}N_2O$	162.0794
$C_{12}H_2N$	160.0187	$C_{11}H_{13}O$	161.0967	$C_9H_{12}N_3$	162.1032
$C_{13}H_4$	160.0313	$C_{11}H_{15}N$	161.1205	$C_{10}H_{10}O_2$	162.0681
161		$C_{11}HN_2$	161.0140	$C_{10}H_{12}NO$	162.0919
$C_5H_9N_2O_4$	161.0563	$C_{12}H_{17}$	161.1331	$C_{11}H_{14}O$	162.1045
$C_5H_{11}N_3O_3$	161.0801	$C_{12}HO$	161.0027	$C_{11}H_{16}N$	162.1284
$C_5H_{13}N_4O_2$	161.1040	$C_{12}H_3N$	161.0266	$C_{11}NO$	161.9980
$C_6H_{11}NO_4$	161.0688	$C_{13}H_5$	161.0391	$C_{11}H_2N_2$	162.0218
$C_6H_{13}N_2O_3$	161.0927	162		$C_{12}H_{18}$	162.1409
		$C_5H_{10}N_2O_4$	162.0641		

FM		FM		FM	
C ₁₂ H ₂ O	162.0106	C ₁₁ H ₁₇ N	163.1362	C ₁₀ H ₁₄ NO	164.1076
C ₁₂ H ₄ N	162.0344	C ₁₁ HNO	163.0058	C ₁₀ H ₁₆ N ₂	164.1315
C ₁₃ H ₆	162.0470	C ₁₁ H ₃ N ₂	163.0297	C ₁₀ N ₂ O	164.0011
163		C ₁₂ H ₁₉	163.1488	C ₁₀ H ₂ N ₃	164.0249
C ₅ H ₁₁ N ₂ O ₄	163.0719	C ₁₂ H ₃ O	163.0184	C ₁₁ H ₁₆ O	164.1202
C ₅ H ₁₃ N ₃ O ₃	163.0958	C ₁₂ H ₅ N	163.0422	C ₁₁ O ₂	163.9898
C ₅ H ₁₅ N ₄ O ₂	163.1196	C ₁₃ H ₇	163.0548	C ₁₁ H ₁₈ N	164.1440
C ₆ H ₁₃ NO ₄	163.0845	164		C ₁₁ H ₂ NO	164.0136
C ₆ H ₁₅ N ₂ O ₃	163.1083	C ₅ H ₁₂ N ₂ O ₄	164.0797	C ₁₁ H ₄ N ₂	164.0375
C ₆ H ₁₇ N ₃ O ₂	163.1322	C ₅ H ₁₄ N ₃ O ₃	164.1036	C ₁₂ H ₂₀	164.1566
C ₆ HN ₃ O ₃	163.0018	C ₅ H ₁₆ N ₄ O ₂	164.1275	C ₁₂ H ₄ O	164.0262
C ₆ H ₃ N ₄ O ₂	163.0257	C ₆ H ₁₄ NO ₄	164.0923	C ₁₂ H ₆ N	164.0501
C ₇ H ₁₅ O ₄	163.0970	C ₆ H ₁₆ N ₂ O ₃	164.1162	C ₁₃ H ₈	164.0626
C ₇ H ₁₇ NO ₃	163.1209	C ₆ N ₂ O ₄	163.9858	165	
C ₇ HNO ₄	161.9905	C ₆ H ₂ N ₃ O ₃	164.0096	C ₅ H ₁₃ N ₂ O ₄	165.0876
C ₇ H ₃ N ₂ O ₃	163.0144	C ₆ H ₄ N ₄ O ₂	164.0335	C ₅ H ₁₅ N ₃ O ₃	165.1114
C ₇ H ₅ N ₃ O ₂	163.0382	C ₇ H ₁₆ O ₄	164.1049	C ₆ H ₁₅ NO ₄	165.1001
C ₇ H ₇ N ₄ O	163.0621	C ₇ H ₂ NO ₄	163.9983	C ₆ HN ₂ O ₄	164.9936
C ₈ H ₃ O ₄	163.0031	C ₇ H ₄ N ₂ O ₃	164.0222	C ₆ H ₃ N ₃ O ₃	165.0175
C ₈ H ₅ NO ₃	163.0269	C ₇ H ₆ N ₃ O ₂	164.0460	C ₆ H ₅ N ₄ O ₂	165.0413
C ₈ H ₇ N ₂ O ₂	163.0508	C ₇ H ₈ N ₄ O	164.0699	C ₇ H ₃ NO ₄	165.0062
C ₈ H ₉ N ₃ O	163.0746	C ₈ H ₄ O ₄	164.0109	C ₇ H ₅ N ₂ O ₃	165.0300
C ₈ H ₁₁ N ₄	163.0985	C ₈ H ₆ NO ₃	164.0348	C ₇ H ₇ N ₃ O ₂	165.0539
C ₉ H ₇ O ₃	163.0395	C ₈ H ₈ N ₂ O ₂	164.0586	C ₇ H ₉ N ₄ O	165.0777
C ₉ H ₉ NO ₂	163.0634	C ₈ H ₁₀ N ₃ O	164.0825	C ₈ H ₅ O ₄	165.0187
C ₉ H ₁₁ N ₂ O	163.0872	C ₈ H ₁₂ N ₄	164.1063	C ₈ H ₇ NO ₃	165.0426
C ₉ H ₁₃ N ₃	163.1111	C ₉ H ₈ O ₃	164.0473	C ₈ H ₉ N ₂ O ₂	165.0664
C ₁₀ H ₁₁ O ₂	163.0759	C ₉ H ₁₀ NO ₂	164.0712	C ₈ H ₁₁ N ₃ O	165.0903
C ₁₀ H ₁₃ NO	163.0998	C ₉ H ₁₂ N ₂ O	164.0950	C ₈ H ₁₃ N ₄	165.1142
C ₁₀ H ₁₅ N ₂	163.1236	C ₉ H ₁₄ N ₃	164.1189	C ₉ H ₉ O ₃	165.0552
C ₁₀ HN ₃	163.0171	C ₉ N ₄	164.0124	C ₉ H ₁₁ NO ₂	165.0790
C ₁₁ H ₁₅ O	163.1123	C ₁₀ H ₁₂ O ₂	164.0837	C ₉ H ₁₃ N ₂ O	165.1029

FM		FM		FM	
$C_9H_{15}N_3$	165.1267	$C_9H_{14}N_2O$	166.1107	$C_9H_{11}O_3$	167.0708
C_9HN_4	165.0202	$C_9H_{16}N_3$	166.1346	$C_9H_{13}NO_2$	167.0947
$C_{10}H_{13}O_2$	165.0916	C_9N_3O	166.0042	$C_9H_{15}N_2O$	167.1185
$C_{10}H_{15}NO$	165.1154	$C_9H_2N_4$	166.0280	$C_9H_{17}N_3$	167.1424
$C_{10}H_{17}N_2$	165.1393	$C_{10}H_{14}O_2$	166.0994	C_9HN_3O	167.0120
$C_{10}HN_2O$	165.0089	$C_{10}H_{16}NO$	166.1233	$C_9H_3N_4$	167.0359
$C_{10}H_3N_3$	165.0328	$C_{10}NO_2$	165.9929	$C_{10}H_{15}O_2$	167.1072
$C_{11}H_{17}O$	165.1280	$C_{10}H_{18}N_2$	166.1471	$C_{10}H_{17}NO$	167.1311
$C_{11}HO_2$	164.9976	$C_{10}H_2N_2O$	166.0167	$C_{10}HNO_2$	167.0007
$C_{11}H_{19}N$	165.1519	$C_{10}H_4N_3$	166.0406	$C_{10}H_{19}N_2$	167.1549
$C_{11}H_3NO$	165.0215	$C_{11}H_{18}O$	166.1358	$C_{10}H_3N_2O$	167.0246
$C_{11}H_5N_2$	165.0453	$C_{11}H_2O_2$	166.0054	$C_{10}H_5N_3$	167.0484
$C_{12}H_{21}$	165.1644	$C_{11}H_{20}N$	166.1597	$C_{11}H_{19}O$	167.1436
$C_{12}H_5O$	165.0340	$C_{11}H_4NO$	166.0293	$C_{11}H_3O_2$	167.0133
$C_{12}H_7N$	165.0579	$C_{11}H_6N_2$	166.0532	$C_{11}H_{21}N$	167.1675
$C_{13}H_9$	165.0705	$C_{12}H_{22}$	166.1722	$C_{11}H_5NO$	167.0371
166		$C_{12}H_6O$	166.0419	$C_{11}H_7N_2$	167.0610
$C_5H_{14}N_2O_4$	166.0954	$C_{12}H_8N$	166.0657	$C_{12}H_{23}$	167.1801
$C_6H_2N_2O_4$	166.0014	$C_{13}H_{10}$	166.0783	$C_{12}H_7O$	167.0497
$C_6H_4N_3O_3$	166.0253	167		$C_{12}H_9N$	167.0736
$C_6H_6N_4O_2$	166.0491	$C_6H_3N_2O_4$	167.0093	$C_{13}H_{11}$	167.0861
$C_7H_4NO_4$	166.0140	$C_6H_5N_3O_3$	167.0331	168	
$C_7H_6N_2O_3$	166.0379	$C_6H_7N_4O_2$	167.0570	$C_6H_4N_2O_4$	168.0171
$C_7H_8N_3O_2$	166.0617	$C_7H_5NO_4$	167.0218	$C_6H_6N_3O_3$	168.0410
$C_7H_{10}N_4O$	166.0856	$C_7H_7N_2O_3$	167.0451	$C_6H_8N_4O_2$	168.0648
$C_8H_6O_4$	166.0266	$C_7H_9N_3O_2$	167.0695	$C_7H_6NO_4$	168.0297
$C_8H_8NO_3$	166.0504	$C_7H_{11}N_4O$	167.0934	$C_7H_8N_2O_3$	168.0535
$C_8H_{10}N_2O_2$	166.0743	$C_8H_7O_4$	167.0344	$C_7H_{10}N_3O_2$	168.0774
$C_8H_{12}N_3O$	166.0981	$C_8H_9NO_3$	167.0583	$C_7H_{12}N_4O$	168.1012
$C_8H_{14}N_4$	166.1220	$C_8H_{11}N_2O_2$	167.0821	$C_8H_8O_4$	168.0422
$C_9H_{10}O_3$	166.0630	$C_8H_{13}N_3O$	167.1060	$C_8H_{10}NO_3$	168.0661
$C_9H_{12}NO_2$	166.0868	$C_8H_{15}N_4$	167.1298	$C_8H_{12}N_2O_2$	168.0899

	FM		FM		FM
$C_8H_{14}N_3O$	168.1138	$C_7H_9N_2O_3$	169.0614	$C_{14}H$	169.0078
$C_8H_{16}N_4$	168.1377	$C_7H_{11}N_3O_2$	169.0852	170	
C_8N_4O	168.0073	$C_7H_{13}N_4O$	169.1091	$C_6H_6N_2O_4$	170.0328
$C_9H_{12}O_3$	168.0786	$C_8H_9O_4$	169.0501	$C_6H_8N_3O_3$	170.0566
$C_9H_{14}NO_2$	168.1025	$C_8H_{11}NO_3$	169.0739	$C_6H_{10}N_4O_2$	170.0805
$C_9H_{16}N_2O$	168.1264	$C_8H_{13}N_2O_2$	169.0978	$C_7H_8NO_4$	170.0453
$C_9N_2O_2$	167.9960	$C_8H_{15}N_3O$	169.1216	$C_7H_{10}N_2O_3$	170.0692
$C_9H_{18}N_3$	168.1502	$C_8H_{17}N_4$	169.1455	$C_7H_{12}N_3O_2$	170.0930
$C_9H_2N_3O$	168.0198	C_8HN_4O	169.0151	$C_7H_{14}N_4O$	170.1169
$C_9H_4N_4$	168.0437	$C_9H_{13}O_3$	169.0865	$C_8H_{10}O_4$	170.0579
$C_{10}H_{16}O_2$	168.1151	$C_9H_{15}NO_2$	169.1103	$C_8H_{12}NO_3$	170.0817
$C_{10}O_3$	167.9847	$C_9H_{17}N_2O$	169.1342	$C_8H_{14}N_2O_2$	170.1056
$C_{10}H_{18}NO$	168.1389	$C_9HN_2O_2$	169.0038	$C_8H_{16}N_3O$	170.1295
$C_{10}H_2NO_2$	168.0085	$C_9H_{19}N_3$	169.1580	$C_8N_3O_2$	169.9991
$C_{10}H_{20}N_2$	168.1628	$C_9H_3N_3O$	169.0277	$C_8H_{18}N_4$	170.1533
$C_{10}H_4N_2O$	168.0324	$C_9H_5N_4$	169.0515	$C_8H_2N_4O$	170.0229
$C_{10}H_6N_3$	168.0563	$C_{10}H_{17}O_2$	169.1229	$C_9H_{14}O_3$	170.0943
$C_{11}H_{20}O$	168.1515	$C_{10}HO_3$	168.9925	$C_9H_{16}NO_2$	170.1182
$C_{11}H_4O_2$	168.0211	$C_{10}H_{19}NO$	169.1467	C_9NO_3	169.9878
$C_{11}H_{22}N$	168.1753	$C_{10}H_3NO_2$	169.0164	$C_9H_{18}N_2O$	170.1420
$C_{11}H_6NO$	168.0449	$C_{10}H_{21}N_2$	169.1706	$C_9H_2N_2O_2$	170.0116
$C_{11}H_8N_2$	168.0688	$C_{10}H_5N_2O$	169.0402	$C_9H_{20}N_3$	170.1659
$C_{12}H_{24}$	168.1879	$C_{10}H_7N_3$	169.0641	$C_9H_4N_3O$	170.0355
$C_{12}H_8O$	168.0575	$C_{11}H_{21}O$	169.1593	$C_9H_6N_4$	170.0594
$C_{12}H_{10}N$	168.0814	$C_{11}H_5O_2$	169.0289	$C_{10}H_{18}O_2$	170.1307
$C_{13}H_{12}$	168.0939	$C_{11}H_{23}N$	169.1832	$C_{10}H_2O_3$	170.0003
C_{14}	168.0000	$C_{11}H_7NO$	169.0528	$C_{10}H_{20}NO$	170.1546
169		$C_{11}H_9N_2$	169.0767	$C_{10}H_4NO_2$	170.0242
$C_6H_5N_2O_4$	169.0249	$C_{12}H_{25}$	169.1957	$C_{10}H_{22}N_2$	170.1784
$C_6H_7N_3O_3$	169.0488	$C_{12}H_9O$	169.0653	$C_{10}H_6N_2O$	170.0480
$C_6H_9N_4O_2$	169.0726	$C_{12}H_{11}N$	169.0892	$C_{10}H_8N_3$	170.0719
$C_7H_7NO_4$	169.0375	$C_{13}H_{13}$	169.1018	$C_{11}H_{22}O$	170.1671

FM		FM		FM	
$C_{11}H_6O_2$	170.0368	$C_9H_7N_4$	171.0672	$C_8H_2N_3O_2$	172.0147
$C_{11}H_{24}N$	170.1910	$C_{10}H_{19}O_2$	171.1385	$C_8H_{20}N_4$	172.1690
$C_{11}H_8NO$	170.0606	$C_{10}H_3O_3$	171.0082	$C_8H_4N_4O$	172.0386
$C_{11}H_{10}N_2$	170.0845	$C_{10}H_{21}NO$	171.1624	$C_9H_{16}O_3$	172.1100
$C_{12}H_{26}$	170.2036	$C_{10}H_5NO_2$	171.0320	C_9O_4	171.9796
$C_{12}H_{10}O$	170.0732	$C_{10}H_{23}N_2$	171.1863	$C_9H_{18}NO_2$	172.1338
$C_{12}H_{12}N$	170.0970	$C_{10}H_7N_2O$	171.0559	$C_9H_2NO_3$	172.0034
$C_{13}H_{14}$	170.1096	$C_{10}H_9N_3$	171.0798	$C_9H_{20}N_2O$	172.1577
$C_{13}N$	170.0031	$C_{11}H_{23}O$	171.1750	$C_9H_4N_2O_2$	172.0273
$C_{14}H_2$	170.0157	$C_{11}H_7O_2$	171.0446	$C_9H_{22}N_3$	172.1815
171		$C_{11}H_{25}N$	171.1988	$C_9H_6N_3O$	172.0511
$C_6H_7N_2O_4$	171.0406	$C_{11}H_9NO$	171.0684	$C_9H_8N_4$	172.0750
$C_6H_9N_3O_3$	171.0644	$C_{11}H_{11}N_2$	171.0923	$C_{10}H_{20}O_2$	172.1464
$C_6H_{11}N_4O_2$	171.0883	$C_{12}H_{11}O$	171.0810	$C_{10}H_4O_3$	172.0160
$C_7H_9NO_4$	171.0532	$C_{12}H_{13}N$	171.1049	$C_{10}H_{22}NO$	172.1702
$C_7H_{11}N_2O_3$	171.0770	$C_{13}H_{15}$	171.1174	$C_{10}H_6NO_2$	172.0399
$C_7H_{13}N_3O_2$	171.1009	$C_{13}HN$	171.0109	$C_{10}H_{24}N_2$	172.1941
$C_7H_{15}N_4O$	171.1247	$C_{14}H_3$	171.0235	$C_{10}H_8N_2O$	172.0637
$C_8H_{11}O_4$	171.0657	172		$C_{10}H_{10}N_3$	172.0876
$C_8H_{13}NO_3$	171.0896	$C_6H_8N_2O_4$	172.0484	$C_{11}H_{24}O$	172.1828
$C_8H_{15}N_2O_2$	171.1134	$C_6H_{10}N_3O_3$	172.0723	$C_{11}H_8O_2$	172.0524
$C_8H_{17}N_3O$	171.1373	$C_6H_{12}N_4O_2$	172.0961	$C_{11}N_{10}NO$	172.0763
$C_8HN_3O_2$	171.0069	$C_7H_{10}NO_4$	172.0610	$C_{11}H_{12}N_2$	172.1001
$C_8H_{19}N_4$	171.1611	$C_7H_{12}N_2O_3$	172.0848	$C_{12}H_{12}O$	172.0888
$C_8H_3N_4O$	171.0308	$C_7H_{14}N_3O_2$	172.1087	$C_{12}H_{14}N$	172.1127
$C_9H_{15}O_3$	171.1021	$C_7H_{16}N_4O$	172.1325	$C_{12}N_2$	172.0062
$C_9H_{17}NO_2$	171.1260	$C_7N_4O_2$	172.0022	$C_{13}H_{16}$	172.1253
C_9HNO_3	170.9956	$C_8H_{12}O_4$	172.0735	$C_{13}O$	171.9949
$C_9H_{19}N_2O$	171.1498	$C_8H_{14}NO_3$	172.0974	$C_{13}H_2N$	172.0187
$C_9H_3N_2O_2$	171.0195	$C_8H_{16}N_2O_2$	172.1213	$C_{14}H_4$	172.0313
$C_9H_{21}N_3$	171.1737	$C_8N_2O_3$	171.9909	173	
$C_9H_5N_3O$	171.0433	$C_8H_{18}N_3O$	172.1451	$C_6H_9N_2O_4$	173.0563

FM		FM		FM	
$C_6H_{11}N_3O_3$	173.0801	$C_{11}H_{13}N_2$	173.1080	$C_9H_6N_2O_2$	174.0429
$C_6H_{13}N_4O_2$	173.1040	$C_{12}H_{13}O$	173.0967	$C_9H_8N_3O$	174.0668
$C_7H_{11}NO_4$	173.0688	$C_{12}H_{15}N$	173.1205	$C_9H_{10}N_4$	174.0907
$C_7H_{13}N_2O_3$	173.0927	$C_{12}HN_2$	173.0140	$C_{10}H_{22}O_2$	174.1620
$C_7H_{15}N_3O_2$	173.1165	$C_{13}H_{17}$	173.1331	$C_{10}H_6O_3$	174.0317
$C_7H_{17}N_4O$	173.1404	$C_{13}HO$	173.0027	$C_{10}H_8NO_2$	174.0555
$C_7HN_4O_2$	173.0100	$C_{13}H_3N$	173.0266	$C_{10}H_{10}N_2O$	174.0794
$C_8H_{13}O_4$	173.0814	$C_{14}H_5$	173.0391	$C_{10}H_{12}N_3$	174.1032
$C_8H_{15}NO_3$	173.1052	174		$C_{11}H_{10}O_2$	174.0681
$C_8H_{17}N_2O_2$	173.1291	$C_6H_{10}N_2O_4$	174.0641	$C_{11}H_{12}NO$	174.0919
$C_8HN_2O_3$	172.9987	$C_6H_{12}N_3O_3$	174.0879	$C_{11}H_{14}N_2$	174.1158
$C_8H_{19}N_3O$	173.1529	$C_6H_{14}N_4O_2$	174.1118	$C_{11}N_3$	174.0093
$C_8H_3N_3O_2$	173.0226	$C_7H_{12}NO_4$	174.0766	$C_{12}H_{14}O$	174.1045
$C_8H_{21}N_4$	173.1768	$C_7H_{14}N_2O_3$	174.1005	$C_{12}H_{16}N$	174.1284
$C_8H_5N_4O$	173.0464	$C_7H_{16}N_3O_2$	174.1244	$C_{12}NO$	173.9980
$C_9H_{17}O_3$	173.1178	$C_7N_3O_3$	173.9940	$C_{12}H_2N_2$	174.0218
C_9HO_4	172.9874	$C_7H_{18}N_4O$	174.1482	$C_{13}H_{18}$	174.1409
$C_9H_{19}NO_2$	173.1416	$C_7H_2N_4O_2$	174.0178	$C_{13}H_2O$	174.0106
$C_9H_3NO_3$	173.0113	$C_8H_{14}O_4$	174.0892	$C_{13}H_4N$	174.0344
$C_9H_{21}N_2O$	173.1655	$C_8H_{16}NO_3$	174.1131	$C_{14}H_6$	174.0470
$C_9H_5N_2O_2$	173.0351	C_8NO_4	173.9827	175	
$C_9H_{23}N_3$	173.1894	$C_8H_{18}N_2O_2$	174.1369	$C_6H_{11}N_2O_4$	175.0719
$C_9H_7N_3O$	173.0590	$C_8H_2N_2O_3$	174.0065	$C_6H_{13}N_3O_3$	175.0958
$C_9H_9N_4$	173.0829	$C_8H_{20}N_3O$	174.1608	$C_6H_{15}N_4O_2$	175.1196
$C_{10}H_{21}O_2$	173.1542	$C_8H_4N_3O_2$	174.0304	$C_7H_{13}NO_4$	175.0845
$C_{10}H_5O_3$	173.0238	$C_8H_{22}N_4$	174.1846	$C_7H_{15}N_2O_3$	175.1083
$C_{10}H_{23}NO$	173.1781	$C_8H_6N_4O$	174.0542	$C_7H_{17}N_3O_2$	175.1322
$C_{10}H_7NO_2$	173.0477	$C_9H_{18}O_3$	174.1256	$C_7HN_3O_3$	175.0018
$C_{10}H_9N_2O$	173.0715	$C_9H_2O_4$	173.9953	$C_7H_{19}N_4O$	175.1560
$C_{10}H_{11}N_3$	173.0954	$C_9H_{20}NO_2$	174.1495	$C_7H_3N_4O_2$	175.0257
$C_{11}H_9O_2$	173.0603	$C_9H_4NO_3$	174.0191	$C_8H_{15}O_4$	175.0970
$C_{11}H_{11}NO$	173.0841	$C_9H_{22}N_2O$	174.1733	$C_8H_{17}NO_3$	175.1209

FM		FM		FM	
C_8HNO_4	174.9905	$C_6H_{16}N_4O_2$	176.1275	$C_{12}O_2$	175.9898
$C_8H_{19}N_2O_2$	175.1447	$C_7H_{14}NO_4$	176.0923	$C_{12}H_{18}N$	176.1440
$C_8H_3N_2O_3$	175.0144	$C_7H_{16}N_2O_3$	176.1162	$C_{12}H_2NO$	176.0136
$C_8H_{21}N_3O$	175.1686	$C_7N_2O_4$	175.9858	$C_{12}H_4N_2$	176.0375
$C_8H_5N_3O_2$	175.0382	$C_7H_{18}N_3O_2$	176.1400	$C_{13}H_{20}$	176.1566
$C_8H_7N_4O$	175.0621	$C_7H_2N_3O_3$	176.0096	$C_{13}H_4O$	176.0262
$C_9H_{19}O_3$	175.1334	$C_7H_{20}N_4O$	176.1639	$C_{13}H_6N$	176.0501
$C_9H_3O_4$	175.0031	$C_7H_4N_4O_2$	176.0335	$C_{14}H_8$	176.0626
$C_9H_{21}NO_2$	175.1573	$C_8H_{16}O_4$	176.1049	177	
$C_9H_5NO_3$	175.0269	$C_8H_{18}NO_3$	176.1287	$C_6H_{13}N_2O_4$	177.0876
$C_9H_7N_2O_2$	175.0508	$C_8H_2NO_4$	175.9983	$C_6H_{15}N_3O_3$	177.1114
$C_9H_9N_3O$	175.0746	$C_8H_{20}N_2O_2$	176.1526	$C_6H_{17}N_4O_2$	177.1353
$C_9H_{11}N_4$	175.0985	$C_8H_2N_2O_3$	176.0222	$C_7H_{13}NO_4$	177.1001
$C_{10}H_7O_3$	175.0395	$C_8H_6N_3O_2$	176.0460	$C_7H_{17}N_2O_3$	177.1240
$C_{10}H_9NO_2$	175.0634	$C_8H_8N_4O$	176.0699	$C_7HN_2O_4$	176.9936
$C_{10}H_{11}N_2O$	175.0872	$C_9H_{20}O_3$	176.1413	$C_7H_{19}N_3O_2$	177.1478
$C_{10}H_{13}N_3$	175.1111	$C_9H_4O_4$	176.0109	$C_7H_3N_3O_3$	177.0175
$C_{11}H_{11}O_2$	175.0759	$C_9H_6NO_3$	176.0348	$C_7H_5N_4O_2$	177.0413
$C_{11}H_{13}NO$	175.0998	$C_9H_8N_2O_2$	176.0586	$C_8H_{17}O_4$	177.1127
$C_{11}H_{15}N_2$	175.1236	$C_9H_{10}N_3O$	176.0825	$C_8H_{19}NO_3$	177.1365
$C_{11}HN_3$	175.0171	$C_9H_{12}N_4$	176.1063	$C_8H_3NO_4$	177.0062
$C_{12}H_{15}O$	175.1123	$C_{10}H_8O_3$	176.0473	$C_8H_5N_2O_3$	177.0300
$C_{12}H_{17}N$	175.1362	$C_{10}H_{10}NO_2$	176.0712	$C_8H_7N_3O_2$	177.0539
$C_{12}HNO$	175.0058	$C_{10}H_{12}N_2O$	176.0950	$C_8H_9N_4O$	177.0777
$C_{12}H_3N_2$	175.0297	$C_{10}H_{14}N_3$	176.1189	$C_9H_5O_4$	177.0187
$C_{13}H_{19}$	175.1488	$C_{10}N_4$	176.0124	$C_9H_7NO_3$	177.0426
$C_{13}H_3O$	175.0184	$C_{11}H_{12}O_2$	176.0837	$C_9H_9N_2O_2$	177.0664
$C_{13}H_5N$	175.0422	$C_{11}N_{14}NO$	176.1076	$C_9H_{11}N_3O$	177.0903
$C_{14}H_7$	175.0548	$C_{11}H_{16}N_2$	176.1315	$C_9H_{13}N_4$	177.1142
176		$C_{11}N_2O$	176.0011	$C_{10}H_9O_3$	177.0552
$C_6H_{12}N_2O_4$	176.0797	$C_{11}H_2N_3$	176.0249	$C_{10}H_{11}NO_2$	177.0790
$C_6H_{14}N_3O_3$	176.1036	$C_{12}H_{16}O$	176.1202	$C_{10}H_{13}N_2O$	177.1029

FM		FM		FM	
$C_{10}H_{15}N_3$	177.1267	$C_9H_{10}N_2O_2$	178.0743	$C_8H_7N_2O_3$	179.0457
$C_{10}HN_4$	177.0202	$C_9H_{12}N_3O$	178.0981	$C_8H_8N_3O_2$	179.0695
$C_{11}H_{13}O_2$	177.0916	$C_9H_{14}N_4$	178.1220	$C_8H_{11}N_4O$	179.0934
$C_{11}H_{15}NO$	177.1154	$C_{10}H_{10}O_3$	178.0630	$C_9H_7O_4$	179.0344
$C_{11}H_{17}N_2$	177.1393	$C_{10}H_{12}NO_2$	178.0868	$C_9H_9NO_3$	179.0583
$C_{11}HN_2O$	177.0089	$C_{10}H_{14}N_2O$	178.1107	$C_9H_{11}N_2O_2$	179.0821
$C_{11}H_3N_3$	177.0328	$C_{10}H_{16}N_3$	178.1346	$C_9H_{13}N_3O$	179.1060
$C_{12}H_{17}O$	177.1280	$C_{10}N_3O$	178.0042	$C_9H_{15}N_4$	179.1298
$C_{12}HO_2$	176.9976	$C_{10}H_2N_4$	178.0280	$C_{10}H_{11}O_3$	179.0708
$C_{12}H_{19}N$	177.1519	$C_{11}H_{14}O_2$	178.0994	$C_{10}H_{13}NO_2$	179.0947
$C_{12}H_3NO$	177.0215	$C_{11}H_{16}NO$	178.1233	$C_{10}H_{15}N_2O$	179.1185
$C_{12}H_5N_2$	177.0453	$C_{11}NO_2$	177.9929	$C_{10}H_{17}N_3$	179.1424
$C_{13}H_{21}$	177.1644	$C_{11}H_{18}N_2$	178.1471	$C_{10}HN_3O$	179.0120
$C_{13}H_5O$	177.0340	$C_{11}H_2N_2O$	178.0167	$C_{10}H_3N_4$	179.0359
$C_{13}H_7N$	177.0579	$C_{11}H_4N_3$	178.0406	$C_{11}H_{15}O_2$	179.1072
$C_{14}H_9$	177.0705	$C_{12}H_{18}O$	178.1358	$C_{11}H_{17}NO$	179.1311
178		$C_{12}H_2O_2$	178.0054	$C_{11}HNO_2$	179.0007
$C_6H_{14}N_2O_4$	178.0954	$C_{12}H_{20}N$	178.1587	$C_{11}H_{19}N_2$	179.1549
$C_6H_{16}N_3O_3$	178.1193	$C_{12}H_4NO$	178.0293	$C_{11}H_3N_2O$	179.0246
$C_6H_{18}N_4O_2$	178.1431	$C_{12}H_6N_2$	178.0532	$C_{11}H_5N_3$	179.0484
$C_7H_{16}NO_4$	178.1080	$C_{13}H_{22}$	178.1722	$C_{12}H_{19}O$	179.1436
$C_7H_{18}N_2O_3$	178.1318	$C_{13}H_6O$	178.0419	$C_{12}H_3O_2$	179.0133
$C_7H_2N_2O_4$	178.0014	$C_{13}H_8N$	178.0657	$C_{12}H_{21}N$	179.1675
$C_7H_4N_3O_3$	178.0253	$C_{14}H_{10}$	178.0783	$C_{12}H_5NO$	179.0371
$C_7H_6N_4O_2$	178.0491	179		$C_{12}H_7N_2$	179.0610
$C_8H_{18}O_4$	178.1205	$C_6H_{15}N_2O_4$	179.1032	$C_{13}H_{23}$	179.1801
$C_8H_4NO_4$	178.0140	$C_6H_{17}N_3O_3$	179.1271	$C_{13}H_7O$	179.0497
$C_8H_6N_2O_3$	178.0379	$C_7H_{17}NO_4$	179.1158	$C_{13}H_9N$	179.0736
$C_8H_8N_3O_2$	178.0617	$C_7H_3N_2O_4$	179.0093	$C_{14}H_{11}$	179.0861
$C_8H_{10}N_4O$	178.0856	$C_7H_5N_3O_3$	179.0331	180	
$C_9H_6O_4$	178.0266	$C_7H_7N_4O_2$	179.0570	$C_6H_{16}N_2O_4$	180.1111
$C_9H_8NO_3$	178.0504	$C_8H_5NO_4$	179.0218	$C_7H_4N_2O_4$	180.0171

FM		FM		FM	
$C_7H_6N_3O_3$	180.0410	$C_{13}H_8O$	180.0575	$C_{12}H_{21}O$	181.1593
$C_7H_8N_4O_2$	180.0648	$C_{13}H_{10}N$	180.0814	$C_{12}H_5O_2$	181.0289
$C_8H_6NO_4$	180.0297	$C_{14}H_{12}$	180.0939	$C_{12}H_{23}N$	181.1832
$C_8H_8N_2O_3$	180.0535	C_{15}	180.0000	$C_{12}H_7NO$	181.0528
$C_8H_{10}N_3O_2$	180.0774	181		$C_{12}H_9N_2$	181.0767
$C_8H_{12}N_4O$	180.1012	$C_7H_5N_2O_4$	181.0249	$C_{13}H_{25}$	181.1957
$C_9H_8O_4$	180.0422	$C_7H_7N_3O_3$	181.0488	$C_{13}H_9O$	181.0653
$C_9H_{10}NO_3$	180.0661	$C_7H_9N_4O_2$	181.0726	$C_{13}H_{11}N$	181.0892
$C_9H_{12}N_2O_2$	180.0899	$C_8H_7NO_4$	181.0375	$C_{14}H_{13}$	181.1018
$C_9H_{14}N_3O$	180.1138	$C_8H_9N_2O_3$	181.0614	$C_{15}H$	181.0078
$C_9H_{16}N_4$	180.1377	$C_8H_{11}N_3O_2$	181.0852	182	
C_9N_4O	180.0073	$C_8H_{13}N_4O$	181.1091	$C_7H_6N_2O_4$	182.0328
$C_{10}H_{12}O_3$	180.0786	$C_9H_9O_4$	181.0501	$C_7H_8N_3O_3$	182.0566
$C_{10}H_{14}NO_2$	180.1025	$C_9H_{11}NO_3$	181.0739	$C_7H_{10}N_4O_2$	182.0805
$C_{10}H_{16}N_2O$	180.1264	$C_9H_{13}N_2O_2$	181.0978	$C_8H_8NO_4$	182.0453
$C_{10}N_2O_2$	179.9960	$C_9H_{15}N_3O$	181.1216	$C_8H_{10}N_2O_3$	182.0692
$C_{10}H_{18}N_3$	180.1502	$C_9H_{17}N_4$	181.1455	$C_8H_{12}N_3O_2$	182.0930
$C_{10}H_2N_3O$	180.0198	C_9HN_4O	181.0151	$C_8H_{14}N_4O$	182.1169
$C_{10}H_4N_4$	180.0437	$C_{10}H_{13}O_3$	181.0863	$C_9H_{10}O_4$	182.0579
$C_{11}H_{16}O_2$	180.1151	$C_{10}H_{15}NO_2$	181.1103	$C_9H_{12}NO_3$	182.0817
$C_{11}O_3$	179.9847	$C_{10}H_{17}N_2O$	181.1342	$C_9H_{14}N_2O_2$	182.1056
$C_{11}H_{18}NO$	180.1389	$C_{10}HN_2O_2$	181.0038	$C_9H_{16}N_3O$	182.1295
$C_{11}H_2NO_2$	180.0085	$C_{10}H_{19}N_3$	181.1580	$C_9N_3O_2$	181.9991
$C_{11}H_{20}N_2$	180.1628	$C_{10}H_3N_3O$	181.0277	$C_9H_{18}N_4$	182.1533
$C_{11}H_4N_2O$	180.0324	$C_{10}H_5N_4$	181.0515	$C_9H_2N_4O$	182.0229
$C_{11}H_6N_3$	180.0563	$C_{11}H_{17}O_2$	181.1229	$C_{10}H_{14}O_3$	182.0943
$C_{12}H_{20}O$	180.1515	$C_{11}HO_3$	180.9925	$C_{10}H_{16}NO_2$	182.1182
$C_{12}H_4O_2$	180.0211	$C_{11}H_{19}NO$	181.1467	$C_{10}NO_3$	181.9878
$C_{12}H_{22}N$	180.1753	$C_{11}H_3NO_2$	181.0164	$C_{10}N_{18}N_2O$	182.1420
$C_{12}H_6NO$	180.0449	$C_{11}H_{21}N_2$	181.1706	$C_{10}H_2N_2O_2$	182.0116
$C_{12}H_8N_2$	180.0688	$C_{11}H_5N_2O$	181.0402	$C_{10}H_{20}N_3$	182.1659
$C_{13}H_{24}$	180.1879	$C_{11}H_7N_3$	181.0641	$C_{10}H_4N_3O$	182.0355

FM		FM		FM	
$C_{10}H_6N_4$	182.0594	$C_9H_{19}N_4$	183.1611	$C_8H_{10}NO_4$	184.0610
$C_{11}H_{18}O_2$	182.1307	$C_9H_3N_4O$	183.0308	$C_8H_{12}N_2O_3$	184.0848
$C_{11}H_2O_3$	182.0003	$C_{10}H_{15}O_3$	183.1021	$C_8H_{14}N_3O_2$	184.1087
$C_{11}H_{20}NO$	182.1546	$C_{10}H_{17}NO_2$	183.1260	$C_8H_{16}N_4O$	184.1325
$C_{11}H_4NO_2$	182.0242	$C_{10}HNO_3$	182.9956	$C_8N_4O_2$	184.0022
$C_{11}H_{22}N_2$	182.1784	$C_{10}H_{19}N_2O$	183.1498	$C_9H_{12}O_4$	184.0735
$C_{11}H_6N_2O$	182.0480	$C_{10}H_3N_2O_2$	183.0195	$C_9H_{14}NO_3$	184.0974
$C_{11}H_8N_3$	182.0719	$C_{10}H_{21}N_3$	183.1737	$C_9H_{16}N_2O_2$	184.1213
$C_{12}H_{22}O$	182.1671	$C_{10}H_5N_3O$	183.0433	$C_9N_2O_3$	184.9909
$C_{12}H_6O_2$	182.0368	$C_{10}H_7N_4$	183.0672	$C_9H_{18}N_3O$	184.1451
$C_{12}H_{24}N$	182.1910	$C_{11}H_{19}O_2$	183.1385	$C_9H_2N_3O_2$	184.0147
$C_{12}H_8NO$	182.0606	$C_{11}H_3O_3$	183.0082	$C_9H_{20}N_4$	184.1690
$C_{12}H_{10}N_2$	182.0845	$C_{11}H_{21}NO$	183.1624	$C_9H_4N_4O$	184.0386
$C_{13}H_{26}$	182.2036	$C_{11}H_5NO_2$	183.0320	$C_{10}H_{16}O_3$	184.1100
$C_{13}H_{10}O$	182.0732	$C_{11}H_{23}N_2$	183.1863	$C_{10}O_4$	183.9796
$C_{13}H_{12}N$	182.0970	$C_{11}H_7N_2O$	183.0559	$C_{10}H_{18}NO_2$	184.1338
$C_{14}H_{14}$	182.1096	$C_{11}H_9N_3$	183.0798	$C_{10}H_2NO_3$	184.0034
$C_{14}N$	182.0031	$C_{12}H_{23}O$	183.1750	$C_{10}H_{20}N_2O$	184.1577
$C_{15}H_2$	182.0157	$C_{12}H_7O_2$	183.0446	$C_{10}H_4N_2O_2$	184.0273
183		$C_{12}H_{25}N$	183.1988	$C_{10}H_{22}N_3$	184.1815
$C_7H_7N_2O_4$	183.0406	$C_{12}H_9NO$	183.0684	$C_{10}H_6N_3O$	184.0511
$C_7H_9N_3O_3$	183.0644	$C_{12}H_{11}N_2$	183.0923	$C_{10}H_8N_4$	184.0750
$C_7H_{11}N_4O_2$	183.0883	$C_{13}H_{27}$	183.2114	$C_{11}H_{20}O_2$	184.1464
$C_8H_9NO_4$	183.0532	$C_{13}H_{11}O$	183.0810	$C_{11}H_4O_3$	184.0160
$C_8H_{11}N_2O_3$	183.0770	$C_{13}H_{13}N$	183.1049	$C_{11}H_{22}NO$	184.1702
$C_8H_{13}N_3O_2$	183.1009	$C_{14}H_{15}$	183.1174	$C_{11}H_6NO_2$	184.0399
$C_8H_{15}N_4O$	183.1247	$C_{14}HN$	183.0109	$C_{11}H_{24}N_2$	184.1941
$C_9H_{11}O_4$	183.0657	$C_{15}H_3$	183.0235	$C_{11}H_8N_2O$	184.0637
$C_9H_{13}NO_3$	183.0896	184		$C_{11}H_{10}N_3$	184.0876
$C_9H_{15}N_2O_2$	183.1134	$C_7H_8N_2O_4$	184.0484	$C_{12}H_{24}O$	184.1828
$C_9H_{17}N_3O$	183.1373	$C_7H_{10}N_3O_3$	184.0723	$C_{12}H_8O_2$	184.0524
$C_9HN_3O_2$	183.0069	$C_7H_{12}N_4O_2$	184.0961	$C_{12}H_{26}N$	184.2067

FM		FM		FM	
$C_{12}H_{10}NO$	184.0763	$C_{10}HO_4$	184.9874	$C_8H_2N_4O_2$	186.0178
$C_{12}H_{12}N_2$	184.1001	$C_{10}H_{23}N_3$	185.1894	$C_9H_{14}O_4$	186.0892
$C_{13}H_{28}$	184.2192	$C_{10}H_7N_3O$	185.0590	$C_9H_{16}NO_3$	186.1131
$C_{13}H_{12}O$	184.0888	$C_{10}H_9N_4$	185.0829	C_9NO_4	185.9827
$C_{13}H_{14}N$	184.1127	$C_{11}H_{21}O_2$	185.1542	$C_9H_{18}N_2O_2$	186.1369
$C_{13}N_2$	184.0062	$C_{11}H_5O_3$	185.0238	$C_9H_2N_2O_3$	186.0065
$C_{14}H_{16}$	184.1253	$C_{11}H_{23}NO$	185.1781	$C_9H_{20}N_3O$	186.1608
$C_{14}O$	183.9949	$C_{11}H_7NO_2$	185.0477	$C_9H_4N_3O_2$	186.0304
$C_{14}H_2N$	184.0187	$C_{11}H_{25}N_2$	185.2019	$C_9H_{22}N_4$	186.1846
$C_{15}H_4$	184.0313	$C_{11}H_9N_2O$	185.0715	$C_9H_6N_4O$	186.0542
185		$C_{11}H_{11}N_3$	185.0954	$C_{10}H_{18}O_3$	186.1256
$C_7H_9N_2O_4$	185.0563	$C_{12}H_{25}O$	185.1906	$C_{10}H_2O_4$	185.9953
$C_7H_{11}N_3O_3$	185.0801	$C_{12}H_9O_2$	185.0603	$C_{10}H_{10}N_4$	186.0907
$C_7H_{13}N_4O_2$	185.1040	$C_{12}H_{27}N$	185.2145	$C_{10}H_{20}NO_2$	186.1495
$C_8H_{11}NO_4$	185.0688	$C_{12}H_{11}NO$	185.0841	$C_{10}H_4NO_3$	186.0191
$C_8H_{13}N_2O_3$	185.0927	$C_{12}H_{13}N_2$	185.1080	$C_{10}H_{22}N_2O$	186.1733
$C_8H_{15}N_3O_2$	185.1165	$C_{13}H_{13}O$	185.0967	$C_{10}H_6N_2O_2$	186.0429
$C_8H_{17}N_4O$	185.1404	$C_{13}H_{15}N$	185.1205	$C_{10}H_{24}N_3$	186.1972
$C_8HN_4O_2$	185.0100	$C_{13}HN_2$	185.0140	$C_{10}H_8N_3O$	186.0668
$C_9H_{21}N_4$	185.1768	$C_{14}H_{17}$	185.1331	$C_{11}H_{22}O_2$	186.1620
$C_9H_{19}N_3O$	185.1529	$C_{14}HO$	185.0027	$C_{11}H_6O_3$	186.0317
$C_9H_5N_4O$	185.0464	$C_{14}H_3N$	185.0266	$C_{11}H_{24}NO$	186.1859
$C_9H_3N_3O_2$	185.0226	$C_{15}H_5$	185.0391	$C_{11}H_8NO_2$	186.0555
$C_9H_{13}O_4$	185.0814	186		$C_{11}H_{26}N_2$	186.2098
$C_9H_{15}NO_3$	185.1052	$C_7H_{10}N_2O_4$	186.0641	$C_{11}H_{10}N_2O$	186.0794
$C_9H_{17}N_2O_2$	185.1291	$C_7H_{12}N_3O_3$	186.0879	$C_{11}H_{12}N_3$	186.1032
$C_9HN_2O_3$	184.9987	$C_7H_{14}N_4O_2$	186.1118	$C_{12}H_{26}O$	186.1985
$C_{10}H_{19}NO_2$	185.1416	$C_8H_{12}NO_4$	186.0766	$C_{12}H_{10}O_2$	186.0681
$C_{10}H_3NO_3$	185.0113	$C_8H_{14}N_2O_3$	186.1005	$C_{12}H_{12}NO$	186.0919
$C_{10}H_{21}N_2O$	185.1655	$C_8H_{16}N_3O_2$	186.1244	$C_{12}H_{14}N_2$	186.1158
$C_{10}H_5N_2O_2$	185.0351	$C_8N_3O_3$	185.9940	$C_{12}N_3$	186.0093
$C_{10}H_{17}O_3$	185.1178	$C_8H_{18}N_4O$	186.1482	$C_{13}H_{14}O$	186.1045

	FM		FM		FM
$C_{13}H_{16}N$	186.1284	$C_{10}H_{25}N_3$	187.2050	$C_9H_{16}O_4$	188.1049
$C_{13}NO$	185.9980	$C_{10}H_9N_3O$	187.0746	$C_9H_{18}NO_3$	188.1287
$C_{13}H_2N_2$	186.0218	$C_{10}H_{11}N_4$	187.0985	$C_9H_2NO_4$	187.9983
$C_{14}H_{18}$	186.1409	$C_{11}H_{11}N_2O$	187.0872	$C_9H_{20}N_2O_2$	188.1526
$C_{14}H_2O$	186.0106	$C_{11}H_{13}N_3$	187.1111	$C_9H_4N_2O_3$	188.0222
$C_{14}H_4N$	186.0344	$C_{11}H_{23}O_2$	187.1699	$C_9H_{22}N_3O$	188.1764
$C_{15}H_6$	186.0470	$C_{11}H_7O_3$	187.0395	$C_9H_6N_3O_2$	188.0460
187		$C_{11}H_{25}NO$	187.1937	$C_9H_{24}N_4$	188.2003
$C_7H_{11}N_2O_4$	187.0719	$C_{11}H_9NO_2$	187.0634	$C_9H_8N_4O$	188.0669
$C_7H_{13}N_3O_3$	187.0958	$C_{12}H_{11}O_2$	187.0759	$C_{10}H_{20}O_3$	188.1413
$C_7H_{15}N_4O_2$	187.1196	$C_{12}H_{13}NO$	187.0998	$C_{10}H_4O_4$	188.0109
$C_8H_{13}NO_4$	187.0845	$C_{12}H_{15}N_2$	187.1236	$C_{10}H_{22}NO_2$	188.1651
$C_8H_{15}N_2O_3$	187.1083	$C_{12}HN_3$	187.0171	$C_{10}H_6NO_3$	188.0348
$C_8H_{17}N_3O_2$	187.1322	$C_{13}H_{15}O$	187.1123	$C_{10}H_{24}N_2O$	188.1890
$C_8HN_3O_3$	187.0018	$C_{13}H_{17}N$	187.1362	$C_{10}H_8N_2O_2$	188.0586
$C_8H_{19}N_4O$	187.1560	$C_{13}HNO$	187.0058	$C_{10}H_{10}N_3O$	188.0825
$C_8H_3N_4O_2$	187.0257	$C_{13}H_3N_2$	187.0297	$C_{10}H_{12}N_4$	188.1063
$C_9H_{15}O_4$	187.0970	$C_{14}H_{19}$	187.1488	$C_{11}H_{24}O_2$	188.1777
$C_9H_{17}NO_3$	187.1209	$C_{14}H_3O$	187.0184	$C_{11}H_8O_3$	188.0473
C_9HNO_4	186.9905	$C_{14}H_5N$	187.0422	$C_{11}H_{10}NO_2$	188.0712
$C_9H_{19}N_2O_2$	187.1447	$C_{15}H_7$	187.0548	$C_{11}H_{12}N_2O$	188.0950
$C_9H_3N_2O_3$	187.0144	188		$C_{11}H_{14}N_3$	188.1189
$C_9H_{21}N_3O$	187.1686	$C_7H_{12}N_2O_4$	188.0797	$C_{11}N_4$	188.0124
$C_9H_5N_3O_2$	187.0382	$C_7H_{14}N_3O_3$	188.1036	$C_{12}H_{12}O_2$	188.0837
$C_9H_{23}N_4$	187.1925	$C_7H_{16}N_4O_2$	188.1275	$C_{12}H_{14}NO$	188.1076
$C_{10}H_7N_4O$	187.0621	$C_8H_{14}NO_4$	188.0923	$C_{12}H_{16}N_2$	188.1315
$C_{10}H_{19}O_3$	187.1334	$C_8H_{16}N_2O_3$	188.1162	$C_{12}N_2O$	188.0011
$C_{10}H_3O_4$	187.0031	$C_8N_2O_4$	187.9858	$C_{12}H_2N_3$	188.0249
$C_{10}H_{21}NO_2$	187.1573	$C_8H_{18}N_3O_2$	188.1400	$C_{13}H_{16}O$	188.1202
$C_{10}H_5NO_3$	187.0269	$C_8H_2N_3O_3$	188.0096	$C_{13}O_2$	187.9898
$C_{10}H_{23}N_2O$	187.1811	$C_8H_{20}N_2O$	188.1639	$C_{13}H_{18}N$	188.1440
$C_{10}H_7N_2O_2$	187.0508	$C_8H_4N_4O_2$	188.0335	$C_{13}H_2NO$	188.0136

	FM		FM		FM
$C_{13}H_4N_2$	188.0375	$C_{11}H_{11}NO_2$	189.0790	$C_9H_{22}N_2O_2$	190.1682
$C_{14}H_{20}$	188.1566	$C_{11}H_{13}N_2O$	189.1029	$C_9H_6N_2O_3$	190.0379
$C_{14}H_4O$	188.0262	$C_{11}H_{15}N_3$	189.1267	$C_9H_8N_3O_2$	190.0617
$C_{14}H_6N$	188.0501	$C_{11}HN_4$	189.0202	$C_9H_{10}N_4O$	190.0856
$C_{15}H_8$	188.0626	$C_{12}H_{13}O_2$	189.0916	$C_{10}H_{22}O_3$	190.1569
189		$C_{12}H_{15}NO$	189.1154	$C_{10}H_6O_4$	190.0266
$C_7H_{13}N_2O_4$	189.0876	$C_{12}H_{17}N_2$	189.1393	$C_{10}H_8NO_3$	190.0504
$C_7H_{15}N_3O_3$	189.1114	$C_{12}HN_2O$	189.0089	$C_{10}H_{10}N_2O_2$	190.0743
$C_7H_{17}N_4O_2$	189.1353	$C_{12}H_3N_3$	189.0328	$C_{10}H_{12}N_3O$	190.0981
$C_8H_{15}NO_4$	189.1001	$C_{13}H_{17}O$	189.1280	$C_{10}H_{14}N_4$	190.1220
$C_8H_{17}N_2O_3$	189.1240	$C_{13}HO_2$	188.9976	$C_{11}H_{10}O_3$	190.0630
$C_8HN_2O_4$	188.9936	$C_{13}H_{19}N$	189.1519	$C_{11}H_{12}NO_2$	190.0868
$C_8H_{19}N_3O_2$	189.1478	$C_{13}H_3NO$	189.0215	$C_{11}H_{14}N_2O$	190.1107
$C_8H_3N_3O_3$	189.0175	$C_{13}H_5N_2$	189.0453	$C_{11}H_{16}N_3$	190.1346
$C_8H_{21}N_4O$	189.1717	$C_{14}H_{21}$	189.1644	$C_{11}N_3O$	190.0042
$C_8H_5N_4O_2$	189.0413	$C_{14}H_5O$	189.0340	$C_{11}H_2N_4$	190.0280
$C_9H_{17}O_4$	189.1127	$C_{14}H_7N$	189.0579	$C_{12}H_{14}O_2$	190.0994
$C_9H_{19}NO_3$	189.1365	$C_{15}H_9$	189.0705	$C_{12}H_{16}NO$	190.1233
$C_9H_3NO_4$	189.0062	190		$C_{12}NO_2$	189.9929
$C_9H_{21}N_2O_2$	189.1604	$C_7H_{14}N_2O_4$	190.0954	$C_{12}H_{18}N_2$	190.1471
$C_9H_5N_2O_3$	189.0300	$C_7H_{16}N_3O_3$	190.1193	$C_{12}H_2N_2O$	190.0167
$C_9H_{23}N_3O$	189.1842	$C_7H_{18}N_4O_2$	190.1431	$C_{12}H_4N_3$	190.0406
$C_9H_7N_3O_2$	189.0539	$C_8H_{16}NO_4$	190.1080	$C_{13}H_{18}O$	190.1358
$C_9H_9N_4O$	189.0777	$C_8H_{18}N_2O_3$	190.1318	$C_{13}H_2O_2$	190.0054
$C_{10}H_{21}O_3$	189.1491	$C_8H_2N_2O_4$	190.0014	$C_{13}H_{20}N$	190.1597
$C_{10}H_5O_4$	189.0187	$C_8H_{20}N_3O_2$	190.1557	$C_{13}H_4NO$	190.0293
$C_{10}H_{23}NO_2$	189.1730	$C_8H_4N_3O_3$	190.0253	$C_{13}H_6N_2$	190.0532
$C_{10}H_7NO_3$	189.0426	$C_8H_{22}N_4O$	190.1795	$C_{14}H_{22}$	190.1722
$C_{10}H_9N_2O_2$	189.0664	$C_8H_6N_4O_2$	190.0491	$C_{14}H_6O$	190.0419
$C_{10}H_{11}N_3O$	189.0903	$C_9H_{18}O_4$	190.1205	$C_{14}H_8N$	190.0657
$C_{10}H_{13}N_4$	189.1142	$C_9H_{20}N_3$	190.1444	$C_{15}H_{10}$	190.0783
$C_{11}H_9O_3$	189.0552	$C_9H_4NO_4$	190.0140	191	
				$C_7H_{15}N_2O_4$	191.1032

FM		FM		FM	
$C_7H_{17}N_3O_3$	191.1271	$C_{13}H_3O_2$	191.0133	$C_{11}H_{18}N_3$	192.1502
$C_7H_{19}N_4O_2$	191.1509	$C_{13}H_{21}N$	191.1675	$C_{11}H_2N_3O$	192.0198
$C_8H_{17}NO_4$	191.1158	$C_{13}H_5NO$	191.0371	$C_{11}H_4N_4$	192.0437
$C_8H_{19}N_2O_3$	191.1396	$C_{13}H_7N_2$	191.0610	$C_{12}H_{16}O_2$	192.1151
$C_8H_3N_2O_4$	191.0093	$C_{14}H_{23}$	191.1801	$C_{12}O_3$	191.9847
$C_8H_{21}N_3O_2$	191.1635	$C_{14}H_7O$	191.0497	$C_{12}H_{18}NO$	192.1389
$C_8H_5N_3O_3$	191.0331	$C_{14}H_9N$	191.0736	$C_{12}H_2NO_2$	192.0085
$C_8H_7N_4O_2$	191.0570	$C_{15}H_{11}$	191.0861	$C_{12}H_{20}N_2$	192.1628
$C_9H_{19}O_4$	191.1284	192		$C_{12}H_4N_2O$	192.0324
$C_9H_{21}NO_3$	191.1522	$C_7H_{16}N_2O_4$	192.1111	$C_{12}H_6N_3$	192.0563
$C_9H_5NO_4$	191.0218	$C_7H_{18}N_3O_3$	192.1349	$C_{13}H_{20}O$	192.1515
$C_9H_7N_2O_3$	191.0457	$C_7H_{20}N_4O_2$	192.1588	$C_{13}H_4O_2$	192.0211
$C_9H_9N_3O_2$	191.0695	$C_8H_{18}NO_4$	192.1236	$C_{13}H_{22}N$	192.1753
$C_9H_{11}N_4O$	191.0934	$C_8H_{20}N_2O_3$	192.1475	$C_{13}H_6NO$	192.0449
$C_{10}H_7O_4$	191.0344	$C_8H_4N_2O_4$	192.0171	$C_{13}H_8N_2$	192.0688
$C_{10}H_9NO_3$	191.0583	$C_8H_6N_3O_3$	192.0410	$C_{14}H_{24}$	192.1879
$C_{10}H_{11}N_2O_2$	191.0821	$C_8H_8N_4O_2$	192.0648	$C_{14}H_8O$	192.0575
$C_{10}H_{13}N_3O$	191.1060	$C_9H_{20}O_4$	192.1362	$C_{14}H_{10}N$	192.0814
$C_{10}H_{15}N_4$	191.1298	$C_9H_6NO_4$	192.0297	$C_{15}H_{12}$	192.0939
$C_{11}H_{11}O_3$	191.0708	$C_9H_8N_2O_3$	192.0535	C_{16}	192.0000
$C_{11}H_{13}NO_2$	191.0947	$C_9H_{10}N_3O_2$	192.0774	193	
$C_{11}H_{15}N_2O$	191.1185	$C_9H_{12}N_4O$	192.1012	$C_7H_{17}N_2O_4$	193.1189
$C_{11}H_{17}N_3$	191.1424	$C_{10}H_8O_4$	192.0422	$C_7H_{19}N_3O_3$	193.1427
$C_{11}HN_3O$	191.0120	$C_{10}H_{10}NO_3$	192.0661	$C_8H_{19}NO_4$	193.1315
$C_{11}H_3N_4$	191.0359	$C_{10}H_{12}N_2O_2$	192.0899	$C_8H_5N_2O_4$	193.0249
$C_{12}H_{15}O_2$	191.1072	$C_{10}H_{14}N_3O$	192.1138	$C_8H_7N_3O_3$	193.0488
$C_{12}H_{17}NO$	191.1311	$C_{10}H_{16}N_4$	192.1377	$C_8H_9N_4O_2$	193.0726
$C_{12}HNO_2$	191.0007	$C_{10}N_4O$	192.0073	$C_9H_7NO_4$	193.0375
$C_{12}H_{19}N_2$	191.1549	$C_{11}H_{12}O_3$	192.0786	$C_9H_9N_2O_3$	193.0614
$C_{12}H_3N_2O$	191.0246	$C_{11}H_{14}NO_2$	192.1025	$C_9H_{11}N_3O_2$	193.0852
$C_{12}H_5N_3$	191.0484	$C_{11}H_{16}N_2O$	192.1264	$C_9H_{13}N_4O$	193.1091
$C_{13}H_{19}O$	191.1436	$C_{11}N_2O_2$	191.9960	$C_9H_7N_3O$	193.0590

FM		FM		FM	
$C_{10}H_9O_4$	193.0501	$C_8H_6N_2O_4$	194.0328	$C_{13}H_8NO$	194.0606
$C_{10}H_{11}NO_3$	193.0739	$C_8H_8N_3O_3$	194.0566	$C_{13}H_{10}N_2$	194.0845
$C_{10}H_{13}N_2O_2$	193.0978	$C_8H_{10}N_4O_2$	194.0805	$C_{14}H_{26}$	194.1036
$C_{10}H_{15}N_3O$	193.1216	$C_9H_8NO_4$	194.0453	$C_{14}H_{10}O$	194.0732
$C_{10}H_{17}N_4$	193.1455	$C_9H_{10}N_2O_3$	194.0692	$C_{14}H_{12}N$	194.0970
$C_{10}HN_4O$	193.0151	$C_9H_{12}N_3O_2$	194.0930	$C_{15}H_{14}$	194.1096
$C_{11}H_{13}O_3$	193.0865	$C_9H_{14}N_4O$	194.1169	$C_{15}N$	194.0031
$C_{11}H_{15}NO_2$	193.1103	$C_{10}H_{10}O_4$	194.0579	$C_{16}H_2$	194.0157
$C_{11}H_{17}N_2O$	193.1342	$C_{10}H_{12}NO_3$	194.0817	195	
$C_{11}HN_2O_2$	193.0038	$C_{10}H_{14}N_2O_2$	194.1056	$C_8H_7N_2O_4$	195.0406
$C_{11}H_{19}N_3$	193.1580	$C_{10}H_{16}N_3O$	194.1295	$C_8H_9N_3O_3$	195.0644
$C_{11}H_3N_3O$	193.0277	$C_{10}N_3O_2$	193.9991	$C_9H_{11}N_4O_2$	195.0883
$C_{11}H_5N_4$	193.0515	$C_{10}H_{18}N_4$	194.1533	$C_9H_9NO_4$	195.0532
$C_{12}H_{17}O_2$	193.1229	$C_{10}H_2N_4O$	194.0229	$C_9H_{11}N_2O_3$	195.0770
$C_{12}HO_3$	192.9925	$C_{11}H_{14}O_3$	194.0943	$C_9H_{13}N_3O_2$	195.1009
$C_{12}H_{19}NO$	193.1467	$C_{11}H_{16}NO_2$	194.1182	$C_9H_{15}N_4O$	195.1247
$C_{12}H_3NO_2$	193.0164	$C_{11}NO_3$	193.9878	$C_{10}H_{11}O_4$	195.0657
$C_{12}H_{21}N_2$	193.1706	$C_{11}H_{18}N_2O$	194.1420	$C_{10}H_{13}NO_3$	195.0896
$C_{12}H_5N_2O$	193.0402	$C_{11}H_2N_2O_2$	194.0116	$C_{10}H_{15}N_2O_2$	195.1134
$C_{12}H_7N_3$	193.0641	$C_{11}H_{20}N_3$	194.1659	$C_{10}H_{17}N_3O$	195.1373
$C_{13}H_{21}O$	193.1593	$C_{11}H_4N_3O$	194.0355	$C_{10}HN_3O_2$	195.0069
$C_{13}H_5O_2$	193.0289	$C_{11}H_6N_4$	194.0594	$C_{10}H_{19}N_4$	195.1611
$C_{13}H_{23}N$	193.1832	$C_{12}H_{18}O_2$	194.1307	$C_{10}H_3N_4O$	195.0308
$C_{13}H_7NO$	193.0528	$C_{12}H_2O_3$	194.0003	$C_{11}H_{15}O_3$	195.1021
$C_{13}H_9N_2$	193.0767	$C_{12}H_{20}NO$	194.1546	$C_{11}H_{17}NO_2$	195.1260
$C_{14}H_{25}$	193.1957	$C_{12}H_4NO_2$	194.0242	$C_{11}HNO_3$	194.9956
$C_{14}H_9O$	193.0653	$C_{12}H_{22}N_2$	194.1784	$C_{11}H_{19}N_2O$	195.1498
$C_{14}H_{11}N$	193.0892	$C_{12}H_6N_2O$	194.0480	$C_{11}H_3N_2O_2$	195.0195
$C_{15}H_{13}$	193.1018	$C_{12}H_8N_3$	194.0719	$C_{11}H_{21}N_3$	195.1737
$C_{16}H$	193.0078	$C_{13}H_{22}O$	194.1671	$C_{11}H_5N_3O$	195.0433
194		$C_{13}H_6O_2$	194.0368	$C_{11}H_7N_4$	195.0672
$C_7H_{18}N_2O_4$	194.1267	$C_{13}H_{24}N$	194.1910	$C_{12}H_{19}O_2$	195.1385

	FM		FM		FM
$C_{12}H_3O_3$	195.0082	$C_{10}H_{20}N_4$	196.1690	$C_8H_{11}N_3O_3$	197.0801
$C_{12}H_{21}NO$	195.1624	$C_{10}H_4N_4O$	196.0386	$C_8H_{13}N_4O_2$	197.1040
$C_{12}H_5NO_2$	195.0320	$C_{11}H_{16}O_3$	196.1100	$C_9H_{11}NO_4$	197.0688
$C_{12}H_{23}N_2$	195.1863	$C_{11}O_4$	195.9796	$C_9H_{13}N_2O_3$	197.0927
$C_{12}H_7N_2O$	195.0559	$C_{11}H_{18}NO_2$	196.1338	$C_9H_{15}N_3O_2$	197.1165
$C_{12}H_9N_3$	195.0798	$C_{11}H_2NO_3$	196.0034	$C_9H_{17}N_4O$	197.1404
$C_{13}H_{23}O$	195.1750	$C_{11}H_{20}N_2O$	196.1577	$C_9HN_4O_2$	197.0100
$C_{13}H_7O_2$	195.0446	$C_{11}H_4N_2O_2$	196.0273	$C_{10}H_{13}O_4$	197.0814
$C_{13}H_{25}N$	195.1988	$C_{11}H_{22}N_3$	196.1815	$C_{10}H_{15}NO_3$	197.1052
$C_{13}H_9NO$	195.0684	$C_{11}H_6N_3O$	196.0511	$C_{10}H_{17}N_2O_2$	197.1291
$C_{13}H_{11}N_2$	195.0923	$C_{11}H_8N_4$	196.0750	$C_{10}HN_2O_3$	196.9987
$C_{14}H_{27}$	195.2114	$C_{12}H_{20}O_2$	196.1464	$C_{10}H_{19}N_3O$	197.1529
$C_{14}H_{11}O$	195.0810	$C_{12}H_4O_3$	196.0160	$C_{10}H_3N_3O_2$	197.0226
$C_{14}H_{13}N$	195.1049	$C_{12}H_{22}NO$	196.1702	$C_{10}H_{21}N_4$	197.1768
$C_{15}H_{15}$	195.1174	$C_{12}H_6NO_2$	196.0399	$C_{10}H_5N_4O$	197.0464
$C_{15}HN$	195.0109	$C_{12}H_{24}N_2$	196.1941	$C_{11}H_{17}O_3$	197.1178
$C_{16}H_3$	195.0235	$C_{12}H_8N_2O$	196.0637	$C_{11}HO_4$	196.9874
196		$C_{12}H_{10}N_3$	196.0876	$C_{11}H_{19}NO_2$	197.1416
$C_8H_8N_2O_4$	196.0484	$C_{13}H_{24}O$	196.1828	$C_{11}H_3NO_3$	197.0113
$C_8H_{10}N_3O_3$	196.0723	$C_{13}H_8O_2$	196.0524	$C_{11}H_{21}N_2O$	197.1655
$C_8H_{12}N_4O_2$	196.0961	$C_{13}H_{26}N$	196.2067	$C_{11}H_5N_2O_2$	197.0351
$C_9H_{10}NO_4$	196.0610	$C_{13}H_{10}NO$	196.0763	$C_{11}H_{23}N_3$	197.1894
$C_9H_{12}N_2O_3$	196.0848	$C_{13}H_{12}N_2$	196.1001	$C_{11}H_7N_3O$	197.0590
$C_9H_{14}N_3O_2$	196.1087	$C_{14}H_{28}$	196.2192	$C_{11}H_9N_4$	197.0829
$C_9H_{16}N_4O$	196.1325	$C_{14}H_{12}O$	196.0888	$C_{12}H_{21}O_2$	197.1542
$C_9N_4O_2$	196.0022	$C_{14}H_{14}N$	196.1127	$C_{12}H_5O_3$	197.0238
$C_{10}H_{12}O_4$	196.0735	$C_{14}N_2$	196.0062	$C_{12}H_{23}NO$	197.1781
$C_{10}H_{14}NO_3$	196.0974	$C_{15}H_{16}$	196.1253	$C_{12}H_7NO_2$	197.0477
$C_{10}H_{16}N_2O_2$	196.1213	$C_{15}O$	195.9949	$C_{12}H_{25}N_2$	197.2019
$C_{10}N_2O_3$	195.9909	$C_{15}H_2N$	196.0187	$C_{12}H_9N_2O$	197.0715
$C_{10}H_{18}N_3O$	196.1451	$C_{16}H_4$	196.0313	$C_{12}H_{11}N_3$	197.0954
$C_{10}H_2N_3O_2$	196.0147	197		$C_{13}H_{25}O$	197.1906
		$C_8H_9N_2O_4$	197.0563		

FM		FM		FM	
$C_{13}H_9O_2$	197.0603	$C_{11}H_2O_4$	197.9953	$C_8H_{13}N_3O_3$	199.0958
$C_{13}H_{27}N$	197.2145	$C_{11}H_{20}NO_2$	198.1495	$C_8H_{15}N_4O_2$	199.1196
$C_{13}H_{11}NO$	197.0841	$C_{11}H_4NO_3$	198.0191	$C_9H_{13}NO_4$	199.0845
$C_{13}H_{13}N_2$	197.1080	$C_{11}H_{22}N_2O$	198.1733	$C_9H_{15}N_2O_3$	199.1083
$C_{14}H_{29}$	197.2270	$C_{11}H_6N_2O_2$	198.0429	$C_9H_{17}N_3O_2$	199.1322
$C_{14}H_{13}O$	197.0967	$C_{11}H_{24}N_3$	198.1972	$C_9HN_3O_3$	199.0018
$C_{14}H_{15}N$	197.1205	$C_{11}H_8N_3O$	198.0668	$C_9H_{19}N_4O$	199.1560
$C_{14}HN_2$	197.0104	$C_{11}H_{10}N_4$	198.0907	$C_9H_3N_4O_2$	199.0257
$C_{15}H_{17}$	197.1331	$C_{12}H_{22}O_2$	198.1620	$C_{10}H_{15}O_4$	199.0970
$C_{15}HO$	197.0027	$C_{12}H_6O_3$	198.0317	$C_{10}H_{17}NO_3$	199.1209
$C_{15}H_3N$	197.0266	$C_{12}H_{24}NO$	198.1859	$C_{10}HNO_4$	198.9905
$C_{16}H_5$	197.0391	$C_{12}H_8NO_2$	198.0555	$C_{10}H_{19}N_2O_2$	199.1447
198		$C_{12}H_{26}N_2$	198.2098	$C_{10}H_3N_2O_3$	199.0144
$C_8H_{10}N_2O_4$	198.0641	$C_{12}H_{10}N_2O$	198.0794	$C_{10}H_{21}N_3O$	199.1686
$C_8H_{12}N_3O_3$	198.0879	$C_{12}H_{12}N_3$	198.1032	$C_{10}H_5N_3O_2$	199.0382
$C_8H_{14}N_4O_2$	198.1118	$C_{13}H_{26}O$	198.1985	$C_{10}H_{23}N_4$	199.1925
$C_9H_{12}NO_4$	198.0766	$C_{13}H_{10}O_2$	198.0681	$C_{10}H_7N_4O$	199.0621
$C_9H_{14}N_2O_3$	198.1005	$C_{13}H_{28}N$	198.2223	$C_{11}H_{19}O_3$	199.1334
$C_9H_{16}N_3O_2$	198.1244	$C_{13}H_{12}NO$	198.0919	$C_{11}H_3O_4$	199.0031
$C_9N_3O_3$	197.9940	$C_{13}H_{14}N_2$	198.1158	$C_{11}H_{21}NO_2$	199.1573
$C_9H_{18}N_4O$	198.1482	$C_{13}N_3$	198.0093	$C_{11}H_5NO_3$	199.0269
$C_9H_2N_4O_2$	198.0178	$C_{14}H_{30}$	198.2349	$C_{11}H_{23}N_2O$	199.1811
$C_{10}H_{14}O_4$	198.0892	$C_{14}H_{14}O$	198.1045	$C_{11}H_7N_2O_2$	199.0508
$C_{10}H_{16}NO_3$	198.1131	$C_{14}H_{16}N$	198.1284	$C_{11}H_{25}N_3$	199.2050
$C_{10}NO_4$	197.9827	$C_{14}NO$	197.9980	$C_{11}H_9N_3O$	199.0746
$C_{10}H_{18}N_2O_2$	198.1369	$C_{14}H_2N_2$	198.0218	$C_{11}H_{11}N_4$	199.0985
$C_{10}H_2N_2O_3$	198.0065	$C_{15}H_{18}$	198.1409	$C_{12}H_{23}O_2$	199.1699
$C_{10}H_{20}N_3O$	198.1608	$C_{15}H_2O$	198.0106	$C_{12}H_7O_3$	199.0395
$C_{10}H_4N_3O_2$	198.0304	$C_{15}H_4N$	198.0344	$C_{12}H_{25}NO$	199.1937
$C_{10}H_{22}N_4$	198.1846	$C_{16}H_6$	198.0470	$C_{12}H_9NO_2$	199.0634
$C_{10}H_6N_4O$	198.0542	199		$C_{12}H_{27}N_2$	199.2176
$C_{11}H_{18}O_3$	198.1256	$C_8H_{11}N_2O_4$	199.0719	$C_{12}H_{11}N_2O$	199.0872

FM		FM		FM	
$C_{12}H_{13}N_3$	199.1111	$C_{10}H_6N_3O_2$	200.0460	$C_{15}H_4O$	200.0262
$C_{13}H_{27}O$	199.2063	$C_{10}H_{24}N_4$	200.2003	$C_{15}H_6N$	200.0501
$C_{13}H_{11}O_2$	199.0759	$C_{10}H_8N_4O$	200.0699	$C_{16}H_8$	200.0626
$C_{13}H_{29}N$	199.2301	$C_{11}H_{20}O_3$	200.1413	201	
$C_{13}H_{13}NO$	199.0998	$C_{11}H_4O_4$	200.0109	$C_8H_{13}N_2O_4$	201.0876
$C_{13}H_{15}N_2$	199.1236	$C_{11}H_{22}NO_2$	200.1651	$C_8H_{15}N_3O_3$	201.1114
$C_{13}HN_3$	199.0171	$C_{11}H_6NO_3$	200.0348	$C_8H_{17}N_4O_2$	201.1353
$C_{14}H_{15}O$	199.1123	$C_{11}H_{24}N_2O$	200.1890	$C_9H_{15}NO_4$	201.1001
$C_{14}H_{17}N$	199.1362	$C_{11}H_8N_2O_2$	200.0586	$C_9H_{17}N_2O_3$	201.1240
$C_{14}HNO$	199.0058	$C_{11}H_{26}N_3$	200.2129	$C_9HN_2O_4$	200.9936
$C_{14}H_3N_2$	199.0297	$C_{11}H_{10}N_3O$	200.0825	$C_9H_{19}N_3O_2$	201.1478
$C_{15}H_{19}$	199.1488	$C_{11}H_{12}N_4$	200.1063	$C_9H_3N_3O_3$	201.0175
$C_{15}H_3O$	199.0184	$C_{12}H_{23}O_2$	200.1777	$C_9H_{21}N_4O$	201.1717
$C_{15}H_5N$	199.0422	$C_{12}H_8O_3$	200.0473	$C_9H_5N_4O_2$	201.0413
$C_{16}H_7$	199.0548	$C_{12}H_{26}NO$	200.2015	$C_{10}H_{17}O_4$	201.1127
200		$C_{12}H_{10}NO_2$	200.0712	$C_{10}H_{19}NO_3$	201.1365
$C_8H_{12}N_2O_4$	200.0797	$C_{12}H_{28}N_2$	200.2254	$C_{10}H_3NO_4$	201.0062
$C_8H_{14}N_3O_3$	200.1036	$C_{12}H_{12}N_2O$	200.0950	$C_{10}H_{21}N_2O_2$	201.1604
$C_8H_{16}N_4O_2$	200.1275	$C_{12}H_{14}N_3$	200.1189	$C_{10}H_5N_2O_3$	201.0300
$C_9H_{14}NO_4$	200.0923	$C_{12}N_4$	200.0124	$C_{10}H_{23}N_3O$	201.1842
$C_9H_{16}N_2O_3$	200.1162	$C_{13}H_{28}O$	200.2141	$C_{10}H_7N_3O_2$	201.0539
$C_9N_2O_4$	199.9858	$C_{13}H_{12}O_2$	200.0837	$C_{10}H_{25}N_4$	201.2081
$C_9H_{18}N_3O_2$	200.1400	$C_{13}H_{14}NO$	200.1076	$C_{10}H_9N_4O$	201.0777
$C_9H_2N_3O_3$	200.0096	$C_{13}H_{16}N_2$	200.1315	$C_{11}H_{21}O_3$	201.1491
$C_9H_{20}N_4O$	200.1639	$C_{13}N_2O$	200.0011	$C_{11}H_5O_4$	201.0187
$C_9H_4N_4O_2$	200.0335	$C_{13}H_2N_3$	200.0249	$C_{11}H_{23}NO_2$	201.1730
$C_{10}H_{16}O_4$	200.1049	$C_{14}H_{16}O$	200.1202	$C_{11}H_7NO_3$	201.0426
$C_{10}H_{18}NO_3$	200.1287	$C_{14}O_2$	199.9898	$C_{11}H_{25}N_2O$	201.1968
$C_{10}H_2NO_4$	199.9983	$C_{14}H_{18}N$	200.1440	$C_{11}H_9N_2O_2$	201.0664
$C_{10}H_{20}N_2O_2$	200.1526	$C_{14}H_2NO$	200.0136	$C_{11}H_{27}N_3$	201.2207
$C_{10}H_4N_2O_3$	200.0222	$C_{14}H_4N_2$	200.0375	$C_{11}H_{11}N_3O$	201.0903
$C_{10}H_{22}N_3O$	200.1764	$C_{15}H_{20}$	200.1566	$C_{11}H_{13}N_4$	201.1142

FM		FM		FM	
$C_{12}H_{25}O_2$	201.1855	$C_{10}H_{18}O_4$	202.1205	$C_{14}H_{20}N$	202.1597
$C_{12}H_9O_3$	201.0552	$C_{10}H_{20}NO_3$	202.1444	$C_{14}H_4NO$	202.0293
$C_{12}H_{27}NO$	201.2094	$C_{10}H_4NO_4$	202.0140	$C_{14}H_6N_2$	202.0532
$C_{12}H_{11}NO_2$	201.0790	$C_{10}H_{22}N_2O_2$	202.1682	$C_{15}H_{22}$	202.1722
$C_{12}H_{13}N_2O$	201.1029	$C_{10}H_6N_2O_3$	202.0379	$C_{15}H_6O$	202.0419
$C_{12}H_{15}N_3$	201.1267	$C_{10}H_{24}N_3O$	202.1921	$C_{15}H_8N$	202.0657
$C_{12}HN_4$	201.0202	$C_{10}H_8N_3O_2$	202.0617	$C_{16}H_{10}$	202.0783
$C_{13}H_{13}O_2$	201.0916	$C_{10}H_{26}N_4$	202.2160	203	
$C_{13}H_{15}NO$	201.1154	$C_{10}H_{10}N_4O$	202.0856	$C_8H_{15}N_2O_4$	203.1032
$C_{13}H_{17}N_2$	201.1393	$C_{11}H_{22}O_3$	202.1569	$C_8H_{17}N_3O_3$	203.1271
$C_{13}HN_2O$	201.0089	$C_{11}H_6O_4$	202.0266	$C_8H_{19}N_4O_2$	203.1509
$C_{13}H_3N_3$	201.0328	$C_{11}H_{24}NO_2$	202.1808	$C_9H_{17}NO_4$	203.1158
$C_{14}H_{17}O$	201.1280	$C_{11}H_8NO_3$	202.0504	$C_9H_{19}N_2O_3$	203.1396
$C_{14}HO_2$	200.9976	$C_{11}H_{26}N_2O$	202.2046	$C_9H_3N_2O_4$	203.0093
$C_{14}H_{19}N$	201.1519	$C_{11}H_{10}N_2O_2$	202.0743	$C_9H_{21}N_3O_2$	203.1635
$C_{14}H_3NO$	201.0215	$C_{11}H_{12}N_3O$	202.0981	$C_9H_5N_3O_3$	203.0331
$C_{14}H_5N_2$	201.0453	$C_{11}H_{14}N_4$	202.0122	$C_9H_{23}N_4O$	203.1873
$C_{15}H_{21}$	201.1644	$C_{12}H_{26}O_2$	202.1934	$C_9H_{17}N_4O_2$	203.0570
$C_{15}H_5O$	201.0340	$C_{12}H_{10}O_3$	202.0630	$C_{10}H_{19}O_4$	203.1284
$C_{15}H_7N$	201.0579	$C_{12}H_{12}NO_2$	202.0868	$C_{10}H_{21}NO_3$	203.1522
$C_{16}H_9$	201.0705	$C_{12}H_{14}N_2O$	202.1107	$C_{10}H_5NO_4$	203.0218
202		$C_{12}H_{16}N_3$	202.1346	$C_{10}H_{23}N_2O_2$	203.1761
$C_8H_{14}N_2O_4$	202.0954	$C_{12}N_3O$	202.0042	$C_{10}H_7N_2O_3$	203.0457
$C_8H_{16}N_3O_3$	202.1193	$C_{12}H_2N_4$	202.0280	$C_{10}H_{25}N_3O$	203.1999
$C_8H_{18}N_4O_2$	202.1431	$C_{13}H_{14}O_2$	202.0994	$C_{10}H_9N_3O_2$	203.0695
$C_9H_{16}NO_4$	202.1080	$C_{13}H_{16}NO$	202.1233	$C_{10}H_{11}N_4O$	203.0934
$C_9H_{18}N_2O_3$	202.1318	$C_{13}NO_2$	201.9929	$C_{11}H_{23}O_3$	203.1648
$C_9H_2N_2O_4$	202.0014	$C_{13}H_{18}N_2$	202.1471	$C_{11}H_7O_4$	203.0344
$C_9H_{20}N_3O_2$	202.1557	$C_{13}H_2N_2O$	202.0167	$C_{11}H_{25}NO_2$	203.1886
$C_9H_4N_3O_3$	202.0253	$C_{13}H_4N_3$	202.0406	$C_{11}H_9NO_3$	203.0583
$C_9H_{22}N_4O$	202.1795	$C_{14}H_{18}O$	202.1358	$C_{11}H_{11}N_2O_2$	203.0821
$C_9H_6N_4O_2$	202.0491	$C_{14}H_2O_2$	202.0054	$C_{11}H_{13}N_3O$	203.1060

FM		FM		FM	
$C_{11}H_{15}N_4$	203.1298	$C_9H_8N_4O_2$	204.0648	$C_{14}H_6NO$	204.0449
$C_{12}H_{11}O_3$	203.0708	$C_{10}H_{20}O_4$	204.1362	$C_{14}H_8N_2$	204.0688
$C_{12}H_{13}NO_2$	203.0947	$C_{10}H_{22}NO_3$	204.1600	$C_{15}H_{24}$	204.1879
$C_{12}H_{15}N_2O$	203.1185	$C_{10}H_6NO_4$	204.0297	$C_{15}H_8O$	204.0575
$C_{12}H_{17}N_3$	203.1424	$C_{10}H_{24}N_2O_2$	204.1839	$C_{15}H_{10}N$	204.0814
$C_{12}HN_3O$	203.0120	$C_{10}H_8N_2O_3$	204.0535	$C_{16}H_{12}$	204.0939
$C_{12}H_3N_4$	203.0359	$C_{10}H_{10}N_3O_2$	204.0774	C_{17}	204.0000
$C_{13}H_{15}O_2$	203.1072	$C_{10}H_{12}N_4O$	204.1012	205	
$C_{13}H_{17}NO$	203.1311	$C_{11}H_{24}O_3$	204.1726	$C_8H_{17}N_2O_4$	205.1159
$C_{13}HNO_2$	203.0007	$C_{11}H_8O_4$	204.0422	$C_8H_{19}N_3O_3$	205.1427
$C_{13}H_{19}N_2$	203.1549	$C_{11}H_{10}NO_3$	204.0661	$C_8H_{21}N_4O_2$	205.1666
$C_{13}H_3N_2O$	203.0246	$C_{11}H_{12}N_2O_2$	204.0899	$C_9H_{19}NO_4$	205.1315
$C_{13}H_5N_3$	203.0484	$C_{11}H_{14}N_3O$	204.1138	$C_9H_{21}N_2O_3$	205.1553
$C_{14}H_{19}O$	203.1436	$C_{11}H_{16}N_4$	204.1377	$C_9H_5N_2O_4$	205.0249
$C_{14}H_3O_2$	203.0133	$C_{11}N_4O$	204.0073	$C_9H_{23}N_3O_2$	205.1791
$C_{14}H_{21}N$	203.1675	$C_{12}H_{12}O_3$	204.0786	$C_9H_7N_3O_3$	205.0488
$C_{14}H_5NO$	203.0371	$C_{12}H_{14}NO_2$	204.1025	$C_9H_9N_4O_2$	205.0726
$C_{14}H_7N_2$	203.0610	$C_{12}H_{18}N_2O$	204.1264	$C_{10}H_{21}O_4$	205.1440
$C_{15}H_{23}$	203.1801	$C_{12}N_2O_2$	203.9960	$C_{10}H_{23}NO_3$	205.1679
$C_{15}H_7O$	203.0497	$C_{12}H_{18}N_3$	204.1502	$C_{10}H_7NO_4$	205.0375
$C_{15}H_9N$	203.0736	$C_{12}H_{22}N_3O$	204.0198	$C_{10}H_9N_2O_3$	205.0614
$C_{16}H_{11}$	203.0861	$C_{12}H_4N_4$	204.0437	$C_{10}H_{11}N_3O_2$	205.0852
204		$C_{13}H_{16}O_2$	204.1151	$C_{10}H_{13}N_4O$	205.1091
$C_8H_{16}N_2O_4$	204.1111	$C_{13}O_3$	203.9847	$C_{11}H_9O_4$	205.0501
$C_8H_{18}N_3O_3$	204.1349	$C_{13}H_{18}NO$	204.1389	$C_{11}H_{11}NO_3$	205.0739
$C_8H_{20}N_4O_2$	204.1588	$C_{13}H_2NO_2$	204.0085	$C_{11}H_{13}N_2O_2$	205.0978
$C_9H_{18}NO_4$	204.1236	$C_{13}H_{20}N_2$	204.1628	$C_{11}H_{15}N_3O$	205.1216
$C_9H_{20}N_2O_3$	204.1475	$C_{13}H_4N_2O$	204.0324	$C_{11}H_{17}N_4$	205.1455
$C_9H_4N_2O_4$	204.0171	$C_{13}H_6N_3$	204.0563	$C_{11}HN_4O$	205.0151
$C_9H_{22}N_3O_2$	204.1713	$C_{14}H_{20}O$	204.1515	$C_{12}H_{13}O_3$	205.0865
$C_9H_6N_3O_3$	204.0410	$C_{14}H_4O_2$	204.0211	$C_{12}H_{15}NO_2$	205.1103
$C_9H_{14}N_4O$	204.1952	$C_{14}H_{22}N$	204.1753	$C_{12}H_{17}N_2O$	205.1342

FM		FM		FM	
$C_{12}HN_2O_2$	205.0038	$C_{10}H_{10}N_2O_3$	206.0692	$C_{15}H_{12}N$	206.0970
$C_{12}H_{19}N_3$	205.1580	$C_{10}H_{12}N_3O_2$	206.0930	$C_{16}H_{14}$	206.1096
$C_{12}H_3N_3O$	205.0277	$C_{10}H_{14}N_4O$	206.1169	$C_{16}N$	206.0031
$C_{12}H_3N_4$	205.0515	$C_{11}H_{10}O_4$	206.0579	$C_{17}H_2$	206.0157
$C_{13}H_{17}O_2$	205.1229	$C_{11}H_{12}NO_3$	206.0817	207	
$C_{13}HO_3$	204.9925	$C_{11}H_{14}N_2O_2$	206.1056	$C_8H_{19}N_2O_4$	207.1345
$C_{13}H_{19}NO$	205.1467	$C_{11}H_{16}N_3O$	206.1295	$C_8H_{21}N_3O_3$	207.1584
$C_{13}H_3NO_2$	205.0164	$C_{11}N_3O_2$	205.9991	$C_9H_{21}NO_4$	207.1471
$C_{13}H_{21}N_2$	205.1706	$C_{11}H_{18}N_4$	206.1533	$C_9H_7N_2O_4$	207.0406
$C_{13}H_3N_2O$	205.0402	$C_{11}H_2N_4O$	206.0229	$C_9H_9N_3O_3$	207.0644
$C_{13}H_7N_3$	205.0641	$C_{12}H_{14}O_3$	206.0943	$C_9H_{11}N_4O_2$	207.0883
$C_{14}H_{21}O$	205.1593	$C_{12}H_{16}NO_2$	206.1182	$C_{10}H_9NO_4$	207.0532
$C_{14}H_3O_2$	205.0289	$C_{12}NO_3$	205.9878	$C_{10}H_{11}N_2O_3$	207.0770
$C_{14}H_{23}N$	205.1832	$C_{12}H_{18}N_2O$	206.1420	$C_{10}H_{13}N_3O_2$	207.1009
$C_{14}H_7NO$	205.0528	$C_{12}H_2N_2O_2$	206.0116	$C_{10}H_{15}N_4O$	207.1247
$C_{14}H_9N_2$	205.0767	$C_{12}H_{20}N_3$	206.1659	$C_{11}H_{11}O_4$	207.0657
$C_{15}H_{25}$	205.1957	$C_{12}H_4N_3O$	206.0355	$C_{11}H_{13}NO_3$	207.0896
$C_{15}H_9O$	205.0653	$C_{12}H_6N_4$	206.0594	$C_{11}H_{15}N_2O_2$	207.1134
$C_{15}H_{11}N$	205.0892	$C_{13}H_{18}O_2$	206.1307	$C_{11}H_{17}N_3O$	207.1373
$C_{16}H_{13}$	205.1018	$C_{13}H_2O_3$	206.0003	$C_{11}HN_3O_2$	207.0069
$C_{17}H$	205.0078	$C_{13}H_{20}NO$	206.1546	$C_{11}H_{19}N_4$	207.1611
206		$C_{13}H_4NO_2$	206.0242	$C_{11}H_3N_4O$	207.0308
$C_8H_{18}N_2O_4$	206.1267	$C_{13}H_{22}N_2$	206.1784	$C_{12}H_{15}O_3$	207.1021
$C_8H_{20}N_3O_3$	206.1506	$C_{13}H_6N_2O$	206.0480	$C_{12}H_{17}NO_2$	207.1260
$C_8H_{22}N_4O_2$	206.1744	$C_{13}H_8N_3$	206.0719	$C_{12}HNO_3$	206.9956
$C_9H_{20}NO_4$	206.1393	$C_{14}H_{22}O$	206.1671	$C_{12}H_{19}N_2O$	207.1498
$C_9H_{22}N_2O_3$	206.1631	$C_{14}H_6O_2$	206.0368	$C_{12}H_3N_2O_2$	207.0195
$C_9H_6N_2O_4$	206.0328	$C_{14}H_{24}N$	206.1910	$C_{12}H_{21}N_3$	207.1737
$C_9H_8N_3O_3$	206.0566	$C_{14}H_8NO$	206.0606	$C_{12}H_3N_3O$	207.0433
$C_9H_{10}N_4O_2$	206.0805	$C_{14}H_{10}N_2$	206.0845	$C_{12}H_7N_4$	207.0672
$C_{10}H_{22}O_4$	206.1518	$C_{15}H_{26}$	206.2036	$C_{13}H_{19}O_2$	207.1385
$C_{10}H_8NO_4$	206.0453	$C_{15}H_{10}O$	206.0732	$C_{13}H_3O_3$	207.0082

	FM		FM		FM
$C_{13}H_{21}NO$	207.1624	$C_{11}H_{20}N_4$	208.1690	$C_9H_{11}N_3O_3$	209.0801
$C_{13}H_5NO_2$	207.0320	$C_{11}H_4N_4O$	208.0386	$C_9H_{13}N_4O_2$	209.1040
$C_{13}H_{23}N_2$	207.1863	$C_{12}H_{16}O_3$	208.1100	$C_{10}H_{11}NO_4$	209.0688
$C_{13}H_7N_2O$	207.0559	$C_{12}O_4$	207.9796	$C_{10}H_{13}N_2O_3$	209.0927
$C_{13}H_9N_3$	207.0798	$C_{12}H_{18}NO_2$	208.1338	$C_{10}H_{15}N_3O_2$	209.1165
$C_{14}H_{23}O$	207.1750	$C_{12}H_2NO_3$	208.0034	$C_{10}H_{17}N_4O$	209.1404
$C_{14}H_7O_2$	207.0446	$C_{12}H_{20}N_2O$	208.1577	$C_{10}HN_4O_2$	209.0100
$C_{14}H_{25}N$	207.1988	$C_{12}H_4N_2O_2$	208.0273	$C_{11}H_{13}O_4$	209.0814
$C_{14}H_9NO$	207.0684	$C_{12}H_{22}N_3$	209.1815	$C_{11}H_{15}NO_3$	209.1052
$C_{14}H_{11}N_2$	207.0923	$C_{12}H_6N_3O$	208.0511	$C_{11}H_{17}N_2O_2$	209.1291
$C_{15}H_{27}$	207.2114	$C_{12}H_8N_4$	208.0750	$C_{11}HN_2O_3$	208.9987
$C_{15}H_{11}O$	207.0810	$C_{13}H_{20}O_2$	208.1464	$C_{11}H_{19}N_3O$	209.1529
$C_{15}H_{13}N$	207.1049	$C_{13}H_4O_3$	208.0160	$C_{11}H_{13}N_3O_2$	209.0226
$C_{16}H_{15}$	207.1174	$C_{13}H_{22}NO$	208.1702	$C_{11}H_{21}N_4$	209.1768
$C_{16}HN$	207.0109	$C_{13}H_6NO_2$	208.0399	$C_{11}H_5N_4O$	209.0464
$C_{17}H_3$	207.0235	$C_{13}H_{24}N_2$	208.1941	$C_{12}H_{17}O_3$	209.1178
208		$C_{13}H_8N_2O$	208.0637	$C_{12}HO_4$	208.9874
$C_8H_{20}N_2O_4$	208.1424	$C_{13}H_{10}N_3$	208.0876	$C_{12}H_{19}NO_2$	209.1416
$C_9H_8N_2O_4$	208.0484	$C_{14}H_{24}O$	208.1828	$C_{12}H_3NO_3$	209.0113
$C_9H_{10}N_3O_3$	208.0723	$C_{14}H_8O_2$	208.0524	$C_{12}H_{21}N_2O$	209.1655
$C_9H_{12}N_4O_2$	208.0961	$C_{14}H_{26}N$	209.2067	$C_{12}H_5N_2O_2$	209.0351
$C_{10}H_{10}NO_4$	208.0610	$C_{14}H_{10}NO$	208.0763	$C_{12}H_{23}N_3$	209.1894
$C_{10}H_{12}N_2O_3$	208.0848	$C_{14}H_{12}N_2$	208.1001	$C_{12}H_7N_3O$	209.0590
$C_{10}H_{14}N_3O_2$	208.1087	$C_{15}H_{28}$	208.2192	$C_{12}H_9N_4$	209.0829
$C_{10}H_{16}N_4O$	208.1325	$C_{15}H_{12}O$	208.0888	$C_{13}H_{21}O_2$	209.1542
$C_{10}N_4O_2$	208.0022	$C_{15}H_{14}N$	208.1127	$C_{13}H_5O_3$	209.0238
$C_{11}H_{12}O_4$	208.0735	$C_{15}N_2$	208.0062	$C_{13}H_{23}NO$	209.1781
$C_{11}H_{14}NO_3$	208.0974	$C_{16}H_{16}$	208.1253	$C_{13}H_7NO_2$	209.0477
$C_{11}H_{16}N_2O_2$	208.1213	$C_{16}O$	207.9949	$C_{13}H_5N_2$	209.2019
$C_{11}N_2O_3$	207.9909	$C_{16}H_2N$	208.0187	$C_{13}H_9N_2O$	209.0715
$C_{11}H_{18}N_3O$	208.1451	$C_{17}H_4$	208.0313	$C_{13}H_{11}N_3$	209.0954
$C_{11}H_2N_3O_2$	208.0147	209		$C_{14}H_{25}O$	209.1906
		$C_9H_9N_2O_4$	209.0563		

	FM		FM		FM
$C_{14}H_9O_2$	209.0603	$C_{12}H_2O_4$	209.9953	$C_9H_{13}N_3O_3$	211.0958
$C_{14}H_{27}N$	209.2145	$C_{12}H_{20}NO_2$	210.1495	$C_9H_{15}N_4O_2$	211.1196
$C_{14}H_{11}NO$	209.0841	$C_{12}H_4NO_3$	210.0191	$C_{10}H_{13}NO_4$	211.0845
$C_{14}H_{13}N_2$	209.1080	$C_{12}H_{22}N_2O$	210.1733	$C_{10}H_{15}N_2O_3$	211.1083
$C_{15}H_{29}$	209.2270	$C_{12}H_6N_2O_2$	210.0429	$C_{10}H_{17}N_3O_2$	211.1322
$C_{15}H_{13}O$	209.0967	$C_{12}H_{24}N_3$	210.1972	$C_{10}HN_3O_3$	211.0018
$C_{15}H_{15}N$	209.1205	$C_{12}H_8N_3O$	210.0668	$C_{10}H_{19}N_4O$	211.1560
$C_{15}HN_2$	209.0140	$C_{12}H_{10}N_4$	210.0907	$C_{10}H_3N_4O_2$	211.0257
$C_{16}H_{17}$	209.1331	$C_{13}H_{22}O_2$	210.1620	$C_{11}H_{15}O_4$	211.0970
$C_{16}HO$	209.0027	$C_{13}H_6O_3$	210.0317	$C_{11}H_{17}NO_3$	211.1209
$C_{16}H_3N$	209.0266	$C_{13}H_{24}NO$	210.1859	$C_{11}HNO_4$	210.9905
$C_{17}H_5$	209.0391	$C_{13}H_8NO_2$	210.0555	$C_{11}H_{19}N_2O_2$	211.1447
210		$C_{13}H_{26}N_2$	210.2098	$C_{11}H_3N_2O_3$	211.0144
$C_9H_{10}N_2O_4$	216.0641	$C_{13}H_{10}N_2O$	210.0794	$C_{11}H_{21}N_3O$	211.1686
$C_9H_{12}N_3O_3$	210.0879	$C_{13}H_{12}N_3$	210.1032	$C_{11}H_5N_3O_2$	211.0382
$C_9H_{14}N_4O_2$	210.1118	$C_{14}H_{26}O$	210.1985	$C_{11}H_{23}N_4$	211.1925
$C_{10}H_{12}NO_4$	210.0766	$C_{14}H_{10}O_2$	210.0681	$C_{11}H_7N_4O$	211.0621
$C_{10}H_{14}N_2O_3$	210.1005	$C_{14}H_{28}N$	210.2223	$C_{12}H_{19}O_3$	211.1334
$C_{10}H_{16}N_3O_2$	210.1244	$C_{14}H_{12}NO$	210.0919	$C_{12}H_3O_4$	211.0031
$C_{10}N_3O_3$	209.9940	$C_{14}H_{14}N_2$	210.1158	$C_{12}H_{21}NO_2$	211.1573
$C_{10}H_{18}N_4O$	210.1482	$C_{14}N_3$	210.0093	$C_{12}H_5NO_3$	211.0269
$C_{10}H_2N_4O_2$	210.0178	$C_{15}H_{30}$	210.2349	$C_{12}H_{23}N_2O$	211.1811
$C_{11}H_{14}O_4$	210.0892	$C_{15}H_{14}O$	210.1045	$C_{12}H_7N_2O_2$	211.0508
$C_{11}H_{16}NO_3$	210.1131	$C_{15}H_6N$	210.1284	$C_{12}H_{25}N_3$	211.2050
$C_{11}NO_4$	209.9827	$C_{15}NO$	209.9980	$C_{12}H_9N_3O$	211.0746
$C_{11}H_{18}N_2O_2$	210.1369	$C_{15}H_2N_2$	210.0218	$C_{12}H_{11}N_4$	211.0985
$C_{11}H_2N_2O_3$	210.0065	$C_{16}H_{18}$	210.1409	$C_{13}H_{23}O_2$	211.1699
$C_{11}H_{23}N_3O$	210.1608	$C_{16}H_2O$	210.0106	$C_{13}H_7O_3$	211.0395
$C_{11}H_4N_3O_2$	210.0304	$C_{16}H_4N$	210.0344	$C_{13}H_{25}NO$	211.1937
$C_{11}H_{22}N_4$	210.1846	$C_{17}H_6$	210.0470	$C_{13}H_9NO_2$	211.0634
$C_{11}H_6N_4O$	210.0542	211		$C_{13}H_{27}N_2$	211.2176
$C_{12}H_{18}O_3$	210.1256	$C_9H_{11}N_2O_4$	211.0719	$C_{13}H_{11}N_2O$	211.0872

	FM		FM		FM
$C_{13}H_{13}N_3$	211.1111	$C_{11}H_{22}N_3O$	212.1764	$C_{15}H_2NO$	212.0136
$C_{14}H_{27}O$	211.2063	$C_{11}H_6N_3O_2$	212.0460	$C_{15}H_4N_2$	212.0375
$C_{14}H_{11}O_2$	211.0759	$C_{11}H_{24}N_4$	212.2003	$C_{16}H_{20}$	212.1566
$C_{14}H_{29}N$	211.2301	$C_{11}H_8N_4O$	212.0699	$C_{16}H_4O$	212.0262
$C_{14}H_{13}NO$	211.0998	$C_{12}H_{20}O_3$	212.1413	$C_{16}H_6N$	212.0501
$C_{14}H_{15}N_2$	211.1236	$C_{12}H_4O_4$	212.0109	$C_{17}H_8$	212.0626
$C_{14}HN_3$	211.0171	$C_{12}H_{22}NO_2$	212.1651	213	
$C_{15}H_{31}$	211.2427	$C_{12}H_6NO_3$	212.0348	$C_9H_{15}N_2O_4$	213.0876
$C_{15}H_{15}O$	211.1123	$C_{12}H_{24}N_2O$	212.1890	$C_9H_{15}N_3O_3$	213.1114
$C_{15}H_{17}N$	211.1362	$C_{12}H_8N_2O_2$	212.0586	$C_9H_{17}N_4O_2$	213.1353
$C_{15}HNO$	211.0058	$C_{12}H_{26}N_3$	212.2129	$C_{10}H_{15}NO_4$	213.1001
$C_{15}H_3N_2$	211.0297	$C_{12}H_{10}N_3O$	212.0825	$C_{10}H_{17}N_2O_3$	213.1240
$C_{16}H_{19}$	211.1488	$C_{12}H_{12}N_4$	212.1063	$C_{10}HN_2O_4$	212.9936
$C_{16}H_3O$	211.0184	$C_{13}H_{24}O_2$	212.1777	$C_{10}H_{19}N_3O_2$	213.1478
$C_{16}H_5N$	211.0422	$C_{13}H_8O_3$	212.0473	$C_{10}H_3N_3O_3$	213.0175
$C_{17}H_7$	211.0548	$C_{13}H_{26}NO$	212.2015	$C_{10}H_{21}N_4O$	213.1717
212		$C_{13}H_{10}NO_2$	212.0712	$C_{10}H_5N_4O_2$	213.0413
$C_9H_{12}N_2O_4$	212.0797	$C_{13}H_{28}N_2$	212.2254	$C_{11}H_{17}O_4$	213.1127
$C_9H_{14}N_3O_3$	212.1036	$C_{13}H_{12}N_2O$	212.0950	$C_{11}H_{19}NO_3$	213.1365
$C_9H_{16}N_4O_2$	212.1275	$C_{13}H_{14}N_3$	212.1189	$C_{11}H_3NO_4$	213.0062
$C_{10}H_{14}NO_4$	212.0923	$C_{13}N_4$	212.0124	$C_{11}H_{21}N_2O_2$	213.1604
$C_{10}H_{16}N_2O_3$	212.1162	$C_{14}H_{28}O$	212.2141	$C_{11}H_5N_2O_3$	213.0300
$C_{10}N_2O_4$	211.9858	$C_{14}H_{12}O_2$	212.0837	$C_{11}H_{23}N_3O$	213.1842
$C_{10}H_{18}N_3O_2$	212.1400	$C_{14}H_{30}N$	212.2380	$C_{11}H_7N_3O_2$	213.0539
$C_{10}H_2N_3O_3$	212.0096	$C_{14}H_{14}NO$	212.1076	$C_{11}H_{25}N_4$	213.2081
$C_{10}H_{20}N_4O$	212.1639	$C_{14}H_{16}N_2$	212.1315	$C_{11}H_9N_4O$	213.0777
$C_{10}H_4N_4O_2$	212.0335	$C_{14}N_2O$	212.0011	$C_{12}H_{21}O_3$	213.1491
$C_{11}H_{16}O_4$	212.1049	$C_{14}H_2N_3$	212.0249	$C_{12}H_5O_4$	213.0187
$C_{11}H_{18}NO_3$	212.1287	$C_{15}H_{32}$	212.2505	$C_{12}H_{23}NO_2$	213.1730
$C_{11}H_2NO_4$	211.9983	$C_{15}H_{16}O$	212.1202	$C_{12}H_7NO_3$	213.0426
$C_{11}H_{20}N_2O_2$	212.1526	$C_{15}O_2$	211.9898	$C_{12}H_{25}N_2O$	213.1968
$C_{11}H_4N_2O_3$	212.0222	$C_{15}H_{18}N$	212.1440	$C_{12}H_9N_2O_2$	213.0664

FM		FM		FM	
$C_{12}H_{27}N_3$	213.2207	$C_{10}H_{18}N_2O_3$	214.1318	$C_{13}H_2N_4$	214.0280
$C_{12}H_{11}N_3O$	213.0903	$C_{10}H_2N_2O_4$	214.0014	$C_{14}H_{30}O$	214.2298
$C_{12}H_{13}N_4$	213.1142	$C_{10}H_{20}N_3O_2$	214.1557	$C_{14}H_{14}O_2$	214.0994
$C_{13}H_{25}O_2$	213.1855	$C_{10}H_4N_3O_3$	214.0253	$C_{14}H_{16}NO$	214.1233
$C_{13}H_9O_3$	213.0552	$C_{10}H_{22}N_4O$	214.1795	$C_{14}NO_2$	213.9929
$C_{13}H_{27}NO$	213.2094	$C_{10}H_6N_4O_2$	214.0491	$C_{14}H_{18}N_2$	214.1471
$C_{13}H_{11}NO_2$	213.0790	$C_{11}H_{18}O_4$	214.1205	$C_{14}H_2N_2O$	214.0167
$C_{13}H_{29}N_2$	213.2332	$C_{11}H_{20}NO_3$	214.1444	$C_{14}H_4N_3$	214.0406
$C_{13}H_{13}N_2O$	213.1029	$C_{11}H_4NO_4$	214.0140	$C_{15}H_{18}O$	214.1358
$C_{13}H_{15}N_3$	213.1267	$C_{11}H_{22}N_2O_2$	214.1682	$C_{15}H_2O_2$	214.0054
$C_{13}HN_4$	213.0202	$C_{11}H_6N_2O_3$	214.0379	$C_{15}H_{20}N$	214.1597
$C_{14}H_{29}O$	213.2219	$C_{11}H_{24}N_3O$	214.1921	$C_{15}H_4NO$	214.0293
$C_{14}H_{13}O_2$	213.0916	$C_{11}H_8N_3O_2$	214.0617	$C_{15}H_6N_2$	214.0532
$C_{14}H_{31}N$	213.2458	$C_{11}H_{26}N_4$	214.2160	$C_{16}H_{22}$	214.1722
$C_{14}H_{15}NO$	213.1154	$C_{11}H_{10}N_4O$	214.0856	$C_{16}H_6O$	214.0419
$C_{14}H_{17}N_2$	213.1393	$C_{12}H_{22}O_3$	214.1569	$C_{16}H_8N$	214.0657
$C_{14}HN_2O$	213.0089	$C_{12}H_6O_4$	214.0266	$C_{17}H_{10}$	214.0783
$C_{14}H_3N_3$	213.0328	$C_{12}H_{24}NO_2$	214.1808	215	
$C_{15}H_{17}O$	213.1280	$C_{12}H_8NO_3$	214.0504	$C_9H_{15}N_2O_4$	215.1032
$C_{15}HO_2$	212.9976	$C_{12}H_{26}N_2O$	214.2046	$C_9H_{17}N_3O_3$	215.1271
$C_{15}H_{19}N$	213.1519	$C_{12}H_{10}N_2O_2$	214.0743	$C_9H_{19}N_4O_2$	215.1509
$C_{15}H_3NO$	213.0215	$C_{12}H_{28}N_3$	214.2285	$C_{10}H_{17}NO_4$	215.1158
$C_{15}H_5N_2$	213.0453	$C_{12}H_{12}N_3O$	214.0981	$C_{10}H_{19}N_2O_3$	215.1396
$C_{16}H_{21}$	213.1644	$C_{12}H_{14}N_4$	214.1220	$C_{10}H_3N_2O_4$	215.0093
$C_{16}H_5O$	213.0340	$C_{13}H_{26}O_2$	214.1934	$C_{10}H_{21}N_3O_2$	215.1635
$C_{16}H_7N$	213.0579	$C_{13}H_{10}O_3$	214.0630	$C_{10}H_5N_3O_3$	215.0331
$C_{17}H_9$	213.0705	$C_{13}H_{28}NO$	214.2172	$C_{10}H_{23}N_4O$	215.1873
214		$C_{13}H_{12}NO_2$	214.0859	$C_{10}H_7N_4O_2$	215.0570
$C_9H_{14}N_2O_4$	214.0954	$C_{13}H_{30}N_2$	214.2411	$C_{11}H_{19}O_4$	215.1284
$C_9H_{16}N_3O_3$	214.1193	$C_{13}H_{14}N_2O$	214.1107	$C_{11}H_{21}NO_3$	215.1522
$C_9H_{18}N_4O_2$	214.1431	$C_{13}H_6N_3$	214.1345	$C_{11}H_5NO_4$	215.0218
$C_{10}H_{16}NO_4$	214.1080	$C_{13}N_3O$	214.0042	$C_{11}H_{23}N_2O_2$	215.1761

FM		FM		FM	
$C_{11}H_7N_2O_3$	215.0457	$C_{15}H_7N_2$	215.0610	$C_{12}H_{16}N_4$	216.1377
$C_{11}H_{25}N_3O$	215.1999	$C_{16}H_{23}$	215.1801	$C_{12}N_4O$	216.0073
$C_{11}H_9N_3O_2$	215.0695	$C_{16}H_7O$	215.0497	$C_{13}H_{28}O_2$	216,2090
$C_{11}H_{27}N_4$	215.2238	$C_{16}H_9N$	215.0736	$C_{13}H_{12}O_3$	216.0786
$C_{11}H_{11}N_4O$	215.0934	$C_{17}H_{11}$	215.0861	$C_{13}H_{14}NO_2$	216.1025
$C_{12}H_{23}O_3$	215.1648	216		$C_{13}H_{16}N_2O$	216.1264
$C_{12}H_7O_4$	215.0344	$C_9H_{16}N_2O_4$	216.1111	$C_{13}N_2O_2$	215.9960
$C_{12}H_{25}NO_2$	215.1886	$C_9H_{18}N_3O_3$	216.1349	$C_{13}H_{18}N_3$	216.1502
$C_{12}H_9NO_3$	215.0583	$C_9H_{20}N_4O_2$	216.1588	$C_{13}H_2N_3O$	216.0198
$C_{12}H_{27}N_2O$	215.2125	$C_{10}H_{18}NO_4$	216.1236	$C_{13}H_4N_4$	216.0437
$C_{12}H_{11}N_2O_2$	215.0821	$C_{10}H_{20}N_2O_3$	216.1475	$C_{14}H_{16}O_2$	216.1151
$C_{12}H_{29}N_3$	215.2363	$C_{10}H_4N_2O_4$	216.0171	$C_{14}O_3$	215.9847
$C_{12}H_{15}N_3O$	215.1060	$C_{10}H_{22}N_3O_2$	216.1713	$C_{14}H_{18}NO$	216.1389
$C_{12}H_{15}N_4$	215.1298	$C_{10}H_6N_3O_3$	216.0410	$C_{14}H_2NO_2$	216.0085
$C_{13}H_{27}O_2$	215.2012	$C_{10}H_{24}N_4O$	216.1952	$C_{14}H_{20}N_2$	216.1628
$C_{13}H_{11}O_3$	215.0708	$C_{10}H_8N_4O_2$	216.0648	$C_{14}H_4N_2O$	216.0324
$C_{13}H_{29}NO$	215.2250	$C_{11}H_{20}O_4$	216.1362	$C_{14}H_6N_3$	216.0563
$C_{13}H_{13}NO_2$	215.0947	$C_{11}H_{22}NO_3$	216.1600	$C_{15}H_{20}O$	216.1515
$C_{13}H_{15}N_2O$	215.1185	$C_{11}H_6NO_4$	216.0297	$C_{15}H_4O_2$	216.0211
$C_{13}H_{17}N_3$	215.1424	$C_{11}H_{24}N_2O_2$	216.1839	$C_{15}H_{22}N$	216.1753
$C_{13}HN_3O$	215.0120	$C_{11}H_8N_2O_3$	216.0535	$C_{15}H_6NO$	216.0449
$C_{13}H_3N_4$	215.0359	$C_{11}H_{26}N_3O$	216.2077	$C_{15}H_8N_2$	216.0688
$C_{14}H_{15}O_2$	215.1072	$C_{11}H_{10}N_3O_2$	216.0774	$C_{16}H_{24}$	216.1879
$C_{14}H_{17}NO$	215.1311	$C_{11}H_{28}N_4$	216.2316	$C_{16}H_8O$	216.0575
$C_{14}HNO_2$	215.0007	$C_{11}H_{12}N_4O$	216.1012	$C_{16}H_{10}N$	216.0814
$C_{14}H_{19}N_2$	215.1541	$C_{12}H_{24}O_3$	216.1726	$C_{17}H_{12}$	216.0939
$C_{14}H_3N_2O$	215.0246	$C_{12}H_8O_4$	216.0422	C_{18}	216.0000
$C_{14}H_5N_3$	215.0484	$C_{12}H_{26}NO_2$	216.1965	217	
$C_{15}H_{19}O$	215.1436	$C_{12}H_{10}NO_3$	216.0661	$C_9H_{17}N_2O_4$	217.1189
$C_{15}H_3O_2$	215.0133	$C_{12}H_{28}N_2O$	216.2203	$C_9H_{19}N_3O_3$	217.1427
$C_{15}H_{21}N$	215.1675	$C_{12}H_{12}N_2O_2$	216.0899	$C_9H_{21}N_4O_2$	217.1666
$C_{15}H_5NO$	215.0371	$C_{12}H_{14}N_3O$	216.1138	$C_{10}H_{19}NO_4$	217.1315

FM		FM		FM	
$C_{10}H_{21}N_2O_3$	217.1553	$C_{14}H_{19}NO$	217.1467	$C_{11}H_{14}N_4O$	218.1169
$C_{10}H_5N_2O_4$	217.0249	$C_{14}H_3NO_2$	217.0164	$C_{12}H_{26}O_3$	218.1883
$C_{10}H_{23}N_3O_2$	217.1791	$C_{14}H_{21}N_2$	217.1706	$C_{12}H_{10}O_4$	218.0579
$C_{10}H_7N_3O_3$	217.0488	$C_{14}H_5N_2O$	217.0402	$C_{12}H_{12}NO_3$	218.0817
$C_{10}H_{25}N_4O$	217.2030	$C_{14}H_7N_3$	217.0641	$C_{12}H_{14}N_2O_2$	218.1056
$C_{10}H_9N_4O_2$	217.0726	$C_{15}H_{21}O$	217.1593	$C_{12}H_{16}N_3O$	218.1295
$C_{11}H_{21}O_4$	217.1440	$C_{15}H_5O_2$	217.0289	$C_{12}N_3O_2$	217.9991
$C_{11}H_{23}NO_3$	217.1679	$C_{15}H_{23}N$	217.1832	$C_{12}H_{18}N_4$	218.1533
$C_{11}H_7NO_4$	217.0375	$C_{15}H_7NO$	217.0528	$C_{12}H_2N_4O$	218.0229
$C_{11}H_{25}N_2O_4$	217.1917	$C_{15}H_9N_2$	217.0767	$C_{13}H_{14}O_3$	218.0943
$C_{11}H_9N_2O_3$	217.0614	$C_{16}H_{25}$	217.1957	$C_{13}H_{16}NO_2$	218.1182
$C_{11}H_{27}N_3O$	217.2156	$C_{16}H_9O$	217.0653	$C_{13}NO_3$	217.9878
$C_{11}H_{11}N_3O_2$	217.0852	$C_{16}H_{11}N$	217.0892	$C_{13}H_{18}N_2O$	218.1420
$C_{11}H_{13}N_4O$	217.1091	$C_{17}H_{13}$	217.1018	$C_{13}H_2N_2O_2$	218.0116
$C_{11}H_{28}N_4$	216.2316	$C_{18}H$	217.0078	$C_{13}H_{20}N_3$	218.1659
$C_{12}H_{25}O_3$	217.1804	218		$C_{13}H_4N_3O$	218.0355
$C_{12}H_9O_4$	217.0501	$C_9H_{18}N_2O_4$	218.1267	$C_{13}H_6N_4$	218.0594
$C_{12}H_{27}NO_2$	217.2043	$C_9H_{20}N_3O_3$	218.1506	$C_{14}H_{18}O_2$	218.1307
$C_{12}H_{11}NO_3$	217.0739	$C_9H_{22}N_4O_2$	218.1744	$C_{14}H_2O_3$	218.0003
$C_{12}H_{13}N_2O_2$	217.0978	$C_{10}H_{20}NO_4$	218.1393	$C_{14}H_{20}NO$	218.1546
$C_{12}H_{15}N_3O$	217.1216	$C_{10}H_{22}N_2O_3$	218.1631	$C_{14}H_4NO_2$	218.0242
$C_{12}H_{17}N_4$	217.1455	$C_{10}H_6N_2O_4$	218.0328	$C_{14}H_{22}N_2$	218.1784
$C_{12}HN_4O$	217.0151	$C_{10}H_{24}N_3O_2$	218.1870	$C_{14}H_6N_2O$	218.0480
$C_{13}H_{13}O_3$	217.0865	$C_{10}H_8N_3O_3$	218.0566	$C_{14}H_8N_3$	218.0719
$C_{13}H_{15}NO_2$	217.1103	$C_{10}H_{26}N_4O$	218.2108	$C_{15}H_{22}O$	218.1671
$C_{13}H_{17}N_2O$	217.1342	$C_{10}H_{10}N_4O_2$	218.0805	$C_{15}H_6O_2$	218.0368
$C_{13}HN_2O_2$	217.0038	$C_{11}H_{22}O_4$	218.1518	$C_{15}H_{24}N$	218.1910
$C_{13}H_{19}N_3$	217.1580	$C_{11}H_{24}NO_3$	218.1757	$C_{15}H_8NO$	218.0606
$C_{13}H_3N_3O$	217.0277	$C_{11}H_8NO_4$	218.0453	$C_{15}H_{10}N_2$	218.0845
$C_{13}H_5N_4$	217.0515	$C_{11}H_{26}N_2O_2$	218.1996	$C_{16}H_{26}$	218.2036
$C_{14}H_{17}O_2$	217.1229	$C_{11}H_{10}N_2O_3$	218.0692	$C_{16}H_{10}O$	218.0732
$C_{14}HO_3$	216.9925	$C_{11}H_{12}N_3O_2$	218.0930	$C_{16}H_{12}N$	218.0970

FM		FM		FM	
C ₁₇ H ₁₄	218.1096	C ₁₃ H ₅ N ₃ O	219.0433	C ₁₁ H ₁₄ N ₃ O ₂	220.1087
C ₁₇ N	218.0031	C ₁₃ H ₇ N ₄	219.0672	C ₁₁ H ₁₆ N ₄ O	220.1325
C ₁₈ H ₂	218.0157	C ₁₄ H ₁₉ O ₂	219.1385	C ₁₁ N ₄ O ₂	220.0022
219		C ₁₄ H ₃ O ₃	219.0082	C ₁₂ H ₁₂ O ₄	220.0735
C ₉ H ₁₉ N ₂ O ₄	219.1345	C ₁₄ H ₂₁ NO	219.1624	C ₁₂ H ₁₄ NO ₃	220.0974
C ₉ H ₂₁ N ₃ O ₃	219.1584	C ₁₄ H ₅ NO ₂	219.0320	C ₁₂ H ₁₆ N ₂ O ₂	220.1213
C ₉ H ₂₃ N ₄ O ₂	219.1822	C ₁₄ H ₂₃ N ₂	219.1863	C ₁₂ N ₂ O ₃	219.9909
C ₁₀ H ₂₁ NO ₄	219.1471	C ₁₄ H ₇ N ₂ O	219.0559	C ₁₂ H ₁₈ N ₃ O	220.1451
C ₁₀ H ₂₃ N ₂ O ₃	219.1710	C ₁₄ H ₉ N ₃	219.0798	C ₁₂ H ₂ N ₃ O ₂	220.0147
C ₁₀ H ₇ N ₂ O ₄	219.0406	C ₁₅ H ₂₃ O	219.1750	C ₁₂ H ₂₀ N ₄	220.1690
C ₁₀ H ₂₅ N ₃ O ₂	219.1948	C ₁₅ H ₇ O ₂	219.0446	C ₁₂ H ₄ N ₄ O	220.0386
C ₁₀ H ₉ N ₃ O ₃	219.0644	C ₁₅ H ₂₅ N	219.1988	C ₁₃ H ₁₆ O ₃	220.1100
C ₁₀ H ₁₁ N ₄ O ₂	219.0883	C ₁₅ H ₉ NO	219.0684	C ₁₃ O ₄	219.9796
C ₁₁ H ₂₃ O ₄	219.1597	C ₁₅ H ₁₁ N ₂	219.0923	C ₁₂ H ₁₈ NO ₂	220.1338
C ₁₁ H ₂₅ NO ₃	219.1835	C ₁₆ H ₂₇	219.2114	C ₁₃ H ₂ NO ₃	220.0034
C ₁₁ H ₉ NO ₄	219.0532	C ₁₆ H ₁₁ O	219.0810	C ₁₃ H ₂₀ N ₂ O	220.1577
C ₁₁ H ₁₁ N ₂ O ₃	219.0770	C ₁₆ H ₁₃ N	219.1049	C ₁₃ H ₄ N ₂ O ₂	220.0273
C ₁₁ H ₁₃ N ₃ O ₂	219.1009	C ₁₇ H ₁₅	219.1174	C ₁₃ H ₂₂ N ₃	220.1815
C ₁₁ H ₁₅ N ₄ O	219.1247	C ₁₇ HN	219.0109	C ₁₃ H ₆ N ₃ O	220.0511
C ₁₂ H ₁₁ O ₄	219.0657	C ₁₈ H ₃	219.0235	C ₁₃ H ₈ N ₄	220.0750
C ₁₂ H ₁₃ NO ₃	219.0896	220		C ₁₄ H ₂₀ O ₂	220.1464
C ₁₂ H ₁₅ N ₂ O ₂	219.1134	C ₉ H ₂₀ N ₂ O ₄	220.1424	C ₁₄ H ₄ O ₃	220.0160
C ₁₂ H ₁₇ N ₃ O	219.1373	C ₉ H ₂₂ N ₃ O ₃	220.1662	C ₁₄ H ₂₂ NO	220.1702
C ₁₂ HN ₃ O ₂	219.0069	C ₉ H ₂₄ N ₄ O ₂	220.1901	C ₁₄ H ₆ NO ₂	220.0399
C ₁₂ H ₉ N ₄	219.1611	C ₁₀ H ₂₂ NO ₄	220.1549	C ₁₄ H ₂₄ N ₂	220.1941
C ₁₂ H ₃ N ₄ O	219.0308	C ₁₀ H ₂₄ N ₂ O ₃	220.1788	C ₁₄ H ₈ N ₂ O	220.0637
C ₁₃ H ₁₅ O ₃	219.1021	C ₁₀ H ₈ N ₂ O ₄	220.0484	C ₁₄ H ₁₀ N ₃	220.0876
C ₁₃ H ₁₇ NO ₂	219.1260	C ₁₀ H ₁₀ N ₃ O ₃	220.0723	C ₁₅ H ₂₄ O	220.1828
C ₁₃ HNO ₃	218.9956	C ₁₀ H ₁₂ N ₄ O ₂	220.0961	C ₁₅ H ₈ O ₂	220.0524
C ₁₃ H ₁₉ N ₂ O	219.1498	C ₁₁ H ₂₄ O ₄	220.1675	C ₁₅ H ₂₆ N	220.2067
C ₁₃ H ₃ N ₂ O ₂	219.0195	C ₁₁ H ₁₀ NO ₄	220.0610	C ₁₅ H ₁₀ NO	220.0763
C ₁₃ H ₂₁ N ₃	219.1737	C ₁₁ H ₁₂ N ₂ O ₃	220.0848	C ₁₅ H ₁₂ N ₂	220.1001

FM		FM		FM	
$C_{16}H_{28}$	220.2192	$C_{13}H_{21}N_2O$	221.1655	$C_{11}H_{16}N_3O_2$	222.1244
$C_{16}H_{12}O$	220.0888	$C_{13}H_5N_2O_2$	221.0351	$C_{11}N_3O_3$	221.9940
$C_{16}H_{14}N$	220.1127	$C_{13}H_{23}N_3$	221.1894	$C_{11}H_{18}N_4O$	222.1482
$C_{16}N_2$	220.0062	$C_{13}H_7N_3O$	221.0590	$C_{11}H_2N_4O_2$	222.0178
$C_{17}H_{16}$	220.1253	$C_{13}H_9N_4$	221.0829	$C_{12}H_{14}O_4$	222.0892
$C_{17}O$	219.9949	$C_{14}H_{21}O_2$	221.1542	$C_{12}H_{16}NO_3$	222.1131
$C_{17}H_2N$	220.0187	$C_{14}H_5O_3$	221.0238	$C_{12}NO_4$	221.9827
$C_{18}H_4$	220.0313	$C_{14}H_{23}NO$	221.1781	$C_{12}H_{18}N_2O_2$	222.1369
221		$C_{14}H_7NO_2$	221.0477	$C_{12}H_2N_2O_3$	222.0065
$C_9H_{21}N_2O_4$	221.1502	$C_{14}H_{25}N_2$	221.2019	$C_{12}H_{20}N_3O$	222.1608
$C_9H_{23}N_3O_3$	221.1741	$C_{14}H_9N_2O$	221.0715	$C_{12}H_4N_3O_2$	222.0304
$C_{10}H_{23}NO_4$	221.1628	$C_{14}H_{11}N_3$	221.0954	$C_{12}H_{22}N_4$	222.1846
$C_{10}H_9N_2O_4$	221.0563	$C_{15}H_{25}O$	221.1906	$C_{12}H_6N_4O$	222.0542
$C_{10}H_{11}N_3O_3$	221.0801	$C_{15}H_9O_2$	221.0603	$C_{13}H_{18}O_3$	222.1256
$C_{10}H_{13}N_4O_2$	221.1040	$C_{15}H_{27}N$	221.2145	$C_{13}H_2O_4$	221.9953
$C_{11}H_{11}NO_4$	221.0688	$C_{15}H_{11}NO$	221.0841	$C_{13}H_{20}NO_2$	222.1495
$C_{11}H_{13}N_2O_3$	221.0927	$C_{15}H_{13}N_2$	221.1080	$C_{13}H_4NO_3$	222.0191
$C_{11}H_{15}N_3O_2$	221.1165	$C_{16}H_{29}$	221.2270	$C_{13}H_{22}N_2O$	222.1733
$C_{11}H_{17}N_4O$	221.1404	$C_{16}H_{13}O$	221.0967	$C_{13}H_6N_2O_2$	222.0429
$C_{11}HN_4O_2$	221.0100	$C_{16}H_{15}N$	221.1205	$C_{13}H_{24}N_3$	222.1972
$C_{12}H_{13}O_4$	221.0814	$C_{16}HN_2$	221.0140	$C_{13}H_8N_3O$	222.0668
$C_{12}H_{15}NO_3$	221.1052	$C_{17}H_{17}$	221.1331	$C_{13}H_{10}N_4$	222.0907
$C_{12}H_{17}N_2O_2$	221.1291	$C_{17}HO$	221.0027	$C_{14}H_{22}O_2$	222.1620
$C_{12}HN_2O_3$	220.9987	$C_{17}H_3N$	221.0266	$C_{14}H_6O_3$	222.0317
$C_{12}H_{19}N_3O$	221.1529	$C_{18}H_5$	221.0391	$C_{14}H_{24}NO$	222.1859
$C_{12}H_3N_3O_2$	221.0226	222		$C_{14}H_8NO_2$	222.0555
$C_{12}H_{21}N_4$	221.1768	$C_9H_{22}N_2O_4$	222.1580	$C_{14}H_{26}N_2$	222.2098
$C_{12}H_5N_4O$	221.0464	$C_{10}H_{10}N_2O_4$	222.0641	$C_{14}H_{10}N_2O$	222.0794
$C_{13}H_{17}O_3$	221.1178	$C_{10}H_{12}N_3O_3$	222.0879	$C_{14}H_{12}N_3$	222.1032
$C_{13}HO_4$	220.9874	$C_{10}H_{14}N_4O_2$	222.1118	$C_{15}H_{26}O$	222.1985
$C_{13}H_{19}NO_2$	221.1416	$C_{11}H_{12}NO_4$	222.0766	$C_{15}H_{10}O_2$	222.0681
$C_{13}H_3NO_3$	221.0113	$C_{11}H_{14}N_2O_3$	222.1005	$C_{15}H_{28}N$	222.2223

FM		FM		FM	
$C_{15}H_{12}NO$	222.0919	$C_{13}H_3O_4$	223.0031	$C_{10}H_{14}N_3O_3$	224.1036
$C_{15}H_{14}N_2$	222.1158	$C_{13}H_{21}NO_2$	223.1573	$C_{10}H_{16}N_4O_2$	224.1275
$C_{15}N_3$	222.0093	$C_{13}H_5NO_3$	223.0269	$C_{11}H_{14}NO_4$	224.0923
$C_{16}H_{30}$	222.2349	$C_{13}H_{23}N_2O$	223.1811	$C_{11}H_{16}N_2O_3$	224.1162
$C_{16}H_{14}O$	222.1045	$C_{13}H_7N_2O_2$	223.0508	$C_{11}N_2O_4$	223.9858
$C_{16}H_{16}N$	222.1284	$C_{13}H_{25}N_3$	223.2050	$C_{11}H_{18}N_3O_2$	224.1400
$C_{16}NO$	221.9980	$C_{13}H_9N_3O$	223.0746	$C_{11}H_2N_3O_3$	224.0096
$C_{16}H_2N_2$	222.0218	$C_{13}H_{11}N_4$	223.0985	$C_{11}H_{20}N_4O$	224.1639
$C_{17}H_{18}$	222.1409	$C_{14}H_{23}O_2$	223.1699	$C_{11}H_4N_4O_2$	224.0335
$C_{17}H_2O$	222.0106	$C_{14}H_7O_3$	223.0395	$C_{12}H_{16}O_4$	224.1049
$C_{17}H_4N$	222.0344	$C_{14}H_{25}NO$	223.1937	$C_{12}H_{18}NO_3$	224.1287
$C_{18}H_6$	222.0470	$C_{14}H_9NO_2$	223.0634	$C_{12}H_2NO_4$	223.9983
223		$C_{14}H_{27}N_2$	223.2176	$C_{12}H_{20}N_2O_2$	224.1526
$C_{10}H_{11}N_2O_4$	223.0719	$C_{14}H_{11}N_2O$	223.0872	$C_{12}H_4N_2O_3$	224.0222
$C_{10}H_{13}N_3O_3$	223.0958	$C_{14}H_{13}N_3$	223.1111	$C_{12}H_{22}N_3O$	224.1764
$C_{10}H_{15}N_4O_2$	223.1196	$C_{15}H_{27}O$	223.2063	$C_{12}H_6N_3O_2$	224.0460
$C_{11}H_{13}NO_4$	223.0845	$C_{15}H_{11}O_2$	223.0759	$C_{12}H_{24}N_4$	224.2003
$C_{11}H_{15}N_2O_3$	223.1083	$C_{15}H_{29}N$	223.2301	$C_{12}H_8N_4O$	224.0699
$C_{11}H_{17}N_3O_2$	223.1322	$C_{15}H_{13}NO$	223.0998	$C_{13}H_{20}O_3$	224.1413
$C_{11}HN_3O_3$	223.0018	$C_{15}H_{15}N_2$	223.1236	$C_{13}H_4O_4$	224.0109
$C_{11}H_{19}N_4O$	223.1560	$C_{15}HN_3$	223.0171	$C_{13}H_{22}NO_2$	224.1651
$C_{11}H_3N_4O_2$	223.0257	$C_{16}H_{31}$	223.2427	$C_{13}H_6NO_3$	224.0348
$C_{12}H_{15}O_4$	223.0970	$C_{16}H_{15}O$	223.1123	$C_{13}H_{24}N_2O$	224.1890
$C_{12}H_{17}NO_3$	223.1209	$C_{16}H_{17}N$	223.1362	$C_{13}H_8N_2O_2$	224.0586
$C_{12}HNO_4$	222.9905	$C_{16}HNO$	223.0058	$C_{13}H_{26}N_3$	224.2129
$C_{12}H_{19}N_2O_2$	223.1447	$C_{16}H_3N_2$	223.0297	$C_{13}H_{10}N_3O$	224.0825
$C_{12}H_3N_2O_3$	223.0144	$C_{17}H_{19}$	223.1488	$C_{13}H_{12}N_4$	224.1063
$C_{12}H_{21}N_3O$	223.1686	$C_{17}H_3O$	223.0184	$C_{14}H_{24}O_2$	224.1777
$C_{12}H_5N_3O_2$	223.0382	$C_{17}H_5N$	223.0422	$C_{14}H_8O_3$	224.0473
$C_{12}H_{23}N_4$	223.1925	$C_{18}H_7$	223.0548	$C_{14}H_{26}NO$	224.2015
$C_{12}H_7N_4O$	223.1621	224		$C_{14}H_{10}NO_2$	224.0712
$C_{13}H_{19}O_3$	223.1334	$C_{10}H_{12}N_2O_4$	224.0797	$C_{14}H_{28}N_2$	224.2254

	FM		FM		FM
$C_{14}H_{12}N_2O$	224.0950	$C_{12}H_{17}O_4$	225.1127	$C_{15}H_3N_3$	225.0328
$C_{14}H_{14}N_3$	224.1189	$C_{12}H_{19}NO_3$	225.1365	$C_{16}H_{33}$	225.2584
$C_{14}N_4$	224.0124	$C_{12}H_3NO_4$	225.0062	$C_{16}H_{17}O$	225.1280
$C_{15}H_{28}O$	224.2141	$C_{12}H_{21}N_2O_2$	225.1604	$C_{16}HO_2$	224.9976
$C_{15}H_{12}O_2$	224.0837	$C_{12}H_5N_2O_3$	225.0300	$C_{16}H_{19}N$	225.1519
$C_{15}H_{30}N$	224.2380	$C_{12}H_{23}N_3O$	225.1842	$C_{16}H_3NO$	225.0215
$C_{15}H_{14}NO$	224.1076	$C_{12}H_7N_3O_2$	225.0539	$C_{16}H_5N_2$	225.0453
$C_{15}H_{16}N_2$	224.1315	$C_{12}H_{25}N_4$	225.2081	$C_{17}H_{21}$	225.1644
$C_{15}N_2O$	224.0011	$C_{12}H_9N_4O$	225.0777	$C_{17}H_5O$	225.0340
$C_{15}H_2N_3$	224.0249	$C_{13}H_{21}O_3$	225.1491	$C_{17}H_7N$	225.0579
$C_{16}H_{32}$	224.2505	$C_{13}H_5O_4$	225.0187	$C_{18}H_9$	225.0705
$C_{16}H_{16}O$	224.1202	$C_{13}H_{23}NO_2$	225.1730	226	
$C_{16}O_2$	223.9898	$C_{13}H_7NO_3$	225.0426	$C_{10}H_{14}N_2O_4$	226.0954
$C_{16}H_{18}N$	224.1440	$C_{13}H_{25}N_2O$	225.1968	$C_{10}H_{16}N_3O_3$	226.1193
$C_{16}H_2NO$	224.0136	$C_{13}H_9N_2O_2$	225.0664	$C_{10}H_{18}N_4O_2$	226.1431
$C_{16}H_4N_2$	224.0375	$C_{13}H_{27}N_3$	225.2207	$C_{11}H_{16}NO_4$	226.1080
$C_{17}H_{20}$	224.1566	$C_{13}H_{11}N_3O$	225.0903	$C_{11}H_{18}N_2O_3$	226.1318
$C_{17}H_4O$	224.0262	$C_{13}H_{13}N_4$	225.1142	$C_{11}H_2N_2O_4$	226.0014
$C_{17}H_6N$	224.0501	$C_{14}H_{25}O_2$	225.1855	$C_{11}H_{20}N_3O_2$	226.1557
$C_{18}H_8$	224.0626	$C_{14}H_9O_3$	225.0552	$C_{11}H_4N_3O_3$	226.0253
225		$C_{14}H_{27}NO$	225.2094	$C_{11}H_{22}N_4O$	226.1795
$C_{10}H_{13}N_2O_4$	225.0876	$C_{14}H_{11}NO_2$	225.0790	$C_{11}H_6N_4O_2$	226.0491
$C_{10}H_{15}N_3O_3$	225.1114	$C_{14}H_{29}N_2$	225.2332	$C_{12}H_{18}O_4$	226.1205
$C_{10}H_{17}N_4O_2$	225.1353	$C_{14}H_{13}N_2O$	225.1029	$C_{12}H_{20}NO_3$	226.1444
$C_{11}H_{15}NO_4$	225.1001	$C_{14}H_{15}N_3$	225.1267	$C_{12}H_4NO_4$	226.0140
$C_{11}H_{17}N_2O_3$	225.1240	$C_{14}HN_4$	225.0202	$C_{12}H_{22}N_2O_2$	226.1682
$C_{11}HN_2O_4$	224.9936	$C_{15}H_{29}O$	225.2219	$C_{12}H_6N_2O_3$	226.0379
$C_{11}H_{19}N_3O$	225.1478	$C_{15}H_{13}O_2$	225.0916	$C_{12}H_{24}N_3O$	226.1929
$C_{11}H_3N_3O_3$	225.0175	$C_{15}H_{31}N$	225.2458	$C_{12}H_8N_3O_2$	226.0617
$C_{11}H_{21}N_4O$	225.1717	$C_{15}H_{15}NO$	225.1154	$C_{12}H_{26}N_4$	226.2160
$C_{11}H_5N_4O_2$	225.0413	$C_{15}H_{17}N_2$	225.1393	$C_{12}H_{10}N_4O$	226.0856
$C_{11}HN_2O_4$	224.9936	$C_{15}HN_2O$	225.0089	$C_{13}H_{22}O_3$	226.1569

FM		FM		FM	
$C_{13}H_6O_4$	226.0266	$C_{17}H_6O$	226.0419	$C_{14}H_{27}O_2$	227.2012
$C_{13}H_{24}NO_2$	226.1808	$C_{17}H_8N$	226.0657	$C_{14}H_{11}O_3$	227.0708
$C_{13}H_8NO_3$	226.0504	$C_{18}H_{10}$	226.0783	$C_{14}H_{29}NO$	227.2250
$C_{13}H_{26}N_2O$	226.2046	227		$C_{14}H_{13}NO_2$	227.0947
$C_{13}H_{10}N_2O_2$	226.0743	$C_{10}H_{15}N_2O_4$	227.1032	$C_{14}H_{31}N_2$	227.2489
$C_{13}H_{28}N_3$	226.2285	$C_{10}H_{17}N_3O_3$	227.1271	$C_{14}H_{15}N_2O$	227.1185
$C_{13}H_{12}N_3O$	226.0981	$C_{10}H_{19}N_4O_2$	227.1509	$C_{14}H_{17}N_3$	227.1424
$C_{13}H_{14}N_4$	226.1220	$C_{11}H_{17}NO_4$	227.1158	$C_{14}HN_3O$	227.0120
$C_{14}H_{26}O_2$	226.1934	$C_{11}H_{19}N_2O_3$	227.1396	$C_{14}H_3N_4$	227.0359
$C_{14}H_{10}O_3$	226.0630	$C_{11}H_3N_2O_4$	227.0093	$C_{15}H_{31}O$	227.2376
$C_{14}H_{28}NO$	226.2172	$C_{11}H_{21}N_3O_2$	227.1635	$C_{15}H_{15}O_2$	227.1072
$C_{14}H_{12}NO_2$	226.0868	$C_{11}H_5N_3O_3$	227.0331	$C_{15}H_{33}N$	227.2615
$C_{14}H_{30}N_2$	226.2411	$C_{11}H_{23}N_4O$	227.1873	$C_{15}H_{17}NO$	227.1311
$C_{14}N_{14}N_2O$	226.1107	$C_{11}H_7N_4O_2$	227.0570	$C_{15}HNO_2$	227.0007
$C_{14}H_{16}N_3$	226.1346	$C_{12}H_{19}O_4$	227.1284	$C_{15}H_{19}N_2$	227.1549
$C_{14}N_3O$	226.0042	$C_{12}H_{21}NO_3$	227.1522	$C_{15}H_3N_2O$	227.0246
$C_{14}H_2N_4$	226.0280	$C_{12}H_5NO_4$	227.0218	$C_{15}H_5N_3$	227.0484
$C_{15}H_{30}$	226.2298	$C_{12}H_{23}N_2O_2$	227.1761	$C_{16}H_{19}O$	227.1436
$C_{15}H_{14}O_2$	226.0994	$C_{12}H_7N_2O_3$	227.0457	$C_{16}H_3O_2$	227.0133
$C_{15}H_{32}N$	226.2536	$C_{12}H_{25}N_3O$	227.1999	$C_{16}H_{21}N$	227.1675
$C_{15}H_{16}NO$	226.1233	$C_{12}H_9N_3O_2$	227.0695	$C_{16}H_5NO$	227.0371
$C_{15}NO_2$	225.9929	$C_{12}H_{27}N_4$	227.2238	$C_{16}H_7N_2$	227.0610
$C_{15}H_{18}N_2$	226.1471	$C_{12}H_{11}N_4O$	227.0934	$C_{17}H_{23}$	227.1801
$C_{15}H_2N_2O$	226.0167	$C_{13}H_{23}O_3$	227.1648	$C_{17}H_7O$	227.0497
$C_{15}H_4N_3$	226.0406	$C_{13}H_7O_4$	227.0344	$C_{17}H_9N$	227.0736
$C_{16}H_{34}$	226.2662	$C_{13}H_{25}NO_2$	227.1886	$C_{18}H_{11}$	227.0861
$C_{16}H_{18}O$	226.1358	$C_{13}H_9NO_3$	227.0583	228	
$C_{16}H_2O_2$	226.0054	$C_{13}H_{27}N_2O$	227.2125	$C_{10}H_{16}N_2O_4$	228.1111
$C_{16}H_{20}N$	226.1597	$C_{13}H_{11}N_2O_2$	227.0821	$C_{10}H_{18}N_3O_3$	228.1349
$C_{16}H_4NO$	226.0293	$C_{13}H_{29}N_3$	227.2363	$C_{10}H_{20}N_4O_2$	228.1588
$C_{16}H_6N_2$	226.0532	$C_{13}H_{13}N_3O$	227.1060	$C_{11}H_{18}NO_4$	228.1236
$C_{17}H_{22}$	226.1722	$C_{13}H_{15}N_4$	227.1298	$C_{11}H_{20}N_2O_3$	228.1475

FM		FM		FM	
$C_{11}H_4N_2O_4$	228.0171	$C_{14}H_2N_3O$	228.0198	$C_{12}H_{23}NO_3$	229.1679
$C_{11}H_{22}N_3O_2$	228.1713	$C_{14}H_4N_4$	228.0437	$C_{12}H_7NO_4$	229.0375
$C_{11}H_6N_3O_3$	228.0410	$C_{15}H_{32}O$	228.2454	$C_{12}H_{25}N_2O_2$	229.1917
$C_{11}H_{24}N_4O$	228.1952	$C_{15}H_{16}O_2$	228.1151	$C_{12}H_9N_2O_3$	229.0614
$C_{11}H_8N_4O_2$	228.0648	$C_{15}O_3$	227.9847	$C_{12}H_{27}N_3O$	229.2156
$C_{12}H_{20}O_4$	228.1362	$C_{15}H_{18}NO$	228.1389	$C_{12}H_{11}N_3O_2$	229.0852
$C_{12}H_{22}NO_3$	228.1600	$C_{15}H_2NO_2$	228.0085	$C_{12}H_{29}N_4$	229.2394
$C_{12}H_6NO_4$	228.0297	$C_{15}H_{20}N_2$	228.1628	$C_{12}H_{13}N_4O$	229.1091
$C_{12}H_{24}N_2O_2$	228.1839	$C_{15}H_4N_2O$	228.0324	$C_{13}H_{25}O_3$	229.1804
$C_{12}H_8N_2O_3$	228.0535	$C_{15}H_6N_3$	228.0563	$C_{13}H_9O_4$	229.0501
$C_{12}H_{26}N_3O$	228.2077	$C_{16}H_{20}O$	228.1515	$C_{13}H_{27}NO_2$	229.2043
$C_{12}H_{10}N_3O_2$	228.0774	$C_{16}H_4O_2$	228.0211	$C_{13}H_{11}NO_3$	229.0739
$C_{12}H_{28}N_4$	228.2316	$C_{16}H_{22}N$	228.1753	$C_{13}H_{29}N_2O$	229.2281
$C_{12}H_{12}N_4O$	228.1012	$C_{16}H_6NO$	228.0449	$C_{13}H_{13}N_2O_2$	229.0978
$C_{13}H_{24}O_3$	228.1726	$C_{16}H_8N_2$	228.0688	$C_{13}H_{31}N_3$	229.2520
$C_{13}H_8O_4$	228.0422	$C_{17}H_{24}$	228.1879	$C_{13}H_{15}N_3O$	229.1216
$C_{13}H_{26}NO_2$	228.1965	$C_{17}H_8O$	228.0575	$C_{13}H_{17}N_4$	229.1455
$C_{13}H_{10}NO_3$	228.0661	$C_{17}H_{10}N$	228.0814	$C_{13}HN_4O$	229.0151
$C_{13}H_{28}N_2O$	228.2203	$C_{18}H_{12}$	228.0939	$C_{14}H_{29}O_2$	229.2168
$C_{13}H_{12}N_2O_2$	228.0899	C_{19}	228.0000	$C_{14}H_{13}O_3$	229.0865
$C_{13}H_{30}N_3$	228.2442	229		$C_{14}H_{31}NO$	229.2407
$C_{13}H_{14}N_3O$	228.1138	$C_{10}H_{17}N_2O_4$	229.1189	$C_{14}H_{15}NO_2$	229.1103
$C_{13}H_{16}N_4$	228.1377	$C_{10}H_{19}N_3O_3$	229.1427	$C_{14}H_{17}N_2O$	229.1342
$C_{13}H_4O$	228.0073	$C_{10}H_{21}N_4O_2$	229.1666	$C_{14}HN_2O_2$	229.0038
$C_{14}H_{28}O_2$	228.2090	$C_{11}H_{19}NO_4$	229.1315	$C_{14}H_{19}N_3$	229.1580
$C_{14}H_{12}O_3$	228.0786	$C_{11}H_{21}N_2O_3$	229.1553	$C_{14}H_3N_3O$	229.0277
$C_{14}H_{30}NO$	228.2329	$C_{11}H_5N_2O_4$	229.0249	$C_{14}H_5N_4$	229.0515
$C_{14}H_{14}NO_2$	228.1025	$C_{11}H_{23}N_3O_2$	229.1791	$C_{15}H_{17}O_2$	229.1229
$C_{14}H_{32}N_2$	228.2567	$C_{11}H_7N_3O_3$	229.0488	$C_{15}HO_3$	228.9925
$C_{14}H_{16}N_2O$	228.1264	$C_{11}H_{25}N_4O$	229.2030	$C_{15}H_{19}NO$	229.1467
$C_{14}N_2O_2$	227.9960	$C_{11}H_9N_4O_2$	229.0726	$C_{15}H_3NO_2$	229.0164
$C_{14}H_{18}N_3$	228.1502	$C_{12}H_{21}O_4$	229.1440	$C_{15}H_{21}N_2$	229.1706

	FM		FM		FM
$C_{15}H_5N_2O$	229.0402	$C_{13}H_{26}O_3$	230.1883	$C_{17}H_{10}O$	230.0732
$C_{15}H_7N_3$	229.0641	$C_{13}H_{10}O_4$	230.0579	$C_{17}H_{12}N$	230.0970
$C_{16}H_{21}O$	229.1593	$C_{13}H_{28}NO_2$	230.2121	$C_{18}H_{14}$	230.1096
$C_{16}H_5O_2$	229.0289	$C_{13}H_{12}NO_3$	230.0817	$C_{18}N$	230.0031
$C_{16}H_{23}N$	229.1832	$C_{13}H_{30}N_2O$	230.2360	$C_{19}H_2$	230.0157
$C_{16}H_7NO$	229.0528	$C_{13}H_{14}N_2O_2$	230.1056	231	
$C_{16}H_9N_2$	229.0767	$C_{13}H_{16}N_3O$	230.1295	$C_{10}H_{19}N_2O_4$	231.1345
$C_{17}H_{25}$	229.1957	$C_{13}N_3O_2$	229.9991	$C_{10}H_{21}N_3O_3$	231.1584
$C_{17}H_{11}N$	229.0892	$C_{13}H_{18}N_4$	230.1533	$C_{10}H_{23}N_4O_2$	231.1822
$C_{17}H_9O$	229.0653	$C_{13}H_2N_4O$	230.0229	$C_{11}H_{21}NO_4$	231.1471
$C_{18}H_{13}$	229.1018	$C_{14}H_{30}O_2$	230.2247	$C_{11}H_{23}N_2O_3$	231.1710
$C_{19}H$	229.0078	$C_{14}H_{14}O_3$	230.0943	$C_{11}H_7N_2O_4$	231.0406
230		$C_{14}H_{16}NO_2$	230.1182	$C_{11}H_{25}N_3O_2$	231.1948
$C_{10}H_{18}N_2O_4$	230.1267	$C_{14}NO_3$	229.9878	$C_{11}H_9N_3O_3$	231.0644
$C_{10}H_{20}N_3O_3$	230.1506	$C_{14}H_{18}N_2O$	230.1420	$C_{11}H_{27}N_4O$	231.2187
$C_{10}H_{22}N_4O_2$	230.1744	$C_{14}H_2N_2O_2$	230.0116	$C_{11}H_{11}N_4O_2$	231.0883
$C_{11}H_{20}NO_4$	230.1393	$C_{14}H_{20}N_3$	230.1659	$C_{12}H_{23}O_4$	231.1597
$C_{11}H_{22}N_2O_3$	230.1631	$C_{14}H_4N_3O$	230.0355	$C_{12}H_{25}NO_3$	231.1835
$C_{11}H_6N_2O_4$	230.0328	$C_{14}H_6N_4$	230.0594	$C_{12}H_9NO_4$	231.0532
$C_{11}H_{24}N_3O_2$	230.1870	$C_{15}H_{18}O_2$	230.1307	$C_{12}H_{27}N_2O_2$	231.2074
$C_{11}H_8N_3O_3$	230.0566	$C_{15}H_2O_3$	230.0003	$C_{12}H_{11}N_2O_3$	231.0770
$C_{11}H_{26}N_4O$	230.2108	$C_{15}H_{20}NO$	230.1546	$C_{12}H_{29}N_3O$	231.2312
$C_{11}H_{10}N_4O_2$	230.0805	$C_{15}H_4NO_2$	230.0242	$C_{12}H_{13}N_3O_2$	231.1009
$C_{12}H_{22}O_4$	230.1518	$C_{15}H_{22}N_2$	230.1784	$C_{12}H_{15}N_4O$	231.1247
$C_{12}H_{24}NO_3$	230.1757	$C_{15}H_6N_2O$	230.0480	$C_{13}H_{27}O_3$	231.1961
$C_{12}H_8NO_4$	230.0453	$C_{15}H_8N_3$	230.0719	$C_{13}H_{11}O_4$	231.0657
$C_{12}H_{26}N_2O_2$	230.1996	$C_{16}H_{22}O$	230.1671	$C_{13}H_{29}NO_2$	231.2199
$C_{12}H_{10}N_2O_3$	230.0692	$C_{16}H_6O_2$	230.0368	$C_{13}H_{13}NO_3$	231.0896
$C_{12}H_{28}N_3O$	230.2234	$C_{16}H_{24}N$	230.1910	$C_{13}H_{15}N_2O_2$	231.1134
$C_{12}H_{12}N_3O_2$	230.0930	$C_{16}H_8NO$	230.0606	$C_{13}H_{17}N_3O$	231.1373
$C_{12}H_{30}N_4$	230.2473	$C_{16}H_{10}N_2$	230.0845	$C_{13}HN_3O_2$	231.0069
$C_{12}H_{14}N_4O$	230.1169	$C_{17}H_{26}$	230.2036	$C_{13}H_{19}N_4$	231.1611

FM		FM		FM	
$C_{13}H_3N_4O$	231.0308	$C_{11}H_{24}N_2O_3$	232.1788	$C_{15}H_{20}O_2$	232.1464
$C_{14}H_{15}O_3$	231.1021	$C_{11}H_8N_2O_4$	232.0484	$C_{15}H_4O_3$	232.0160
$C_{14}H_{17}NO_2$	231.1260	$C_{11}H_{26}N_3O_2$	232.2026	$C_{15}H_{22}NO$	232.1702
$C_{14}HNO_3$	230.9956	$C_{11}H_{10}N_3O_3$	232.0723	$C_{15}H_6NO_2$	232.0399
$C_{14}H_{19}N_2O$	231.1498	$C_{11}H_{28}N_4O$	232.2265	$C_{15}H_{24}N_2$	232.1941
$C_{14}H_3N_2O_2$	231.0195	$C_{11}H_{12}N_4O_2$	232.0961	$C_{15}H_8N_2O$	232.0637
$C_{14}H_{21}N_3$	231.1737	$C_{12}H_{24}O_4$	232.1675	$C_{15}H_{10}N_3$	232.0876
$C_{14}H_5N_3O$	231.0433	$C_{12}H_{26}NO_3$	232.1914	$C_{16}H_{24}O$	232.1828
$C_{14}H_7N_4$	231.0672	$C_{12}H_{10}NO_4$	232.0610	$C_{16}H_8O_2$	232.0524
$C_{15}H_{19}O_2$	231.1385	$C_{12}H_{28}N_2O_2$	232.2152	$C_{16}H_{26}N$	232.2067
$C_{15}H_3O_3$	231.0082	$C_{12}H_{12}N_2O_3$	232.0848	$C_{16}H_{10}NO$	232.0768
$C_{15}H_{21}NO$	231.1624	$C_{12}H_{14}N_3O_2$	232.1087	$C_{16}H_{12}N_2$	232.1001
$C_{15}H_5NO_2$	231.0320	$C_{12}H_{16}N_4O$	232.1325	$C_{17}H_{28}$	232.2192
$C_{15}H_{23}N_2$	231.1863	$C_{12}N_4O_2$	232.0022	$C_{17}H_{12}O$	232.0888
$C_{15}H_7N_2O$	231.0559	$C_{13}H_{28}O_3$	232.2039	$C_{17}H_{14}N$	232.1127
$C_{15}H_9N_3$	231.0798	$C_{13}H_{12}O_4$	232.0735	$C_{17}N_2$	232.0062
$C_{16}H_{23}O$	291.1750	$C_{13}H_{14}NO_3$	232.0974	$C_{18}H_{16}$	232.1253
$C_{16}H_7O_2$	231.0446	$C_{13}H_{16}N_2O_2$	232.1213	$C_{18}O$	231.9949
$C_{16}H_{25}N$	231.1988	$C_{13}N_2O_3$	231.9909	$C_{18}H_2N$	232.0187
$C_{16}H_9NO$	231.0684	$C_{13}H_{18}N_3O$	232.1451	$C_{19}H_4$	232.0313
$C_{16}H_{11}N_2$	231.0923	$C_{13}H_2N_3O_2$	232.0147	233	
$C_{17}H_{27}$	231.2114	$C_{13}H_{20}N_4$	232.1690	$C_{10}H_{21}N_2O_4$	233.1502
$C_{17}H_{11}O$	231.0810	$C_{13}H_4N_4O$	232.0386	$C_{10}H_{23}N_3O_3$	233.1741
$C_{17}H_{13}N$	231.1049	$C_{14}H_{16}O_3$	232.1100	$C_{10}H_{25}N_4O_2$	233.1979
$C_{18}H_{15}$	231.1174	$C_{14}O_4$	231.9796	$C_{11}H_{23}NO_4$	233.1628
$C_{18}HN$	231.0109	$C_{14}H_{18}NO_2$	232.1338	$C_{11}H_{25}N_2O_3$	233.1866
$C_{19}H_3$	231.0235	$C_{14}H_2NO_3$	232.0034	$C_{11}H_9N_2O_4$	233.0563
232		$C_{14}H_{20}N_2O$	232.1577	$C_{11}H_{27}N_3O_2$	233.2105
$C_{10}H_{20}N_2O_4$	232.1424	$C_{14}H_4N_2O_2$	232.0273	$C_{11}H_{11}N_3O_3$	233.0801
$C_{10}H_{22}N_3O_3$	232.1662	$C_{14}H_{22}N_3$	232.1815	$C_{11}H_{13}N_4O_2$	233.1040
$C_{10}H_{24}N_4O_2$	232.1901	$C_{14}H_6N_3O$	232.0511	$C_{12}H_{25}O_4$	233.1753
$C_{11}H_{22}NO_4$	232.1549	$C_{14}H_8N_4$	232.0750	$C_{12}H_{27}NO_3$	233.1992

FM		FM		FM	
$C_{12}H_{11}NO_4$	233.0688	$C_{16}H_{11}NO$	233.0841	$C_{13}H_4N_3O_2$	234.0304
$C_{12}H_{13}N_2O_3$	233.0927	$C_{16}H_{13}N_2$	233.1080	$C_{13}H_{22}N_4$	234.1846
$C_{12}H_{15}N_3O_2$	233.1165	$C_{17}H_{29}$	233.2270	$C_{13}H_6N_4O$	234.0542
$C_{12}H_{17}N_4O$	233.1404	$C_{17}H_{13}O$	233.0967	$C_{14}H_{18}O_3$	234.1256
$C_{12}HN_4O_2$	233.0100	$C_{17}H_{15}N$	233.1205	$C_{14}H_2O_4$	233.9953
$C_{13}H_{13}O_4$	233.0814	$C_{17}HN_2$	233.0140	$C_{14}H_{20}NO_2$	234.1495
$C_{13}H_{15}NO_3$	233.1052	$C_{18}H_{17}$	233.1331	$C_{14}H_4NO_3$	234.0191
$C_{13}H_{17}N_2O_2$	233.1291	$C_{18}HO$	233.0027	$C_{14}H_{22}N_2O$	234.1733
$C_{13}HN_2O_3$	232.9987	$C_{18}H_3N$	233.0266	$C_{14}H_6N_2O_2$	234.0429
$C_{13}H_{19}N_3O$	233.1529	$C_{19}H_5$	233.0391	$C_{14}H_{24}N_3$	234.1972
$C_{13}H_3N_3O_2$	233.0226	234		$C_{14}H_8N_3O$	234.0668
$C_{13}H_{21}N_4$	233.1768	$C_{10}H_{22}N_2O_4$	234.1580	$C_{14}H_{10}N_4$	234.0907
$C_{13}H_5N_4O$	233.0464	$C_{10}H_{24}N_3O_3$	234.1819	$C_{15}H_{22}O_2$	234.1620
$C_{14}H_{17}O_3$	233.1178	$C_{10}H_{26}N_4O_2$	234.2057	$C_{15}H_6O_3$	234.0317
$C_{14}HO_4$	232.9874	$C_{11}H_{24}NO_4$	234.1706	$C_{15}H_{24}NO$	234.1859
$C_{14}H_{19}NO_2$	233.1416	$C_{11}H_{26}N_2O_3$	234.1945	$C_{15}H_8NO_2$	234.0555
$C_{14}H_3NO_3$	233.0113	$C_{11}H_{10}N_2O_4$	234.0641	$C_{15}H_{26}N_2$	234.2098
$C_{14}H_{21}N_2O$	233.1655	$C_{11}H_{12}N_3O_3$	234.0879	$C_{15}H_{10}N_2O$	234.0794
$C_{14}H_5N_2O_2$	233.0351	$C_{11}H_{14}N_4O_2$	234.1118	$C_{15}H_{12}N_3$	234.1032
$C_{14}H_{23}N_3$	233.1894	$C_{12}H_{26}O_4$	234.1832	$C_{16}H_{26}O$	234.1985
$C_{14}H_7N_3O$	233.0590	$C_{12}H_{12}NO_4$	234.0766	$C_{16}H_{10}O_2$	234.0681
$C_{14}H_9N_4$	233.0829	$C_{12}H_{14}N_2O_3$	234.1005	$C_{16}H_{28}N$	234.2223
$C_{15}H_{21}O_2$	233.1542	$C_{12}H_{16}N_3O_2$	234.1244	$C_{16}H_{12}NO$	234.0919
$C_{15}H_5O_3$	233.0238	$C_{12}N_3O_3$	233.9940	$C_{16}H_{14}N_2$	234.1158
$C_{15}H_{23}NO$	233.1781	$C_{12}H_{18}N_4O$	234.1482	$C_{16}N_3$	234.0093
$C_{15}H_7NO_2$	233.0477	$C_{12}H_2N_4O_2$	234.0178	$C_{17}H_{30}$	234.2349
$C_{15}H_{25}N_2$	233.2019	$C_{13}H_{14}O_4$	234.0892	$C_{17}H_{14}O$	234.1045
$C_{15}H_9N_2O$	233.0715	$C_{13}H_{16}NO_3$	234.1131	$C_{17}H_{16}N$	234.1284
$C_{15}H_{11}N_3$	233.0954	$C_{13}NO_4$	233.9827	$C_{17}NO$	233.9980
$C_{16}H_{25}O$	233.1906	$C_{13}H_{18}N_2O_2$	234.1369	$C_{17}H_2N_2$	234.0218
$C_{16}H_9O_2$	233.0603	$C_{13}H_2N_2O_3$	234.0065	$C_{18}H_{18}$	234.1409
$C_{16}H_{27}N$	233.2145	$C_{13}H_{20}N_3O$	234.1608	$C_{18}H_2O$	234.0106

FM		FM		FM	
$C_{18}H_4N$	234.0344	$C_{14}H_{11}N_4$	235.0985	$C_{12}H_2N_3O_3$	236.0096
$C_{19}H_6$	234.0470	$C_{15}H_{23}O_2$	235.1699	$C_{12}H_{20}N_4O$	236.1639
235		$C_{15}H_7O_3$	235.0395	$C_{12}H_4N_4O_2$	236.0335
$C_{10}H_{23}N_2O_4$	235.1659	$C_{15}H_{25}NO$	235.1937	$C_{13}H_{16}O_4$	236.1049
$C_{10}H_{25}N_3O_3$	235.1897	$C_{15}H_9NO_2$	235.0634	$C_{13}H_{18}NO_3$	236.1287
$C_{11}H_{25}NO_4$	235.1784	$C_{15}H_{27}N_2$	235.2176	$C_{13}H_2NO_4$	235.9983
$C_{11}H_{11}N_2O_4$	235.0719	$C_{15}H_{11}N_2O$	235.0872	$C_{13}H_{20}N_2O_2$	236.1526
$C_{11}H_{13}N_3O_3$	235.0958	$C_{15}H_{13}N_3$	235.1111	$C_{13}H_4N_2O_3$	236.0222
$C_{11}H_{15}N_4O_2$	235.1196	$C_{16}H_{27}O$	235.2063	$C_{13}H_{22}N_3O$	236.1764
$C_{12}H_{13}NO_4$	235.0845	$C_{16}H_{11}O_2$	235.0759	$C_{13}H_6N_3O_2$	236.0460
$C_{12}H_{15}N_2O_3$	235.1083	$C_{16}H_{29}N$	235.2301	$C_{13}H_{24}N_4$	236.2003
$C_{12}H_{17}N_3O_2$	235.1322	$C_{16}H_{13}NO$	235.0998	$C_{13}H_8N_4O$	236.0699
$C_{12}HN_3O_3$	235.0018	$C_{16}H_{15}N_2$	235.1236	$C_{14}H_{20}O_3$	236.1413
$C_{12}H_{19}N_4O$	235.1560	$C_{16}HN_3$	235.0171	$C_{14}H_4O_4$	236.0109
$C_{12}H_3N_4O_2$	235.0257	$C_{17}H_{31}$	235.2427	$C_{14}H_{22}NO_2$	236.1651
$C_{13}H_{15}O_4$	235.0970	$C_{17}H_{15}O$	235.1123	$C_{14}H_6NO_3$	236.0348
$C_{13}H_{17}NO_3$	235.1209	$C_{17}H_{17}N$	235.1362	$C_{14}H_{24}N_2O$	236.1890
$C_{13}HNO_4$	234.9905	$C_{17}HNO$	235.0058	$C_{14}H_8N_2O_2$	236.0586
$C_{13}H_{19}N_2O_2$	235.1447	$C_{17}H_3N_2$	235.0297	$C_{14}H_{26}N_3$	236.2129
$C_{13}H_3N_2O_3$	235.0144	$C_{18}H_{19}$	235.1488	$C_{14}H_{10}N_3O$	236.0825
$C_{13}H_{21}N_3O$	235.1686	$C_{18}H_3O$	235.0184	$C_{14}H_{12}N_4$	236.1063
$C_{13}H_5N_3O_2$	235.0382	$C_{18}H_5N$	235.0422	$C_{15}H_{24}O_2$	236.1777
$C_{13}H_{23}N_4$	235.1925	$C_{19}H_7$	235.0548	$C_{15}H_8O_3$	236.0473
$C_{13}H_7N_4O$	235.0621	236		$C_{15}H_{26}NO$	236.2015
$C_{14}H_{19}O_3$	235.1334	$C_{10}H_{24}N_2O_4$	236.1737	$C_{15}H_{10}NO_2$	236.0712
$C_{14}H_3O_4$	235.0031	$C_{11}H_{12}N_2O_4$	236.0797	$C_{15}H_{28}N_2$	236.2254
$C_{14}H_{21}NO_2$	235.1573	$C_{11}H_{14}N_3O_3$	236.1036	$C_{15}H_{12}N_2O$	236.0950
$C_{14}H_5NO_3$	235.0269	$C_{11}H_{16}N_4O_2$	236.1275	$C_{15}H_{14}N_3$	236.1189
$C_{14}H_{23}N_2O_2$	235.1811	$C_{12}H_{14}NO_4$	236.0923	$C_{15}N_4$	236.0124
$C_{14}H_7N_2O_2$	235.0508	$C_{12}H_{16}N_2O_3$	236.1162	$C_{16}H_{28}O$	236.2141
$C_{14}H_{25}N_3$	235.2050	$C_{12}N_2O_4$	235.9858	$C_{16}H_{12}O_2$	236.0837
$C_{14}H_9N_3O$	235.0746	$C_{12}H_{18}N_3O_2$	236.1400	$C_{16}H_{30}N$	236.2380

	FM		FM		FM
$C_{16}H_{14}NO$	236.1076	$C_{13}H_{25}N_4$	237.2081	$C_{18}H_{21}$	237.1644
$C_{16}H_{16}N_2$	236.1315	$C_{13}H_9N_4O$	237.0777	$C_{18}H_5O$	237.0340
$C_{16}N_2O$	236.0011	$C_{14}H_{21}O_3$	237.1491	$C_{18}H_7N$	237.0579
$C_{16}H_2N_3$	236.0249	$C_{14}H_5O_4$	237.0187	$C_{19}H_9$	237.0705
$C_{17}H_{32}$	236.2505	$C_{14}H_{23}NO_2$	237.1730	238	
$C_{17}H_{16}O$	236.1202	$C_{14}H_7NO_3$	237.0426	$C_{11}H_{14}N_2O_4$	238.0954
$C_{17}O_2$	235.9898	$C_{14}H_{25}N_2O$	237.1968	$C_{11}H_{16}N_3O_3$	238.1193
$C_{17}H_{18}N$	236.1440	$C_{14}H_9N_2O_2$	237.0664	$C_{11}H_{18}N_4O_2$	238.1431
$C_{17}H_2NO$	236.0136	$C_{14}H_{27}N_3$	237.2207	$C_{12}H_{16}NO_4$	238.1080
$C_{17}H_4N_2$	236.0375	$C_{14}H_{11}N_3O$	237.0903	$C_{12}H_{18}N_2O_3$	238.1318
$C_{18}H_{20}$	236.1566	$C_{14}H_{13}N_4$	237.1142	$C_{12}H_2N_2O_4$	238.0014
$C_{18}H_4O$	236.0262	$C_{15}H_{25}O_2$	237.1855	$C_{12}H_{20}N_3O_2$	238.1557
$C_{18}H_6N$	236.0501	$C_{15}H_9O_3$	237.0552	$C_{12}H_4N_3O_3$	238.0253
$C_{19}H_8$	236.0626	$C_{15}H_{27}NO$	237.2094	$C_{12}H_{22}N_4O$	238.1795
237		$C_{15}H_{11}NO_2$	237.0790	$C_{12}H_6N_4O_2$	238.0491
$C_{11}H_{13}N_2O_4$	237.0876	$C_{15}H_{29}N_2$	237.2332	$C_{13}H_{18}O_4$	238.1205
$C_{11}H_{15}N_3O_3$	237.1114	$C_{15}H_{13}N_2O$	237.1029	$C_{13}H_{20}NO_3$	238.1444
$C_{11}H_{17}N_4O_2$	237.1353	$C_{15}H_{15}N_3$	237.1267	$C_{13}H_4NO_4$	238.0140
$C_{12}H_{15}NO_4$	237.1001	$C_{15}HN_4$	237.0202	$C_{13}H_{22}N_2O_2$	238.1682
$C_{12}H_{17}N_2O_3$	237.1240	$C_{16}H_{29}O$	237.2219	$C_{13}H_6N_2O_3$	238.0379
$C_{12}HN_2O_4$	236.9936	$C_{16}H_{13}O_2$	237.0916	$C_{13}H_{24}N_3O$	238.1921
$C_{12}H_{19}N_3O_2$	237.1478	$C_{16}H_{31}N$	237.2458	$C_{13}H_8N_3O_2$	238.0617
$C_{12}H_3N_3O_3$	237.0175	$C_{16}H_{15}NO$	237.1154	$C_{13}H_{26}N_4$	238.2160
$C_{12}H_{21}N_4O$	237.1717	$C_{16}H_{17}N_2$	237.1393	$C_{13}H_{10}N_4O$	238.0856
$C_{12}H_5N_4O_2$	237.0413	$C_{16}HN_2O$	237.0089	$C_{14}H_{22}O_3$	238.1569
$C_{13}H_{17}O_4$	237.1127	$C_{16}H_3N_3$	237.0328	$C_{14}H_6O_4$	238.0266
$C_{13}H_{19}NO_3$	237.1365	$C_{17}H_{33}$	237.2584	$C_{14}H_{24}NO_2$	238.1808
$C_{13}H_3NO_4$	237.0062	$C_{17}H_{17}O$	237.1280	$C_{14}H_8NO_3$	238.0504
$C_{13}H_{21}N_2O_2$	237.1604	$C_{17}HO_2$	236.9976	$C_{14}H_{26}N_2O$	238.2046
$C_{13}H_5N_2O_3$	237.0300	$C_{17}H_{19}N$	237.1519	$C_{14}H_{10}N_2O_2$	238.0743
$C_{13}H_{23}N_3O$	237.1842	$C_{17}H_3NO$	237.0215	$C_{14}H_{28}N_3$	238.2285
$C_{13}H_7N_3O_2$	237.0539	$C_{17}H_5N_2$	237.0453	$C_{14}H_{12}N_3O$	238.0981

FM		FM		FM	
$C_{14}H_{14}N_4$	238.1220	$C_{12}H_{17}NO_4$	239.1158	$C_{15}HN_3O$	239.0120
$C_{15}H_{26}O_2$	238.1934	$C_{12}H_{19}N_2O_3$	239.1396	$C_{15}H_3N_4$	239.0359
$C_{15}H_{10}O_3$	238.0630	$C_{12}H_3N_2O_4$	239.0093	$C_{16}H_{31}O$	239.2376
$C_{15}H_{28}NO$	238.2172	$C_{12}H_{21}N_3O_2$	239.1635	$C_{16}H_{15}O_2$	239.1072
$C_{15}H_{12}NO_2$	238.0868	$C_{12}H_5N_3O_3$	239.0331	$C_{16}H_{33}N$	239.2615
$C_{15}H_{30}N_2$	238.2411	$C_{12}H_{23}N_4O$	239.1873	$C_{16}H_{17}NO$	239.1311
$C_{15}H_{14}N_2O$	238.1107	$C_{12}H_7N_4O_2$	239.0570	$C_{16}HNO_2$	239.0007
$C_{15}H_{16}N_3$	238.1346	$C_{13}H_{19}O_4$	239.1284	$C_{16}H_{19}N_2$	239.1549
$C_{15}N_3O$	238.0042	$C_{13}H_{21}NO_3$	239.1522	$C_{16}H_3N_2O$	239.0246
$C_{15}H_2N_4$	238.0280	$C_{13}H_5NO_4$	239.0218	$C_{16}H_5N_3$	239.0484
$C_{16}H_{30}O$	238.2298	$C_{13}H_{23}N_2O_2$	239.1761	$C_{17}H_{35}$	239.2740
$C_{16}H_{14}O_2$	238.0994	$C_{13}H_7N_2O_3$	239.0457	$C_{17}H_{19}O$	239.1436
$C_{16}H_{32}N$	238.2536	$C_{13}H_{25}N_3O$	239.1999	$C_{17}H_3O_2$	239.0133
$C_{16}H_{16}NO$	238.1233	$C_{13}H_9N_3O_2$	239.0695	$C_{17}H_{21}N$	239.1675
$C_{16}NO_2$	237.9929	$C_{13}H_{27}N_4$	239.2238	$C_{17}H_5NO$	239.0371
$C_{16}H_{18}N_2$	238.1471	$C_{13}H_{11}N_4O$	239.0934	$C_{17}H_7N_2$	239.0610
$C_{16}H_2N_2O$	238.0167	$C_{14}H_{23}O_3$	239.1648	$C_{18}H_{23}$	239.1801
$C_{16}H_4N_3$	238.0406	$C_{14}H_7O_4$	239.0344	$C_{18}H_7O$	239.0497
$C_{17}H_{34}$	238.2662	$C_{14}H_{25}NO_2$	239.1886	$C_{18}H_9N$	239.0736
$C_{17}H_{18}O$	238.1358	$C_{14}H_9NO_3$	239.0583	$C_{19}H_{11}$	239.0861
$C_{17}H_2O_2$	238.0054	$C_{14}H_{27}N_2O$	239.2125	240	
$C_{17}H_{20}N$	238.1597	$C_{14}H_{11}N_2O_2$	239.0821	$C_{11}H_{16}N_2O_4$	240.1111
$C_{17}H_4NO$	238.0293	$C_{14}H_{29}N_3$	239.2363	$C_{11}H_{18}N_3O_3$	240.1349
$C_{17}H_6N_2$	238.0532	$C_{14}H_{13}N_3O$	239.1060	$C_{11}H_{20}N_4O_2$	240.1588
$C_{18}H_{22}$	238.1722	$C_{14}H_{15}N_4$	239.1298	$C_{12}H_{18}NO_4$	240.1236
$C_{18}H_6O$	238.0419	$C_{15}H_{27}O_2$	239.2012	$C_{12}H_{20}N_2O_3$	240.1475
$C_{18}H_8N$	238.0657	$C_{15}H_{11}O_3$	239.0708	$C_{12}H_4N_2O_4$	240.0171
$C_{19}H_{10}$	238.0783	$C_{15}H_{29}NO$	239.2250	$C_{12}H_{22}N_3O_2$	240.1713
239		$C_{15}H_{13}NO_2$	239.0947	$C_{12}H_6N_3O_3$	240.0410
$C_{11}H_{15}N_2O_4$	239.1032	$C_{15}H_{31}N_2$	239.2489	$C_{12}H_{24}N_4O$	240.1952
$C_{11}H_{17}N_3O_3$	239.1271	$C_{15}H_{15}N_2O$	239.1185	$C_{12}H_8N_4O_2$	240.0648
$C_{11}H_{19}N_4O_2$	239.1509	$C_{15}H_{17}N_3$	239.1424	$C_{13}H_{20}O_4$	240.1362

	FM		FM		FM
$C_{13}H_{22}NO_3$	240.1600	$C_{16}H_{18}NO$	240.1389	$C_{13}H_{27}N_3O$	241.2156
$C_{13}H_6NO_4$	240.0297	$C_{16}H_2NO_2$	240.0085	$C_{13}H_{11}N_3O_2$	241.0852
$C_{13}H_{24}N_2O_2$	240.1839	$C_{16}H_{20}N_2$	240.1628	$C_{13}H_{29}N_4$	241.2394
$C_{13}H_8N_2O_3$	240.0535	$C_{16}H_4N_2O$	240.0324	$C_{13}H_{13}N_4O$	241.1091
$C_{13}H_{26}N_3O$	240.2077	$C_{16}H_6N_3$	240.0563	$C_{14}H_{25}O_3$	241.1804
$C_{13}H_{10}N_3O_2$	240.0774	$C_{17}H_{36}$	240.2819	$C_{14}H_9O_4$	241.0501
$C_{13}H_{28}N_4$	240.2316	$C_{17}H_{20}O$	240.1515	$C_{14}H_{27}NO_2$	241.2043
$C_{13}H_{12}N_4O$	240.1012	$C_{17}H_4O_2$	240.0211	$C_{14}H_{11}NO_3$	241.0739
$C_{14}H_{24}O_3$	240.1726	$C_{17}H_{22}N$	240.1753	$C_{14}H_{29}N_2O$	241.2281
$C_{14}H_8O_4$	240.0422	$C_{17}H_6NO$	240.0449	$C_{14}H_{13}N_2O_2$	241.0978
$C_{14}H_{26}NO_2$	240.1965	$C_{17}H_8N_2$	240.0688	$C_{14}H_{31}N_3$	241.2520
$C_{14}H_{10}NO_3$	240.0661	$C_{18}H_{24}$	240.1879	$C_{14}H_{15}N_3O$	241.1216
$C_{14}H_{28}N_2O$	240.2203	$C_{18}H_8O$	240.0575	$C_{14}H_{17}N_4$	241.1455
$C_{14}H_{12}N_2O_2$	240.0899	$C_{18}H_{10}N$	240.0814	$C_{14}HN_4O$	241.0151
$C_{14}H_{30}N_3$	240.2442	$C_{19}H_{12}$	240.0939	$C_{15}H_{29}O_2$	241.2168
$C_{14}H_{14}N_3O$	240.1138	C_{20}	240.0000	$C_{15}H_{13}O_3$	241.0865
$C_{14}H_{16}N_4$	240.1377	241		$C_{15}H_{31}NO$	241.2407
$C_{14}N_4O$	240.0073	$C_{11}H_{17}N_2O_4$	241.1189	$C_{15}H_{15}NO_2$	241.1103
$C_{15}H_{28}O_2$	240.2090	$C_{11}H_{19}N_3O_3$	241.1427	$C_{15}H_{33}N_2$	241.2646
$C_{15}H_{12}O_3$	240.0786	$C_{11}H_{21}N_4O_2$	241.1666	$C_{15}H_{17}N_2O$	241.1342
$C_{15}H_{30}NO$	240.2329	$C_{12}H_{19}NO_4$	241.1315	$C_{15}HN_2O_2$	241.0038
$C_{15}H_{14}NO_2$	240.1015	$C_{12}H_{21}N_2O_3$	241.1553	$C_{15}H_{19}N_3$	241.1580
$C_{15}H_{32}N_2$	240.2567	$C_{12}H_5N_2O_4$	241.0249	$C_{15}H_3N_3O$	241.0277
$C_{15}H_{16}N_2O$	240.1264	$C_{12}H_{23}N_3O_2$	241.1791	$C_{15}H_5N_4$	241.0515
$C_{15}N_2O_2$	239.9960	$C_{12}H_7N_3O_3$	241.0488	$C_{16}H_{33}O$	241.2533
$C_{15}H_{18}N_3$	240.1502	$C_{12}H_{25}N_4O$	241.2030	$C_{16}H_{17}O_2$	241.1229
$C_{15}H_2N_3O$	240.0198	$C_{12}H_9N_4O_2$	241.0726	$C_{16}HO_3$	240.9925
$C_{15}H_4N_4$	240.0437	$C_{13}H_{21}O_4$	241.1440	$C_{16}H_{35}N$	241.2771
$C_{16}H_{32}O$	240.2454	$C_{13}H_{23}NO_3$	241.1679	$C_{16}H_{19}NO$	241.1467
$C_{16}H_{16}O_2$	240.1151	$C_{13}H_7NO_4$	241.0375	$C_{16}H_{13}NO_2$	241.0164
$C_{16}O_3$	239.9847	$C_{13}H_{25}N_2O_2$	241.1917	$C_{16}H_{21}N_2$	241.1706
$C_{16}H_{34}N$	240.2693	$C_{13}H_9N_2O_3$	241.0614	$C_{16}H_5N_2O$	241.0402

	FM		FM		FM
$C_{16}H_7N_3$	241.0641	$C_{14}H_{10}O_4$	242.0579	$C_{17}H_8NO$	242.0606
$C_{17}H_{21}O$	241.1593	$C_{14}H_{28}NO_2$	242.2121	$C_{17}H_{10}N_2$	242.0845
$C_{17}H_5O_2$	241.0289	$C_{14}H_{12}NO_3$	242.0817	$C_{18}H_{26}$	242.2036
$C_{17}H_{23}N$	241.1832	$C_{14}H_{30}N_2O$	242.2360	$C_{18}H_{10}O$	242.0732
$C_{17}H_7NO$	241.0528	$C_{14}H_{14}N_2O_2$	242.1056	$C_{18}H_{12}N$	242.0970
$C_{17}H_9N_2$	241.0767	$C_{14}H_{32}N_3$	242.2598	$C_{19}H_{14}$	242.1096
$C_{18}H_{25}$	241.1957	$C_{14}H_{16}N_3O$	242.1295	$C_{19}N$	242.0031
$C_{18}H_9O$	241.0653	$C_{14}N_3O_2$	241.9991	$C_{20}H_2$	242.0157
$C_{18}H_{11}N$	241.0892	$C_{14}H_{18}N_4$	242.1533	243	
$C_{19}H_{13}$	241.1018	$C_{14}H_{22}N_4O$	242.0229	$C_{11}H_{19}N_2O_4$	243.1345
$C_{20}H$	241.0078	$C_{15}H_{30}O_2$	242.2247	$C_{11}H_{21}N_3O_3$	243.1584
242		$C_{15}H_{14}O_3$	242.0943	$C_{11}H_{23}N_4O_2$	243.1822
$C_{11}H_{18}N_2O_4$	242.1267	$C_{15}H_{32}NO$	242.2485	$C_{12}H_{21}NO_4$	243.1471
$C_{11}H_{20}N_3O_3$	242.1506	$C_{15}H_{16}NO_2$	242.1182	$C_{12}H_{23}N_2O_3$	243.1710
$C_{11}H_{22}N_4O_2$	242.1744	$C_{15}NO_3$	241.9878	$C_{12}H_7N_2O_4$	243.0406
$C_{12}H_{20}NO_4$	242.1393	$C_{15}H_{34}N_2$	242.2724	$C_{12}H_{25}N_3O_2$	243.1948
$C_{12}H_{22}N_2O_3$	242.1631	$C_{15}H_{18}N_2O$	242.1420	$C_{12}H_9N_3O_3$	243.0644
$C_{12}H_6N_2O_4$	242.0328	$C_{15}H_2N_2O_2$	242.0116	$C_{12}H_{27}N_4O$	243.2187
$C_{12}H_{24}N_3O_2$	242.1870	$C_{15}H_{20}N_3$	242.1659	$C_{12}H_{11}N_4O_2$	243.0883
$C_{12}H_8N_3O_3$	242.0566	$C_{15}H_4N_3O$	242.0355	$C_{13}H_{23}O_4$	243.1597
$C_{12}H_{26}N_4O$	242.2108	$C_{15}H_6N_4$	242.0594	$C_{13}H_{25}NO_3$	243.1835
$C_{12}H_{10}N_4O_2$	242.0805	$C_{16}H_{34}O$	242.2611	$C_{13}H_9NO_4$	243.0532
$C_{13}H_{22}O_4$	242.1518	$C_{16}H_{18}O_2$	242.1307	$C_{13}H_{27}N_2O_2$	243.2074
$C_{13}H_{24}NO_3$	242.1757	$C_{16}H_2O_3$	242.0003	$C_{13}H_{11}N_2O_3$	243.0770
$C_{13}H_8NO_4$	242.0453	$C_{16}H_{20}NO$	242.1546	$C_{13}H_{29}N_3O$	243.2312
$C_{13}H_{26}N_2O_2$	242.1996	$C_{16}H_4NO_2$	242.0242	$C_{13}H_{13}N_3O_2$	243.1009
$C_{13}H_{10}N_2O_3$	242.0692	$C_{16}H_{22}N_2$	242.1784	$C_{13}H_{31}N_4$	243.2551
$C_{13}H_{28}N_3O$	242.2234	$C_{16}H_6N_2O$	242.0480	$C_{13}H_{15}N_4O$	243.1247
$C_{13}H_{12}N_3O_2$	242.0930	$C_{16}H_8N_3$	242.0719	$C_{14}H_{27}O_3$	243.1961
$C_{13}H_{30}N_4$	242.2473	$C_{17}H_{22}O$	242.1671	$C_{14}H_{11}O_4$	243.0657
$C_{13}H_{14}N_4O$	242.1169	$C_{17}H_6O_2$	242.0368	$C_{14}H_{29}NO_2$	243.2199
$C_{14}H_{26}O_3$	242.1883	$C_{17}H_{24}N$	242.1910	$C_{14}H_{13}NO_3$	243.0896

	FM		FM		FM
$C_{14}H_{31}N_2O$	243.2438	$C_{19}H_{15}$	243.1174	$C_{14}H_2N_3O_2$	244.0147
$C_{14}H_{15}N_2O_2$	243.1134	$C_{19}HN$	243.0109	$C_{14}H_{20}N_4$	244.1690
$C_{14}H_{33}N_3$	243.2677	$C_{20}H_3$	243.0235	$C_{14}H_4N_4O$	244.0386
$C_{14}H_{17}N_3O$	243.1373	244		$C_{15}H_{32}O_2$	244.2403
$C_{14}HN_3O_2$	243.0069	$C_{11}H_{20}N_2O_4$	244.1424	$C_{15}H_{16}O_3$	244.1100
$C_{14}H_{19}N_4$	243.1611	$C_{11}H_{22}N_3O_3$	244.1662	$C_{15}O_4$	243.9796
$C_{14}H_3N_4O$	243.0308	$C_{11}H_{24}N_4O_2$	244.1901	$C_{15}H_{18}NO_2$	244.1338
$C_{15}H_{31}O_2$	243.2325	$C_{12}H_{22}NO_4$	244.1549	$C_{15}H_2NO_3$	244.0034
$C_{15}H_{15}O_3$	243.1021	$C_{12}H_{24}N_2O_3$	244.1788	$C_{15}H_{20}N_2O$	244.1577
$C_{15}H_{33}NO$	243.2564	$C_{12}H_8N_2O_4$	244.0484	$C_{15}H_4N_2O_2$	244.0273
$C_{15}H_{17}NO_2$	243.1260	$C_{12}H_{26}N_3O_2$	244.2026	$C_{15}H_{22}N_3$	244.1815
$C_{15}HNO_3$	242.9956	$C_{12}H_{10}N_3O_3$	244.0723	$C_{15}H_6N_3O$	244.0511
$C_{15}H_{19}N_2O$	243.1498	$C_{12}H_{28}N_4O$	244.2265	$C_{15}H_8N_4$	244.0750
$C_{15}H_3N_2O_2$	243.0195	$C_{12}H_{12}N_4O_2$	244.0961	$C_{16}H_{20}O_2$	244.1464
$C_{15}H_{21}N_3$	243.1737	$C_{13}H_{24}O_4$	244.1675	$C_{16}H_4O_3$	244.0160
$C_{15}H_5N_3O$	243.0433	$C_{13}H_{26}NO_3$	244.1914	$C_{16}H_{22}NO$	244.1702
$C_{15}H_7N_4$	243.0672	$C_{13}H_{10}NO_4$	244.0610	$C_{16}H_6NO_2$	244.0399
$C_{16}H_{19}O_2$	243.1385	$C_{13}H_{28}N_2O_2$	244.2152	$C_{16}H_{24}N_2$	244.1941
$C_{16}H_3O_3$	243.0082	$C_{13}H_{12}N_2O_3$	244.0848	$C_{16}H_8N_2O$	244.0637
$C_{16}H_{21}NO$	243.1624	$C_{13}H_{30}N_3O$	244.2391	$C_{16}H_{10}N_3$	244.0876
$C_{16}H_5NO_2$	243.0320	$C_{13}H_{14}N_3O_2$	244.1087	$C_{17}H_{24}O$	244.1828
$C_{16}H_{23}N_2$	243.1863	$C_{13}H_{32}N_4$	244.2629	$C_{17}H_8O_2$	244.0524
$C_{16}H_7N_2O$	243.0559	$C_{13}H_{16}N_4O$	244.1325	$C_{17}H_{26}N$	244.2067
$C_{16}H_9N_3$	243.0798	$C_{13}N_4O_2$	244.0022	$C_{17}H_{10}NO$	244.0763
$C_{17}H_{23}O$	243.1750	$C_{14}H_{28}O_3$	244.2039	$C_{17}H_{12}N_2$	244.1001
$C_{17}H_7O_2$	243.0446	$C_{14}H_{12}O_4$	244.0735	$C_{18}H_{28}$	244.2192
$C_{17}H_{25}N$	243.1988	$C_{14}H_{30}NO_2$	244.2278	$C_{18}H_{12}O$	244.0888
$C_{17}H_9NO$	243.0684	$C_{14}H_{14}NO_3$	244.0974	$C_{18}H_{14}N$	244.1127
$C_{17}H_{11}N_2$	243.0923	$C_{14}H_{32}N_2O$	244.2516	$C_{18}N_2$	244.0062
$C_{18}H_{27}$	243.2114	$C_{14}H_{16}N_2O_2$	244.1213	$C_{19}H_{16}$	244.1253
$C_{18}H_{11}O$	243.0810	$C_{14}N_2O_3$	243.9909	$C_{19}O$	243.9949
$C_{18}H_{13}N$	243.1049	$C_{14}H_{18}N_3O$	244.1451	$C_{19}H_2N$	244.0187

	FM		FM		FM
$C_{20}H_4$	244.0313	$C_{15}HO_4$	244.9874	$C_{12}H_{24}NO_4$	246.1706
245		$C_{15}H_{19}NO_2$	245.1416	$C_{12}H_{26}N_2O_3$	246.1945
$C_{11}H_{21}N_2O_4$	245.1502	$C_{15}H_3NO_3$	245.0113	$C_{12}H_{10}N_2O_4$	246.0641
$C_{11}H_{23}N_3O_3$	245.1741	$C_{15}H_{21}N_2O$	245.1655	$C_{12}H_{28}N_3O_2$	246.2183
$C_{11}H_{25}N_4O_2$	245.1979	$C_{15}H_5N_2O_2$	245.0351	$C_{12}H_{12}N_3O_3$	246.0879
$C_{12}H_{23}NO_4$	245.1628	$C_{15}H_{23}N_3$	245.1894	$C_{12}H_{30}N_4O$	246.2422
$C_{12}H_{25}N_2O_3$	245.1866	$C_{15}H_7N_3O$	245.0590	$C_{12}H_{14}N_4O_2$	246.1118
$C_{12}H_9N_2O_4$	245.0653	$C_{15}H_9N_4$	245.0829	$C_{13}H_{26}O_4$	246.1832
$C_{12}H_{27}N_3O_2$	245.2105	$C_{16}H_{21}O_2$	245.1542	$C_{13}H_{28}NO_3$	246.2070
$C_{12}H_{11}N_3O_3$	245.0801	$C_{16}H_5O_3$	245.0238	$C_{13}H_{12}NO_4$	246.0766
$C_{12}H_{29}N_4O$	245.2343	$C_{16}H_{23}NO$	245.1781	$C_{13}H_{30}N_2O_2$	246.2309
$C_{12}H_{13}N_4O_2$	245.1040	$C_{16}H_7NO_2$	245.0477	$C_{13}H_{14}N_2O_3$	246.1005
$C_{13}H_{25}O_4$	245.1753	$C_{16}H_{25}N_2$	245.2019	$C_{13}H_{16}N_3O_2$	246.1244
$C_{13}H_{27}NO_3$	245.1992	$C_{16}H_9N_2O$	245.0715	$C_{13}N_3O_3$	245.9940
$C_{13}H_{11}NO_4$	245.0688	$C_{16}H_{11}N_3$	245.0954	$C_{13}H_{18}N_4O$	246.1482
$C_{13}H_{29}N_2O_2$	245.2230	$C_{17}H_{25}O$	245.1906	$C_{13}H_2N_4O_2$	246.0178
$C_{13}H_{13}N_2O_3$	245.0927	$C_{17}H_9O_2$	245.0603	$C_{14}H_{30}O_3$	246.2196
$C_{13}H_{31}N_3O$	245.2469	$C_{17}H_{27}N$	245.2145	$C_{14}H_{14}O_4$	246.0892
$C_{13}H_{15}N_3O_2$	245.1165	$C_{17}H_{11}NO$	245.0841	$C_{14}H_{16}NO_3$	246.1131
$C_{13}H_{17}N_4O$	245.1404	$C_{17}H_{13}N_2$	245.1080	$C_{14}NO_4$	245.9827
$C_{13}HN_4O_2$	245.0100	$C_{18}H_{29}$	245.2270	$C_{14}H_{18}N_2O_2$	246.1369
$C_{14}H_{29}O_3$	245.2117	$C_{18}N_{13}O$	245.0967	$C_{14}H_2N_2O_3$	246.0065
$C_{14}H_{13}O_4$	245.0814	$C_{18}H_{15}N$	245.1205	$C_{14}H_{20}N_3O$	246.1608
$C_{14}H_{31}NO_2$	245.2356	$C_{18}HN_2$	245.0140	$C_{14}H_4N_3O_2$	246.0304
$C_{14}H_{15}NO_3$	245.1052	$C_{19}H_{17}$	245.1331	$C_{14}H_{22}N_4$	246.1846
$C_{14}H_{17}N_2O_2$	245.1291	$C_{19}HO$	245.0027	$C_{14}H_6N_4O$	246.0542
$C_{14}HN_2O_3$	244.9987	$C_{19}H_3N$	245.0266	$C_{15}H_{18}O_3$	246.1256
$C_{14}H_{19}N_3O$	245.1529	$C_{20}H_5$	245.0391	$C_{15}H_2O_4$	245.9953
$C_{14}H_3N_3O_2$	245.0226	246		$C_{15}H_{20}NO_2$	246.1495
$C_{14}H_{21}N_4$	245.1768	$C_{11}H_{22}N_2O_4$	246.1580	$C_{15}H_4NO_3$	246.0191
$C_{14}H_5N_4O$	245.0464	$C_{11}H_{24}N_3O_3$	246.1819	$C_{15}H_{22}N_2O$	246.1733
$C_{15}H_{17}O_3$	245.1178	$C_{11}H_{26}N_4O_2$	246.2057	$C_{15}H_6N_2O_2$	246.0429

	FM		FM		FM
$C_{15}H_{24}N_3$	246.1972	$C_{12}H_{29}N_3O_2$	247.2261	$C_{16}H_9NO_2$	247.0634
$C_{15}H_8N_3O$	246.0668	$C_{12}H_{13}N_3O_3$	247.0958	$C_{16}H_{27}N_2$	247.2176
$C_{15}H_{10}N_4$	246.0907	$C_{12}H_{15}N_4O_2$	247.1196	$C_{16}H_{11}N_2O$	247.0872
$C_{16}H_{22}O_2$	246.1620	$C_{13}H_{27}O_4$	247.1910	$C_{16}H_{13}N_3$	247.1111
$C_{16}H_6O_3$	246.0317	$C_{13}H_{29}NO_3$	247.2148	$C_{17}H_{27}O$	247.2063
$C_{16}H_{24}NO$	246.1859	$C_{13}H_{13}NO_4$	247.0845	$C_{17}H_{11}O_2$	247.0759
$C_{16}H_8NO_2$	246.0555	$C_{13}H_{15}N_2O_3$	247.1083	$C_{17}H_{29}N$	247.2301
$C_{16}H_{26}N_2$	246.2098	$C_{13}H_{17}N_3O_2$	247.1322	$C_{17}H_{13}NO$	247.0998
$C_{16}H_{10}N_2O$	246.0794	$C_{13}HN_3O_3$	247.0018	$C_{17}H_{15}N_2$	247.1236
$C_{16}H_{12}N_3$	246.1032	$C_{13}H_{19}N_4O$	247.1560	$C_{17}HN_3$	247.0171
$C_{17}H_{26}O$	246.1985	$C_{13}H_3N_4O_2$	247.0257	$C_{18}H_{31}$	247.2427
$C_{17}H_{10}O_2$	246.0681	$C_{14}H_{15}O_4$	247.0970	$C_{18}H_{15}O$	247.1123
$C_{17}H_{28}N$	246.2223	$C_{14}H_{17}NO_3$	247.1209	$C_{18}H_{17}N$	247.1362
$C_{17}H_{12}NO$	246.0919	$C_{14}HNO_4$	246.9905	$C_{18}HNO$	247.0058
$C_{17}H_{14}N_2$	246.1158	$C_{14}H_{19}N_2O_2$	247.1447	$C_{18}H_3N_2$	247.0297
$C_{17}N_3$	246.0093	$C_{14}H_3N_2O_3$	247.0144	$C_{19}H_{19}$	247.1488
$C_{18}H_{30}$	246.2349	$C_{14}H_{21}N_3O$	247.1686	$C_{19}H_3O$	247.0184
$C_{18}H_{14}O$	246.1045	$C_{14}H_5N_3O_2$	247.0382	$C_{19}H_5N$	247.0422
$C_{18}H_{16}N$	246.1284	$C_{14}H_{23}N_4$	247.1925	$C_{20}H_7$	247.0548
$C_{18}NO$	245.9980	$C_{14}H_7N_4O$	247.0621	248	
$C_{18}H_2N_2$	246.0218	$C_{15}H_{19}O_3$	247.1334	$C_{11}H_{24}N_2O_4$	248.1737
$C_{19}H_{18}$	246.1409	$C_{15}H_3O_4$	247.0031	$C_{11}H_{26}N_3O_3$	248.1976
$C_{19}H_2O$	246.0106	$C_{15}H_{21}NO_2$	247.1573	$C_{11}H_{28}N_4O_2$	248.2214
$C_{19}H_4N$	246.0344	$C_{15}H_5NO_3$	247.0269	$C_{12}H_{26}NO_4$	248.1863
$C_{20}H_6$	246.0470	$C_{15}H_{23}N_2O$	247.1811	$C_{12}H_{28}N_2O_3$	248.2101
247		$C_{15}H_7N_2O_2$	247.0508	$C_{12}H_{12}N_2O_4$	248.0797
$C_{11}H_{23}N_2O_4$	247.1659	$C_{15}H_{25}N_3$	247.2050	$C_{12}H_{14}N_3O_3$	248.1036
$C_{11}H_{25}N_3O_3$	247.1897	$C_{15}H_9N_3O$	247.0746	$C_{12}H_{16}N_4O_2$	248.1275
$C_{11}H_{27}N_4O_2$	247.2136	$C_{15}H_{11}N_4$	247.0985	$C_{13}H_{28}O_4$	248.1988
$C_{12}H_{25}NO_4$	247.1784	$C_{16}H_{23}O_2$	247.1699	$C_{13}H_{14}NO_4$	248.0923
$C_{12}H_{27}N_2O_3$	247.2023	$C_{16}H_7O_3$	247.0395	$C_{13}H_{16}N_2O_3$	248.1162
$C_{12}H_{11}N_2O_4$	247.0719	$C_{16}H_{25}NO$	247.1937	$C_{13}N_2O_4$	247.9858

FM		FM		FM	
$C_{13}H_{18}N_3O_2$	248.1400	$C_{17}H_{30}N$	248.2380	$C_{14}H_{21}N_2O_2$	249.1604
$C_{13}H_2N_3O_3$	248.0096	$C_{17}H_{14}NO$	248.1076	$C_{14}H_5N_2O_3$	249.0300
$C_{13}H_{20}N_4O$	248.1639	$C_{17}H_{16}N_2$	248.1315	$C_{14}H_{23}N_3O$	249.1842
$C_{13}H_4N_4O_2$	248.0335	$C_{17}N_2O$	248.0011	$C_{14}H_7N_3O_2$	249.0539
$C_{14}H_{16}O_4$	248.1049	$C_{17}H_2N_3$	248.0249	$C_{14}H_{25}N_4$	249.2081
$C_{14}H_{18}NO_3$	248.1287	$C_{18}H_{32}$	248.2505	$C_{14}H_9N_4O$	249.0777
$C_{14}H_2NO_4$	247.9983	$C_{18}H_{16}O$	248.1202	$C_{15}H_{21}O_3$	249.1491
$C_{14}H_{20}N_2O_2$	248.1526	$C_{18}O_2$	247.9898	$C_{15}H_5O_4$	249.0187
$C_{14}H_4N_2O_3$	248.0222	$C_{18}H_{18}N$	248.1440	$C_{15}H_{23}NO_2$	249.1730
$C_{14}H_{22}N_3O$	248.1764	$C_{18}H_2NO$	248.0136	$C_{15}H_7NO_3$	249.0426
$C_{14}H_6N_3O_2$	248.0460	$C_{18}H_4N_2$	248.0375	$C_{15}H_{25}N_2O$	249.1968
$C_{14}H_{24}N_4$	248.2003	$C_{19}H_{20}$	248.1566	$C_{15}H_9N_2O_2$	249.0664
$C_{14}H_8N_4O$	248.0699	$C_{19}H_4O$	248.0262	$C_{15}H_{27}N_3$	249.2200
$C_{15}H_{20}O_3$	248.1413	$C_{19}H_6N$	248.0501	$C_{15}H_{11}N_3O$	249.0903
$C_{15}H_4O_4$	248.0109	$C_{20}H_8$	248.0626	$C_{15}H_{13}N_4$	249.1142
$C_{15}H_{22}NO_2$	248.1651	249		$C_{16}H_{25}O_2$	249.1855
$C_{15}H_6NO_3$	248.0348	$C_{11}H_{25}N_2O_4$	249.1815	$C_{16}H_9O_3$	249.0552
$C_{15}H_{24}N_2O$	248.1890	$C_{11}H_{27}N_3O_3$	249.2054	$C_{16}H_{27}NO$	249.2094
$C_{15}H_8N_2O_2$	248.0586	$C_{12}H_{27}NO_4$	249.1941	$C_{16}H_{11}NO_2$	249.0790
$C_{15}H_{26}N_3$	248.2129	$C_{12}H_{13}N_2O_4$	249.0876	$C_{16}H_{29}N_2$	249.2332
$C_{15}H_{10}N_3O$	248.0825	$C_{12}H_{15}N_3O_3$	249.1114	$C_{16}H_{13}N_2O$	249.1029
$C_{15}H_{12}N_4$	248.1063	$C_{12}H_{17}N_4O_2$	249.1353	$C_{16}H_{15}N_3$	249.1267
$C_{16}H_{24}O_2$	248.1777	$C_{13}H_{15}NO_4$	249.1001	$C_{16}HN_4$	249.0202
$C_{16}H_8O_3$	248.0473	$C_{13}H_{17}N_2O_3$	249.1240	$C_{17}H_{29}O$	249.2219
$C_{16}H_{26}NO$	248.2015	$C_{13}HN_2O_4$	248.9936	$C_{17}H_{13}O_2$	249.0916
$C_{16}H_{10}NO_2$	248.0712	$C_{13}H_{19}N_3O_2$	249.1478	$C_{17}H_{31}N$	249.2458
$C_{16}H_{28}N_2$	248.2254	$C_{13}H_3N_3O_3$	249.0175	$C_{17}H_{15}NO$	249.1154
$C_{16}H_{12}N_2O$	248.0950	$C_{13}H_{21}N_4O$	249.1717	$C_{17}H_{17}N_2$	249.1393
$C_{16}H_{14}N_3$	248.1189	$C_{13}H_5N_4O_2$	249.0413	$C_{17}HN_2O$	249.0089
$C_{16}N_4$	248.0124	$C_{14}H_{17}O_4$	249.1127	$C_{17}H_3N_3$	249.0328
$C_{17}H_{28}O$	248.2141	$C_{14}H_{19}NO_3$	249.1365	$C_{18}H_{33}$	249.2584
$C_{17}H_{12}O_2$	248.0837	$C_{14}H_3NO_4$	249.0062	$C_{18}H_{17}O$	249.1290

	FM		FM		FM
$C_{18}HO_2$	248.9976	$C_{15}H_8NO_3$	250.0504		
$C_{18}H_{19}N$	249.1519	$C_{15}H_{26}N_2O$	250.2046		
$C_{18}H_3NO$	249.0215	$C_{15}H_{10}N_2O_2$	250.0743		
$C_{18}H_5N_2$	249.0453	$C_{15}H_{28}N_3$	250.2285		
$C_{19}H_{21}$	249.1644	$C_{15}H_{12}N_3O$	250.0981		
$C_{19}H_5O$	249.0340	$C_{15}H_{14}N_4$	250.1220		
$C_{19}H_7N$	249.0579	$C_{16}H_{26}O_2$	256.1934		
$C_{20}H_9$	249.0705	$C_{16}H_{10}O_3$	250.0630		
250		$C_{16}H_{28}NO$	250.2172		
$C_{11}H_{26}N_2O_4$	250.1894	$C_{16}H_{12}NO_2$	250.0868		
$C_{12}H_{14}N_2O_4$	250.0954	$C_{16}H_{30}N_2$	250.2411		
$C_{12}H_{16}N_3O_3$	250.1193	$C_{16}H_{14}N_2O$	250.1107		
$C_{12}H_{18}N_4O_2$	250.1431	$C_{16}H_{16}N_3$	250.1346		
$C_{13}H_{16}NO_4$	250.1080	$C_{16}N_3O$	250.0042		
$C_{13}H_{18}N_2O_3$	250.1318	$C_{16}H_2N_4$	250.0280		
$C_{13}H_2N_2O_4$	250.0014	$C_{17}H_{30}O$	250.2298		
$C_{13}H_{20}N_3O_2$	250.1557	$C_{17}H_{14}O_2$	250.0994		
$C_{13}H_4N_3O_3$	250.0253	$C_{17}H_{32}N$	250.2536		
$C_{13}H_{22}N_4O$	250.1795	$C_{17}H_{16}NO$	250.1233		
$C_{13}H_6N_4O_2$	250.0491	$C_{17}NO_2$	249.9929		
$C_{14}H_{18}O_4$	250.1205	$C_{17}H_{18}N_2$	250.1471		
$C_{14}H_{20}NO_3$	250.1444	$C_{17}H_2N_2O$	250.0167		
$C_{14}H_4NO_4$	250.0140	$C_{17}H_4N_3$	250.0406		
$C_{14}H_{22}N_2O_2$	250.1682	$C_{18}H_{34}$	250.2662		
$C_{14}H_6N_2O_3$	250.0379	$C_{18}H_{18}O$	250.1358		
$C_{14}H_{24}N_3O$	250.1921	$C_{18}H_2O_2$	250.0054		
$C_{14}H_8N_3O_2$	250.0617	$C_{18}H_{20}N$	250.1597		
$C_{14}H_{26}N_4$	250.2160	$C_{18}H_4NO$	250.0293		
$C_{14}H_{10}N_4O$	250.0856	$C_{18}H_6N_2$	250.0532		
$C_{15}H_{22}O_3$	250.1569	$C_{19}H_{22}$	250.1722		
$C_{15}H_6O_4$	250.0266	$C_{19}H_6O$	250.0419		
$C_{15}H_{24}NO_2$	250.1808	$C_{19}H_8N$	250.0657		
		$C_{20}H_{10}$	250.0783		

(a) If only C, H, N, O, F, P, I are present, the approximate expected % (M + 1) and % (M + 2) intensities can be calculated by use of the following formulas:

$$\% (M + 1) = 100 \left[\frac{(M + 1)}{(M)} \right]$$

$$\approx 1.1 \times \text{number of C atoms} + 0.36 \times \text{number of N atoms.}$$

$$\% (M + 2) = 100 \left[\frac{(M + 2)}{(M)} \right]$$

$$\approx \frac{(1.1 \times \text{number of C atoms})^2}{200}$$

$$+ 0.20 \times \text{number of O atoms.}$$

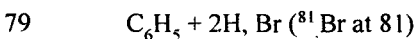
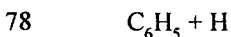
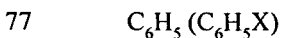
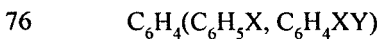
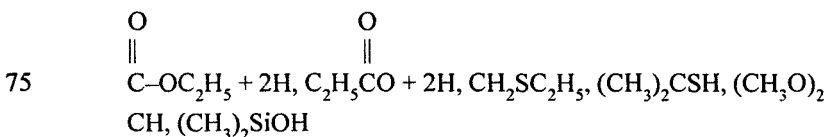
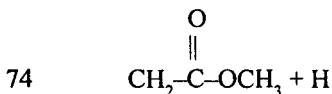
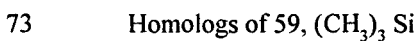
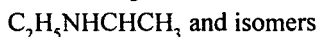
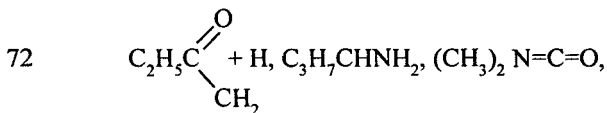
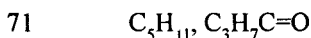
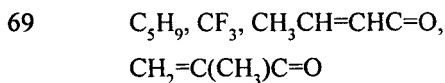
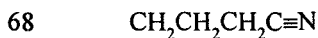
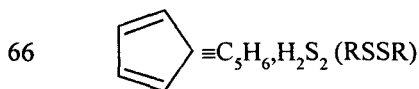
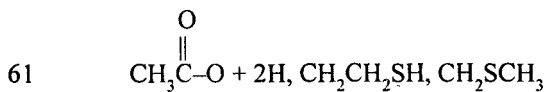
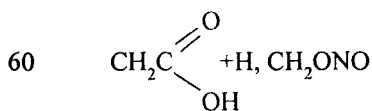
Table 5.4

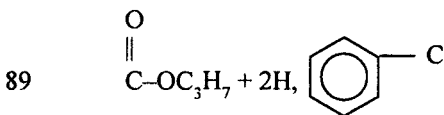
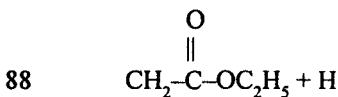
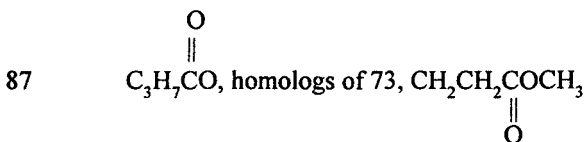
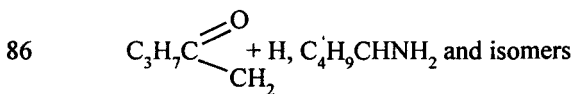
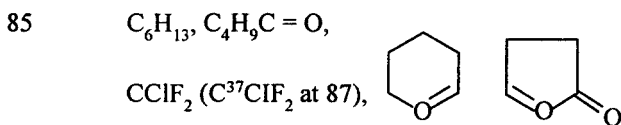
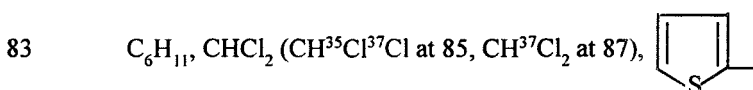
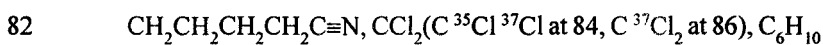
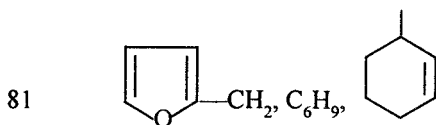
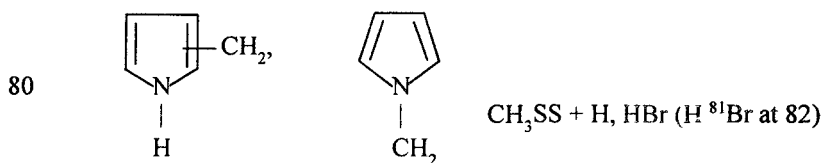
COMMON FRAGMENT IONS

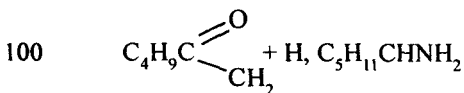
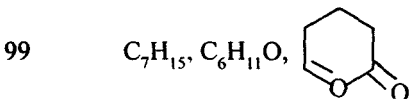
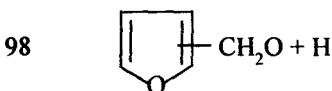
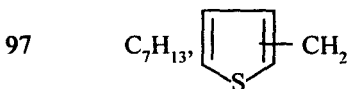
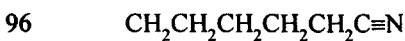
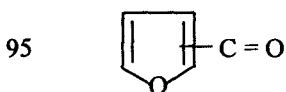
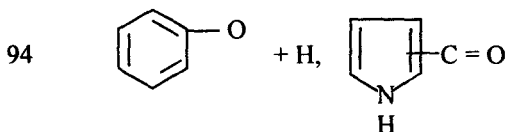
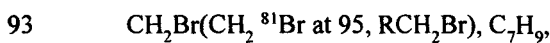
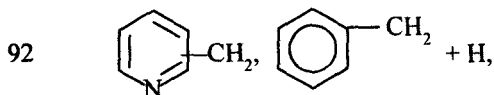
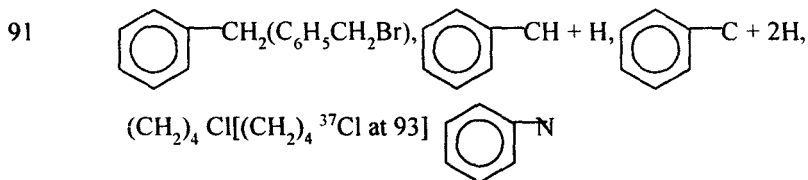
All fragments listed bear + 1 charges. To be used in conjunction with Table 5.5. Not all members of homologous and isomeric series are given. The list is meant to be suggestive rather than exhaustive. Structural inferences are listed in parentheses.

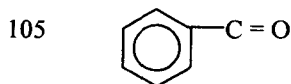
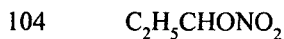
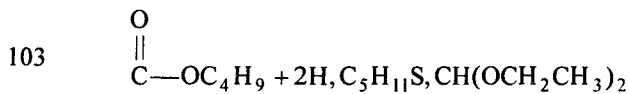
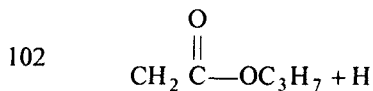
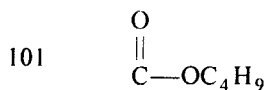
m/z	(Structural Inference)
Ions*	
14	CH ₂
15	CH ₃
16	O
17	OH
18	H ₂ O, NH ₄
19	F, H ₃ O
26	C≡N, C ₂ H ₂
27	C ₂ H ₃
28	C ₂ H ₄ , CO, N ₂ (air), CH=NH
29	C ₂ H ₅ , CHO
30	CH ₂ NH ₂ (RCH ₂ NH ₂), NO
31	CH ₂ OH(RCH ₂ OH), OCH ₃
32	O ₂ (air)
33	SH, CH ₂ F

- 34 H_2S
- 35 Cl (^{37}Cl at 37)
- 36 HCl (H^{37}Cl at 38)
- 39 C_3H_3
- 40 $\text{CH}_2\text{C}=\text{N}$, Ar (air)
- 41 C_3H_5 , $\text{CH}_2\text{C}=\text{N} + \text{H}^a$, $\text{C}_2\text{H}_2\text{NH}$
- 42 C_3H_6 , $\text{C}_2\text{H}_2\text{O}$
- 43 C_3H_7 , $\text{CH}_3\text{C}=\text{O}$, $\text{CH}_3\text{C}=\text{OG}$, ($\text{G} = \text{R}, \text{Ar}, \text{NH}_2, \text{OR}, \text{OH}$), $\text{C}_2\text{H}_5\text{N}$
- 44 $\begin{array}{c} \text{H} \\ | \\ \text{CH}_2\text{C}=\text{O} \end{array} + \text{H}$ (Aldehydes, McLafferty Rearrangement),
 CH_3CHNH_2 , CO_2 , $\text{NH}_2\text{C}=\text{O}$ ($\text{RC}=\text{ONH}_2$), $(\text{CH}_3)_2\text{N}$
- 45 $\begin{array}{c} \text{CH}_3 \\ | \\ \text{CHOH}, \text{CH}_2\text{CH}_2\text{OH}, \text{CH}_2\text{OCH}_3 \text{ (RCH}_2\text{OCH}_3\text{)}, \\ \text{O} \\ || \\ \text{C-OH}, \text{CH}_3\text{CH-O} + \text{H(CH}_3\text{CHOHR)} \end{array}$
- 46 NO_2
- 47 CH_2SH (RCH_2SH), CH_3S
- 48 $\text{CH}_3\text{S} + \text{H}$
- 49 CH_2Cl (CH_2 ^{37}Cl at 51)
- 51 CHF_2 , C_4H_3
- 53 C_4H_5
- 54 $\text{CH}_2\text{CH}_2\text{C}\equiv\text{N}$
- 55 C_4H_7 , $\text{CH}_2=\text{CHC}=\text{O}$
- 56 C_4H_8
- 57 C_4H_9 , $\text{C}_2\text{H}_5\text{C}=\text{O}$
- 58 $\text{CH}_3-\text{C} \begin{array}{l} \nearrow \text{O} \\ \searrow \text{CH}_2 \end{array} + \text{H}$, $\text{C}_2\text{H}_5\text{CHNH}_2$, $(\text{CH}_3)_2\text{NCH}_2$, $\text{C}_2\text{H}_5\text{NHCH}_2$, $\text{C}_2\text{H}_2\text{S}$
- 59 $(\text{CH}_3)_2\text{COH}$, $\text{CH}_2\text{OC}_2\text{H}_5$, $\begin{array}{c} \text{O} \\ || \\ \text{C-OCH}_3 \end{array}$ (RCO_2CH_3).
 $\text{NH}_2\text{C}=\text{O} + \text{H}$,
 $\begin{array}{c} | \\ \text{CH}_2 \\ | \\ \text{CH}_3\text{OCHCH}_3, \text{CH}_3\text{CHCH}_2\text{OH}, \text{C}_2\text{H}_5\text{CHOH} \end{array}$

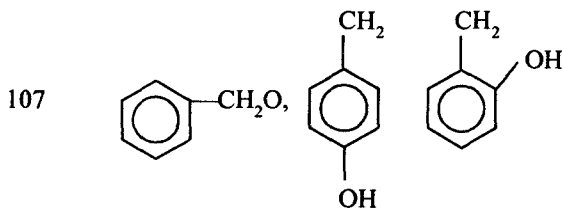
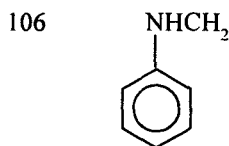
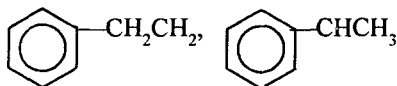




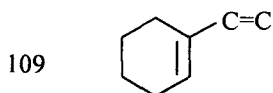
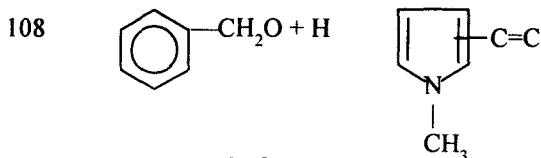


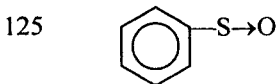
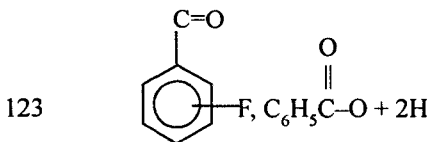
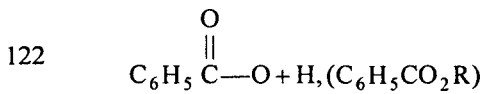
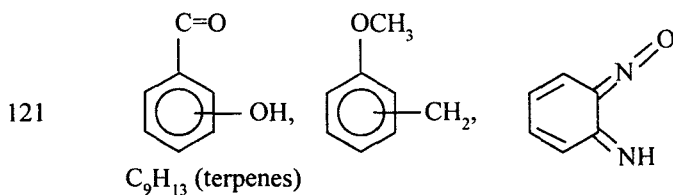
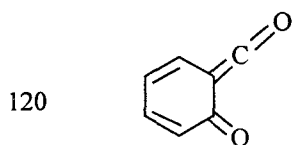
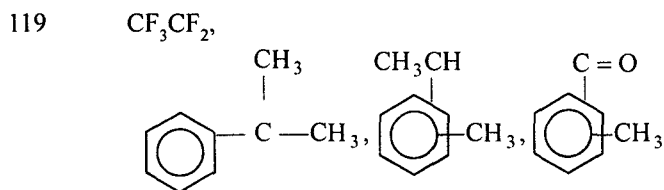
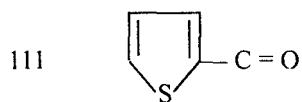


$[\text{C}_6\text{H}_5(\text{C}=\text{O})\text{G}, \text{G} = \text{OH}, \text{OR}, \text{OAr}, \text{halogen}, \text{NH}_2],$



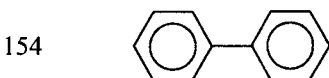
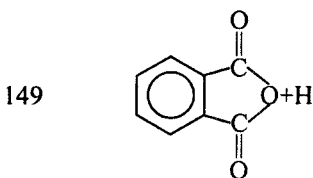
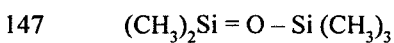
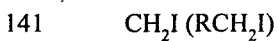
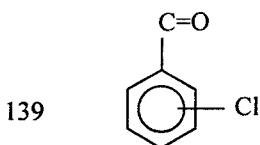
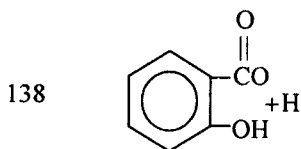
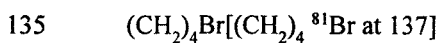
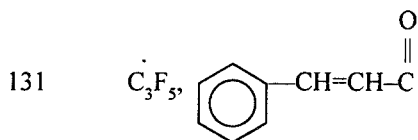
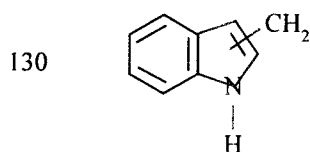
$\text{C}_2\text{H}_4\text{Br}(\text{C}_2\text{H}_4 \text{ } ^{81}\text{Br} \text{ at } 109)$





127 I

128 HI



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

Table 5.5
Common Fragments Lost

This list is suggestive rather than comprehensive. It should be used in conjunction with Table 5.4. 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 $\text{CH}_2=\text{CHCH}_3$, $\text{CH}_2=\text{C}=\text{O}$, $\text{H}_2\text{C} \begin{array}{c} \text{H}_2 \\ \diagup \text{C} \diagdown \\ \text{---} \text{CH}_2 \end{array}$, NCO , NCNH_2
- 43 $\text{C}_3\text{H}_7^\bullet$ (propyl ketones, $\text{ArCH}_2-\text{C}_3\text{H}_7$), $\text{CH}_3-\overset{\text{O}}{\parallel}{\text{C}}^\bullet$ (methyl ketones, CH_3CG , where G = various functional groups), $\text{CH}_2=\overset{\text{O}}{\parallel}{\text{C}}^\bullet$, (CH_3^\bullet and $\text{CH}_2=\text{CH}_2$), HCNO
- 44 $\text{CH}_2=\text{CHOH}$, CO_2 (esters, anhydrides), N_2O , CONH_2 , NHCH_2CH_3
- 45 CH_3CHOH , $\text{CH}_3\text{CH}_2\text{O}^\bullet$ (ethyl esters), CO_2H , $\text{CH}_3\text{CH}_2\text{NH}_2$
- 46 (H_2O and $\text{CH}_2=\text{CH}_2$), $\text{CH}_3\text{CH}_2\text{OH}$, $^\bullet\text{NO}_2$ (ArNO_2)
- 47 $\text{CH}_3\text{S}^\bullet$
- 48 CH_3SH , SO (sulfoxides), O_3
- 49 $^\bullet\text{CH}_2\text{Cl}$
- 51 $^\bullet\text{CHF}_2$
- 52 C_4H_4 , C_2N_2
- 53 C_4H_5
- 54 $\text{CH}_2=\text{CH}-\text{CH}=\text{CH}_2$
- 55 $\text{CH}_2=\text{CHCHCH}_3$
- 56 $\text{CH}_2=\text{CHCH}_2\text{CH}_3$, $\text{CH}_3\text{CH}=\text{CHCH}_3$, 2CO
- 57 $\text{C}_4\text{H}_9^\bullet$ (butyl ketones), $\text{C}_2\text{H}_5\text{CO}$ (ethyl ketones, $\text{EtC} = \text{OG}$, G = various structural units)
- 58 $^\bullet\text{NCS}$, ($\text{NO} + \text{CO}$), CH_3COCH_3 , C_4H_{10}
- 59 $\text{CH}_3\overset{\text{O}}{\parallel}{\text{C}}^\bullet$, $\text{CH}_3-\overset{\text{O}}{\parallel}{\text{C}}-\text{NH}_2$, $\begin{array}{c} \text{H} \\ | \\ \text{S} \\ \triangle \end{array}$
- 60 $\text{C}_3\text{H}_7\text{OH}$, $\text{CH}_2=\text{C}(\text{OH})_2$ (acetate esters)^a
- 61 $\text{CH}_3\text{CH}_2\text{S}^\bullet$, $\begin{array}{c} \text{H} \\ | \\ \text{S}^\bullet \\ \triangle \end{array}$
- 62 (H_2S and $\text{CH}_2=\text{CH}_2$)
- 63 $^\bullet\text{CH}_2\text{CH}_2\text{Cl}$

64	C_5H_4, S_2, SO_2
68	$\begin{array}{c} CH_3 \\ \\ CH_2=C-CH=CH_2 \end{array}$
69	$CF_3^\bullet, C_5H_9^\bullet$
71	$C_5H_{11}^\bullet$
73	$\begin{array}{c} O \\ \\ CH_3CH_2OC^\bullet \end{array}$
74	C_4H_9OH
75	C_6H_3
76	C_6H_4, CS_2
77	C_6H_5, CS_2H
78	C_6H_6, CS_2H_2, C_5H_4N
79	Br^\bullet, C_5H_5N
80	HBr
85	$^\bullet CClF_2$
100	$CF_2=CF_2$
119	$CF_3-CF_2^\bullet$
122	C_6H_5COOH
127	I^\bullet
128	HI

^aMclafferty Rearrangement**Problems:**

- (1) List the possible formulas of molecules with $M^+ = 100$. Assume that C, H and O may be present.

Strategy: A good approach to this kind of problem is to begin by calculating the possible hydrocarbon formulas. First divide the molecular weight by 12 to find the maximum number of carbons possible. Each carbon is equal in mass to 12 hydrogens, so the next step is to replace 1 C by 12H, giving another possible formula.

Oxygen containing formulas can be calculated by realising that one oxygen is equal in mass to CH_4 .

Ans.: Dividing M^+ by 12 gives $100/12 = 8$ (remainder 4), so a possible hydrocarbon formula is C_8H_4 . Replacing 1 C by 12H gives the second possible hydrocarbon formula C_7H_{16} .

Starting with the hydrocarbon formula C_8H_4 and replacing CH_4 by O gives C_7O as possible (but unlikely) formula. Doing the same with C_7H_{16} gives $\text{C}_6\text{H}_{12}\text{O}$. Again replacing CH_4 by O gives $\text{C}_5\text{H}_8\text{O}_2$, and repeating the process a third time gives $\text{C}_4\text{H}_4\text{O}_3$. Thus, there are five likely formulas for a substance with $MW = 100$.

(2) Write as many molecular formulas as you can for compounds that have the following molecular ions in their mass spectra. Assume that all the compounds contain C^1 and H, and that O may or may not be present.

(a) $M^+ = 86$, (b) $M^+ = 128$, (c) $M^+ = 156$

Ans. (a) C_6H_{14} , $\text{C}_5\text{H}_{10}\text{O}$, $\text{C}_4\text{H}_6\text{O}_2$, $\text{C}_3\text{H}_2\text{O}_3$
 (b) C_9H_{20} , $\text{C}_9\text{H}_4\text{O}$, C_{10}H_8 , $\text{C}_8\text{H}_{16}\text{O}$, $\text{C}_7\text{H}_{12}\text{O}_2$, $\text{C}_6\text{H}_8\text{O}_3$, $\text{C}_5\text{H}_4\text{O}_4$
 (c) $\text{C}_{11}\text{H}_{24}$, $\text{C}_{12}\text{H}_{12}$, $\text{C}_{11}\text{H}_8\text{O}$, $\text{C}_{10}\text{H}_{20}\text{O}$, $\text{C}_{10}\text{H}_4\text{O}_2$, $\text{C}_9\text{H}_{16}\text{O}_2$, $\text{C}_8\text{H}_{12}\text{O}_3$,
 $\text{C}_7\text{H}_8\text{O}_4$, $\text{C}_6\text{H}_4\text{O}_5$

(3) What are the masses of the charged fragments produced in the following cleavage pathways?

(a) Alpha cleavage of 2-pentanone ($\text{CH}_3\text{COCH}_2\text{CH}_2\text{CH}_3$)

Ans. 43, 71

(b) Dehydration of cyclohexanol (hydroxycyclohexane)

Ans. 82

(c) McLafferty rearrangement of 4-methyl-2-pentanone [$\text{CH}_3\text{COCH}_2\text{CH}(\text{CH}_3)_2$]

Ans. 58

(d) Alpha cleavage of triethylamine [$(\text{CH}_3\text{CH}_2)_3\text{N}$]

Ans. 86

STRUCTURAL DATA OBTAINABLE FROM DIFFERENT SPECTRA

Characteristic and readily obtainable structural data from each type of spectrum are collected below:

UV	Conjugation, substituents on sp^2 C atoms.
IR	Functional groups.
NMR	Carbon chain.
MS	Molecular formula, functional groups, carbon skeleton.

Details

UV The following data can be obtained from a UV spectrum.

1. The nature of conjugated system and substituents, from the empirical rules for calculation of λ_{\max} of (a) polyenes, (b) enones and (c) aromatic carbonyl compounds.
2. The presence of aromatic units from the λ_{\max} 200 nm and λ_{\max} 260 nm (benzenoid) bands.
3. By comparing the shape of the spectrum of the unknown with spectra of known compounds it is possible to identify the nature of the chromophoric units (cf. model compounds).
4. Weakly absorbing chromophores (i.e., simple ketones, sulphides etc., or $n \rightarrow \sigma^*$ or $n \rightarrow \pi^*$ transitions) are indicated by weak bands in the absence of strong chromophores.

IR The IR spectrum is extremely useful for the identification of functional groups in the unknown. The tables given in the chapter on IR spectroscopy should be consulted. Briefly IR is helpful in identifying the following:

1. $-\text{OH}$; $-\text{COOH}$;
2. $-\text{NH}_2$; $-\text{NH}$; $-\text{CONH}_2$; $-\text{CONH}$;
3. $\text{C}\equiv\text{C}$; $\text{HC}\equiv\text{C}$; $-\text{CN}$; $\text{C}=\text{C}=\text{C}$;
4. Aromatic rings, nature of substitution in the ring.
5. Carbonyl functions.
6. Enes and their cis-trans stereochemistry.

7. Alkyl units $-\text{CH}(\text{CH}_3)_2$; $\text{CH}(\text{CH}_3)_3$

Note that absence of bands is also informative because if the functional group is present it must give its IR bands. The vibrations never stop.

NMR The NMR spectrum gives valuable data about the carbon chain.
PMR (Proton Magnetic Resonance) or ^1H NMR. The following information can be obtained.

1. The number of groups of equivalent protons and hence of the nature of C atoms (δ values) in the chain (whether CH_3 , CH_2 , CH , etc.). The integration gives the number of protons in each group of equivalent protons.
2. The adjacent groups of protons (J, splitting patterns).
3. Decoupling experiments identify the neighbouring groups of protons.
4. NOE and J values indicate stereochemistry.
5. Paramagnetic shift reagents simplify complex spectra.

^{13}C -NMR The following information can be obtained:

1. The number of equivalent groups of C atoms.
2. The number of H atoms attached to each C atom (off-resonance decoupling).
3. Calculation of the chemical shifts of C atoms in the proposed structure and comparison with the observed values, for confirmation.
4. Carbonyl functional groups.

The NMR spectrum is the most useful spectrum because it can give almost the complete structure of the unknown compound which may need only marginal information for confirmation.

MS The mass spectrum provides data, some of which cannot be obtained from other spectra.

1. Accurate molecular weight and molecular formula M^{+0} . This will be very valuable in those cases where only a small amount

of the unknown compound is available. Ion formulae can also be obtained from high resolution MS.

2. The class of compounds to which the unknown belongs can be deduced from $M + 1$ abundance and the general appearance of the spectrum.
- 3.. Functional groups from high m/z peaks and characteristic ion series.
4. Information about the C-skeleton from fragment peaks.

Reference Books used:

1. *Spectrometric Identification of Organic Compounds* by Silverstein, Bassler, Morrill, 5/e (John Wiley & Sons. Inc.).
2. *Absorption Spectroscopy of Organic Molecules* by V.M. Parikh (Addison Wesley Publishing Company, California).
3. *Application of Absorption Spectroscopy of Organic Compounds* by John R. Dyer (Prentice Hall of India Private Limited, New Delhi, 1991).
4. *Organic Spectroscopy* by V.R. Dani. (Tata McGraw – Hill Publishing Company Limited, New Delhi, 1995).



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