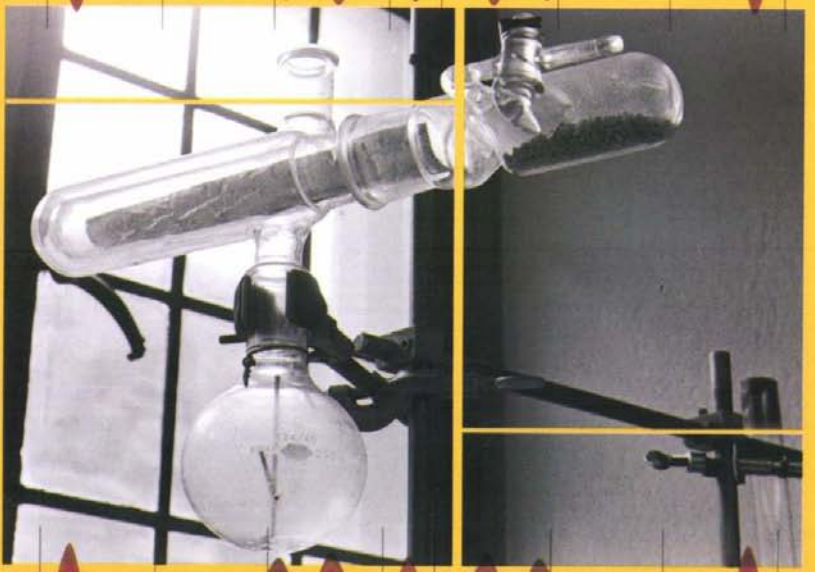
A Handbook of Spectroscopic Data

Chemistry

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

B.D.Mistry



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Contents

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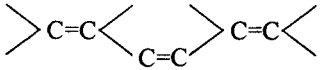
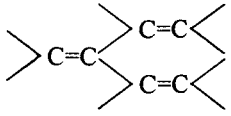
Ultraviolet Spectroscopy

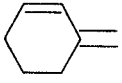
1.1 Calculating Absorption Maxima of Unsaturated Compounds

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:

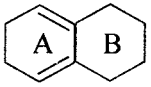
i)  A linear conjugation; for example, 1,3,5 hexatriene, isoprene,etc.

ii)  A cross conjugation.

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

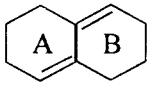
iv)  A semicyclic diene; one of the double bonds forms part of a ring and the other is exocyclic, or outside the ring. When only one of of the two sp^2 hybridized carbons of a double bond is a part of the ring under

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

v) 

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.

vi) 

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 exocylic to two rings)	+5nm
v)	Substitutents 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 (λmax) 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 λmax 220 nm (∈ 10,050) which is quite different from the calcualted 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 λmax and ϵ_{max} of UV absorption.

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

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

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

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

$>\overset{\delta}{C}=\overset{\gamma}{C}-\overset{\beta}{C}=\overset{\alpha}{C}-C=O$

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

$$\underset{\text{Enone}}{\beta-C=C-C=O} \quad \text{and} \quad \underset{\text{Dienone}}{\delta-C=C-C=C-C=O}$$

Z = C, enone, Z = H, aldehyde

Z = OH, acid, Z = OR, ester

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 >C=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
Alkoxyl ($-OCH_3$)	α	+ 35nm
	β	+ 30nm
	γ	+ 17nm
	δ	31nm

Acetoxyl (–O–$COCH_3$)	α, β or δ	+ 6nm
Dialkyl aniino (–NR_2)	β	+ 95nm
Chlorine (–Cl)	α	+ 15nm
	β	+ 12nm
Thioalkyl (–SR)	β	+ 85nm
Bromine (–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

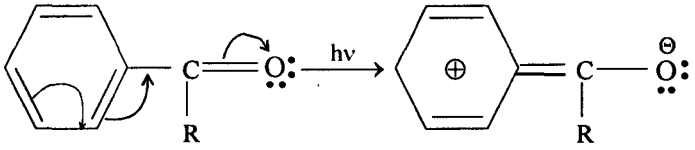
There are two types of aromatic molecules: benzenoid and nonbenzenoid. Their spectra show considerable resemblance. In fact, the presence or absence of certain features in UV spectra, such as a low intensity band (known as a fine structure band) at or about 255 nm, is often used to detect the aromatic 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-structue 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. $-NR_2$, –OH, etc. which allow for the n → π conjugation and –C = 0 and $-NO_2$ 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 substitutents:



Auxochrome substituents:

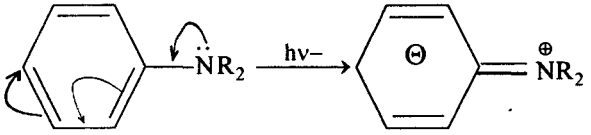


Table 1.3: Scotts rules for calculation of λmax of the ET (electron transfer) band of aromatic carbonyl compounds

Parent chromophore : Ar=C_6H_5

Z = Alkyl or ring residue, (e.g.; ArCOR)		246 nm
Z = H, (Ar CHO)		250 nm
Z = OH, OAlk, (ArCOOH and ArCOOR)		230 nm
Increment for each substitutent 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]

In heterocyclic chemistry model compounds are essential for the interpretation of most spectra. No rules are available for the predicition of the wavelength maxima of aromatic compounds except in the case of aromatic carbonyl compounds where acetophenone is taken as the parent chromophore, and increments allotted on the usual basis (Table 1.3)

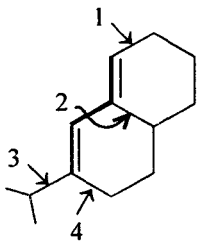
– Cl	o–, m–	+ 0 nm
	p–	+ 10 nm
– Br	o–, m–	+ 2 nm
	p–	+ 15 nm
– NH_2	o–, m–	+ 13 nm
	p–	+ 58 nm
– $NHCOCH_3$	o–, m–	+ 20 nm
	p–	+ 45 nm
– $NHCH_3$	P–	+ 73 nm
– $N(CH_3)_2$	o–, m–	+ 20 nm
	p–	+ 85 nm

[a]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

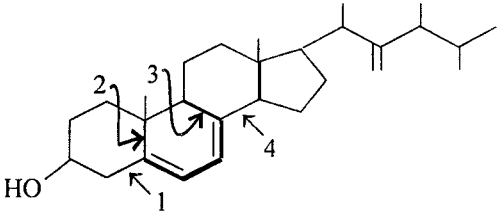
(1) Abietic acid



Basic heteroannular diene	214 nm
Exocyclic double bonds (1 × 5)	05 nm
Substituents R (4 × 5)	20 nm
Calculated λmax	239 nm
Observed	241 nm

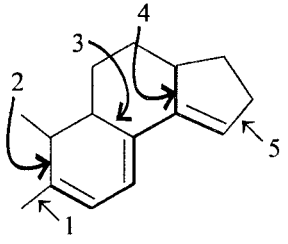
[Chromophore is shown by **heavy lines**; numbers indicate substituents.]

(2) Ergosterol



Basic homoannular diene	253 nm
Exocyclic double bonds (2 × 5)	10 nm
Substituents R (4 × 5)	20 nm
Calculated λmax	283 nm
Observed	282 nm

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

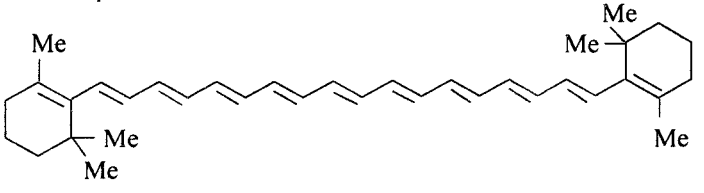


In compounds containing both homoannular and heteroannular double bonds, the diene system which requires least energy for excitation (i.e. the one with the longer wavelength of absorption) is used as a base.

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 λmax	323 nm
Observed	319 nm

II. Polyenes

(1) All trans β–carotene



Basic λmax value		114 nm
M = number of alkyl substituents, 5 × 10	add	50 nm
n = number of conjugated double bonds,		
11 × [48 – (1.7 × 11)]	add	322.3 nm
R_{endo} = number of rings with endocyclic double bonds,		
2 × 16.5, substract		33.0 nm
R_{exo} = number of rings with exocyclic double bonds,		
0 × 10, substract		00.0 nm
Calculated λmax		453.30 nm
Observed		452.00 nm

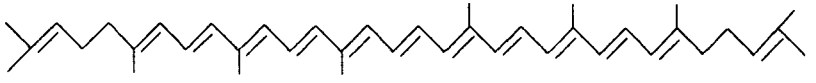
$\epsilon_{max} = 1.74 \times 11 \times 10^4$

$= 19.1 \times 10^4$ (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 λmax		114 nm
M = 5 × 8	add	40 nm
n = 11 × 148 –(1.7 × 11)	add	322.3 nm

(**Note:** Double bonds at ends are not in conjugation with others)

R_{endo}	substract	00.0 nm
R_{exo}	substract	00.0 nm
	Calculated λmax	476.30 nm
	Observed	474.00 nm

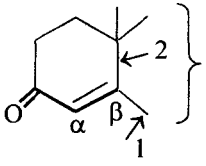
$\epsilon_{max} = 1.74 \times 11 \times 10^4$

$= 19.1 \times 10^4$ (calculated)

$= 18.6 \times 10^4$ (observed)

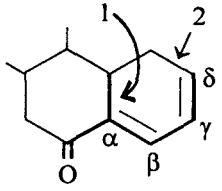
III. Enones

(1) Cholest–4–en–3–one



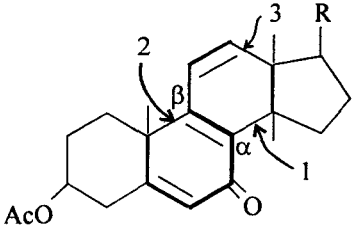
Parent base	215 nm
Substituents β, β (2 × 12) add	24 nm
Exocyclic = C< add	05 nm
Calculated λ_{max}^{EtOH}	244 nm
Observed	241 nm

(2) Cholesta–2,4–dien–6–one



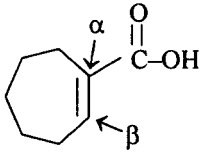
Parent base		215 nm
Extended conjugation	add	30 nm
Homoannular component	add	39 nm
Substituents α (1 × 10)	add	10 nm
δ (1 × 18)	add	18 nm
Calculated λ_{max}^{EtOH}		312 nm
Observed		314 nm

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



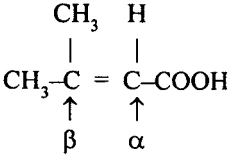
Parent base		215 nm
Extended conjugation	add	30 nm
Homoannular component	add	39 nm
Exocyclic double bond	add	5 nm
Substituents α (1 × 10)	add	10 nm
β (1 × 12)	add	12 nm
δ (1 × 18)	add	18 nm
Calculated λ_{max}^{EtOH}		329 nm
Observed		327 nm

(4) Cycloheptene–1–carboxylic acid



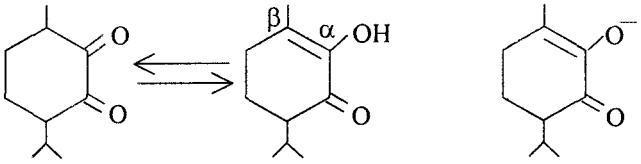
Parent base		195 nm
Substituents α (1 × 10)	add	10 nm
β (1 × 12)	add	12 nm
C=C endocyclic to 7-member ring,	add	05 nm
Calculated λ_{max}^{EtOH}		222 nm

(5) 3–Methyl–2–butenoic acid



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

Dicarbonyl compounds

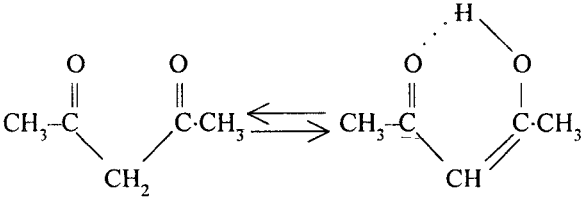


Diosphenol

Parent base		215 nm
Substituents	2β (2 × 12)	24 nm
	α-OH (1 × 35)	35 nm
	Calculated λ_{max}^{EtOH}	274 nm
	Observed λ_{max}^{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

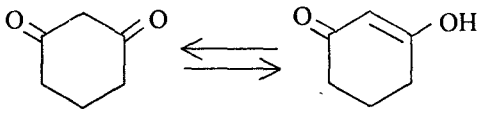
aβ-diketone

$\lambda_{max}^{Isooctane}$ 272, ϵ_{max} 12,000

$\lambda_{max}^{H_2O}$ 274, ϵ_{max} 2050

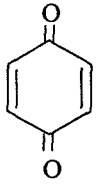
However, in the case of acetyl acetone agreement with the calculated wavelength (257 nm) is indifferent. This may be due to the fact that the strong internal hydrogen bond forces the carbonyl group and the double bond into a configuration different from that which is present in cyclic structures, e.g.,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



λ_{max}^{hexane} = 242 nm (ϵ 24,000) ($\pi \rightarrow \pi^*$ K-band)

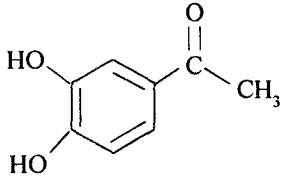
281 nm (ϵ 400) $\}$ $n \rightarrow \pi^*$

434 nm (ϵ 20) $\}$ R – band

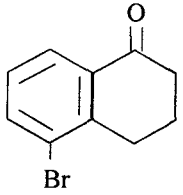
The colour of the simpler members is due to the weak $n \rightarrow \pi^*$ transition which is also present in α-diketones. The $n \rightarrow \pi^*$ transitions of α-diketones in the diketo form gives rise to two bands one in the usual region near 290 nm ($\epsilon \sim 30$) and a second ($\epsilon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

IV. Aromatic carbonyl compounds

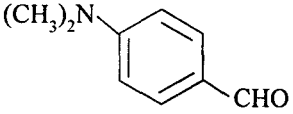
1.



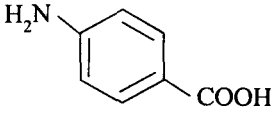
Base value	246 nm
OH in m	07 nm
OH in p	25 nm
	278 nm

2. 

Base value	246 nm
Br in m	02 nm
$-CH_2$ in o	03 nm
	251 nm

3. 

Base value	250 nm
NMe_2 in p	85 nm
	335 nm

4. 

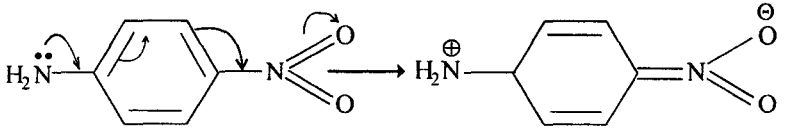
Base value	230 nm
NH_2 in p	58 nm
	288 nm

Another approach to predicting, the λmax 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:

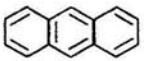
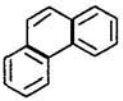
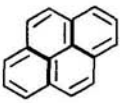
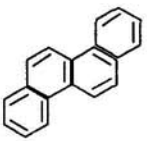
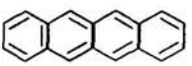
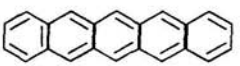
a. Both groups are either electron donating or electron withdrawing: Only the effect of the group causing the larger shift is used. For example, the λmax of p-nitrobenzoic acid would be expected to be the same as that of nitrobenzene, ~(203.5 + 65.0) = ~268.5 (in alcohol solvent).

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 benzens 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	λmax, nm	∈max	λmax, nm	∈max	λmax, nm	∈max
 Benzene	184	47,000	203	7,400	255	230
 Napthalene	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
 Napthacene	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 (CH_3OH solvent)

Base Value: 203. 5 nm

Substitutent	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 Benzens:

Compound	$\pi \rightarrow \pi^*$ Transition K Band		B Band	
	λmax (nm)	∈max	λmax (nm)	∈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

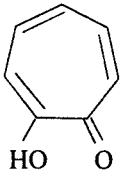
Compound	Solvent	Primary band $\pi \rightarrow \pi^*$ Transition K Band		Secondary band $\pi \rightarrow \pi^*$ Transition B Band		$n \rightarrow \pi^*$ Transition R Band	
		λ_{max} (nm)	ϵ_{max}	λ_{max} (nm)	ϵ_{max}	λ_{max} (nm)	ϵ_{max}
Benzene	Hexane	204	7,900	256	200		
Toluene	Methanol(2%)	206.5	7,000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

Compound	Solvent	Primary band $\pi \rightarrow \pi^*$ Transition K Band		Secondary 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)	ϵ_{max}
m-Xylene	Methanol	212	7,200	265	300		
p-Xylene	Methanol	212	8,000	274	460		
Benzaidehyde	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 sylfone	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 $\pi \rightarrow \pi^*$ Transition K Band		Secondary 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)	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 (Napthacene)	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	l[a]		
Pyrrole	Hexane	209	6,730	240	300[a]		
Thiophene	Hexane	231	7,100	269.5	1.5[a]		
Pyrazole	Ethanol	214	3,160	-	-		

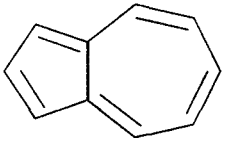
[a] These weak bands may be due to impurities rather than a forbidden transition ($n \rightarrow \pi^*$) of a hetero aromatic molecule.

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.



tropolone

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.



azulene

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

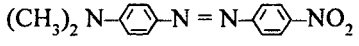
Solvent	Cutoff wavelength, nm	Solvent	Cutoff wavelength, nm
	200-250		250-300
Acetonitrile	210	Benzene	280
n-Butanol	210	Carbon tetrachloride	265
Chloroform	245	N,N-Dimethylformamide	270
Cyclohexane	210	Methyl formate	260
Decahydronapthalene	200	Tetrachloroethylene	290
1, 1-Dichloroethane	235	Xylene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

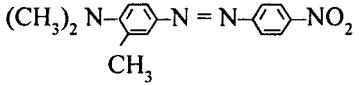
Solvent	Cutoff wavelength, nm	Solvent	Cutoff wavelength, nm
Dioxane	225		
Dodecane	200		300-350
Ethanol	210	Acetone	330
Ethyl ether	210	Benzonitrile	300
Heptane	210	Bromofon-n	335
		Pyridine	305
Hexane	210		
Methanol	215		
Methylcyclohexane	210		350-400
isooctane	210		
isopropanol	215		
Water	210	Nitromethane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

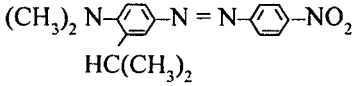
* **Cutoff wavelengths:** i.e. useful wavelength range is beyond the indicated wavelength.

Exercises and problems:

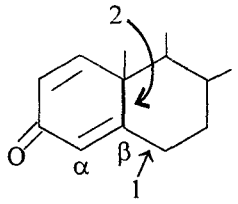
(1) Explain the differences in the electron spectra of compounds (2) and (3) compared to compound (1)

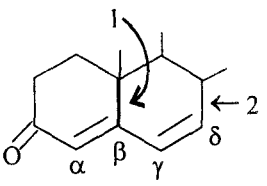
1. 
$\lambda max = 475, \epsilon = 32{,}000$

2. 
$\lambda max = 438, \epsilon = 22{,}000$

3. 
$\lambda max = 420, \epsilon = 18{,}600$

(2) Identify which one of the following two isomers has the electronic absorption band with $\lambda max = 241$ nm and $\epsilon max = 18000$

(1) 

(2) 

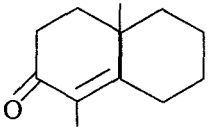
(3) Which structural features may produce a bathochromic or a hypsochromic effect in an organic compound.

(4) Aniline absorbs at 230 nm (∈8600), however, in acid solution the main absorption band is seen at 203 nm (∈7500) and is comparable with benzene. Explain.

(5) o-Nitrophenol gives a UV band at λmax 350 nm when the spectrum is recorded in 0.1 N HCl solution, but the band is observed at λmax 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?

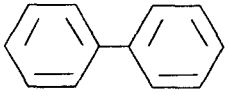
(7) Explain the substitution pattern on the following enone and calculate the position of K band.



(8) The position of absorption of acetone shifts in different solvents: 279 nm (hexane); 272 nm (ethanol) and 264.5 (water). Explain.

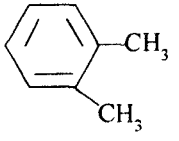
(9) At what wavelength the coloured compounds absorb?

(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

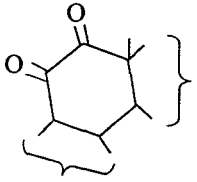
K-Band, λmax → 252,



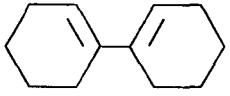
o-xylene

ϵmax → 19,000 λmax 262,
planar conformation ϵmax 270

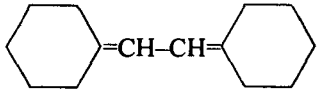
(11) How will you confirm the presence of α-diketone system in the following steroid?



(12) Why the λmax for the diene (I) is observed at lower nm than (II)

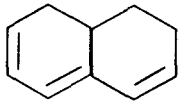


(I)

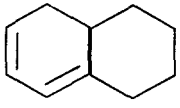


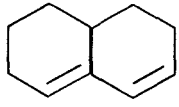
(II)

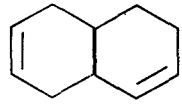
(13) The following triene on partial hydrogenation gives three products. Which are separated by glc. How UV spectroscopy and application of Woodward-Fieser rules will help to identify the products.



$\xrightarrow[pt]{H_2(1eq.)}$ unknown structure $C_{10}H_{14}$







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 → π* 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 (λ = 420 nm), with an accopanying drop of the band intensity (ϵ = 18,600).

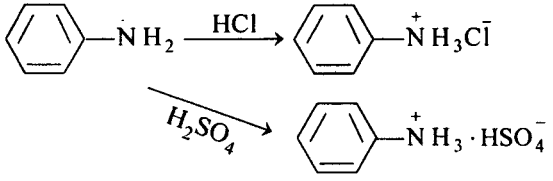
(2) For isomer 1 we find

λ = 215 nm
+ 24 nm (2 × 12)
239 nm

For isomer 2 λ = 215 nm
+ 12 nm (β-substituent)
+ 18 nm (δ-substituent)
+ 30 nm (extra double bond in conjugation)
+ 05 nm (exocyclic double bond)
280 nm

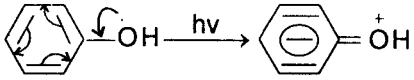
Hence, the absorption spectrum has been measured for isomer I.

(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.

(4) 

Due to the removal of conjugation of the Ione 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 (ϵ7500) and is comparable with benzene.

(5) In 0.1 N HCl solution o-Nitrophenol gives a UV band at λmax 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 ∈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.

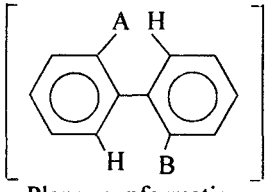
(6) Singlet excited state of the brightening agent is converted into triplet state which emits radiation in the visible range.

(7) One α–substituent, two β–ring residues and one exocyclic double bond: 215 + 10 + 24 + 5 = 254 nm.

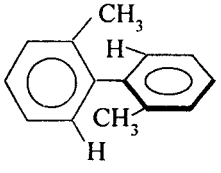
(8) This is the expected shift of the n → π* transition of acetone to shorter wavelength (blue shift) by changing to solvents of increased polarity.

(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.

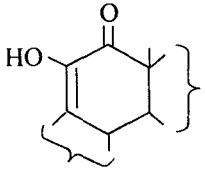


Planar conformation
(A = CH_3 and B = CH_3)
2,2'–Dimethylbiphenyl



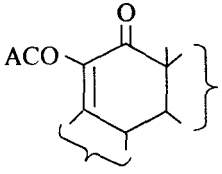
Twist conformation
2,2'–dimethylbiphenyl
B-Band λmax 270, ∈max 800

(11) It will largely exist in the enolic form as revealed by the observed λmax 281 nm (∈max 9,700) which matches with the Cal. λmax (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 → 330 nm.



λ_{max}^{obs} = 281 nm (ϵ_{max} 9700)

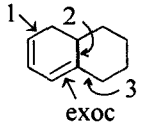
λ_{max}^{calc} = 215 + 2 × 12 + 5 + 35 = 279 nm..

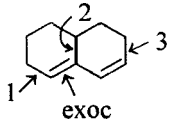


(215 + 2 × 12 + 5 + 6 (OAC)
= 250 nm

(12) In both the dienes, there are 4 ring residues as substituents. In diene (II), the two double bonds are exocyclic, thus in it λmax will be higher by 2 × 5 = 10 nm.

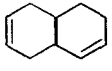
(13) The markedly differed values are expected from each of the structures.





base value	253 nm	214 nm
3 alkyl substituents 3 × 5	15 nm	15 nm
exocyclic C=C	05 nm	05 nm
Calculated or expected	273 nm	234 nm

λmax



< 200 nm (not conj)

□□□

2

Infrared Spectroscopy

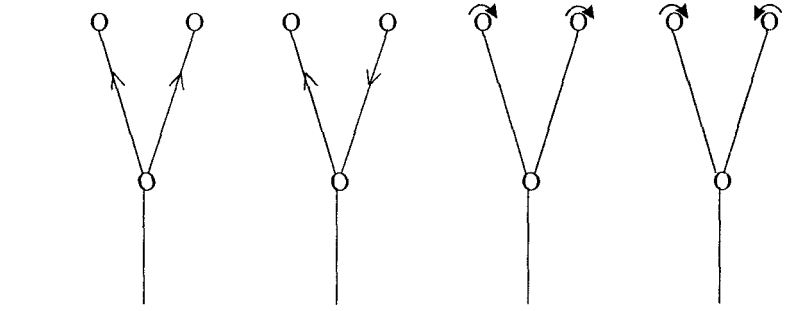


Table 2.la: Characteristic infrarred absorption frequencies of common classes of organic compounds

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	8.51-8.77	s., br.
		840-790	11.90.12.66	m.
$-C(CH_3)_3$	C–H def.	1395-1365	7.17-7.33	s, d. ratio 1:2
	Skeletal	1255-1200	7.97-8.33	s., br., d.
		750-720	13.33-13.89	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 $-(CH_2)_4$ or more	750-720	13.33-13.89	s.
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.**	3310-3300	3.02-3.03	m.
Terminal/ monosubstituted (RC≡CH)	C–H def.	600-650	16.7-15.4	s.
	C≡C str.	2140-2100	4.67-4.76	w.
Nonterminal/ unsymmetrically disubstituted $R_1C{\equiv}CR_2$	C≡C str.	2260-2190	4.42-4.57	υ.

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.
Prirnary 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	C(C)(C)–C–O str.	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				
Fonnates	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	3.47-3.77	w.-m., d.
		975-780	10.26-12.82	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	2.83-2.88	s.
		3420-3380	2.92-2.96	s.
bonded NH	N–H str.	3360-3320	2.98-3.01	m.
		3220-3180	3.11-3.15	m.
Free or bonded NH	N–H def. plus C–N str.	1650-1620 (amide II band)	6.06- 6.17	s.
		1620-1590 (amide II band)	6.17-6.29	s.
Secondary, free NH	N–H, cis str.	3440-3420	2.91-2.93	s.
	N–H, trans str.	3460-3430	2.89-2.92	s.
bonded NH	N–H, cis str.	3180-3140	3.15-3.19	m.
	N–H, trans str.	3330-3270	3.00-3.06	m.
	N–H, cis and trans. str.	3100-3070	3.23-3.26	w.
	N–H def.	Ca.700 (amide V band)	Ca 14.30	conc. dependent
	N–H def. plus C–N str.	1305-1200 (amide III band)	7.67-8.33	m.
Acyclic compound	N–H def. plus C–N str.	1570-1515 (amide II band)	6.37-6.60	s.
		1550-1510 (amide II band)	6.45-6.62	s.

		770-620 (amide IV band)	13 00-16.13	m.
		630-530 (amide VI band)	15.87-18.87	s.

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

9. Unsaturated nitrogen compounds

a) Nitriles				
saturated alkyl	C ≡ N str.	2260-2240	4.42-4.46	m.
α, β unsaturated alkyl	C ≡ N str.	2235-2215	4.47-4.51	s.,v.
Aryl	C ≡ N str.	2240-2220	4.46-4.50	m.
Iso-	C ≡ 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. (R–N–N–O)	N–O str.	1310-1250	7.63-8.00	m., –s.

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_2Cl)	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_2SO_2)	S=O str., asym	1160-1120	8 62-8.93	v., -s.
Sylfonic acids	S=O str., sym.	1260-1150	7.94-8.70	s.
(RSO_3H)	S=O str., asyin.	1080-1010	9.26-9.90	s.
Sylfites $(RO)_2SO$	S=O str.	1220-1170	8.20-8.55	s.
Sylfoxides (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, $CR_1R_2=CH_2$)	C–H str.
3030-2500	3.30-4.00	w., mlt.	Amino acid hydrochlorides	

3000-2001				
2975-2950	3.36-3.39	m.	Alkanes ($-CH_3$)	C–H str.
2940-2915	3.40-3.43	m.	Alkanes ($-CH_2-$)	C–H str.
2905-2875	3.44-3.48	w.	Alkanes (–CH–) ·	C–H str.
2880-2860	3.47-3.50	m.	Alkanes ($-CH_3$)	C–H str.
2880-2650	3.47-3.77	w.-m., d.	Aldehydes (–CHO)	C–H str.
2870-2845	3.49-3.52	m.	Alkanes ($-CH_2-$)	C–H str.
2835-2815	3.53-3.55	m.	Ethers ($-O-CH_3$)	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 ($O-CH_2-O-$)	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 ($C=NH^+$)	NH^+ str.
2280-2260	4.39-4.43	s.	Diazonium salts $(R-C=N=N)^+$	
2280-2080	4.39-4.81	v.	Organo-silicon compounds	Si–H str.
2275-2240	4.40-4.46	v.	isocyanates	N=C=O str.
2260-2240	4.43-4.46	w.-m.	Saturated nitrites	C≡N str.
2240-2220	4.46-4.51	m.-s.	Aryl nitrites	C≡N str.
2235-2215	4.47-4.52	s.	Acyclic α, β unsat. nitriles	C≡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≡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≡CH)	C≡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.
2000-1501				
ca. 2000	ca. 5.00	w.	Amino acid hydrochlorides	
1970-1950	5.08-5.13	m.	Allenes (C=C=C)	C≡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.	Acychc 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.
i750-1735	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.
i740-1720	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	C=O str.
			secondary amide.	
			amide I bind	
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 ($CR_1R_2=CH_2$)	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_6H_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	6.29-636	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	6.33-637	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.
1500-1001				
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.

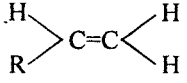
1430-1400	7.0-7.14	v.	Ketones, esters, α-methylene C–H scissor	C–H def.
1430-1350	7.00-7.41	s.	Sulfites	S=O str.
1420-1410	7.04-7-09	s.	Alkenes ($RCH=CH_2$ or $R_1R_2C=CH_2$)	C–H def.
1420-1390	7.04-7.20	w.	Alcohols	O–H def.
1410-1310	7.10-7.60	s.	Phenols, tert. alcohols	O–H def.
1400-1300	7.15-7.69	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	735-7.64	s.	Aromatic tert. amines	C–N vib.
1350-1300	7.41-7.69	s.	Sulfones, sulfonamides	S= 0 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	$-\overset{\overset{O}{\parallel}}{C}-O-R$ 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	

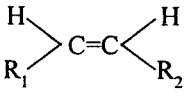
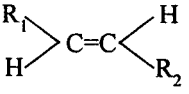
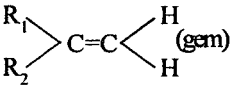
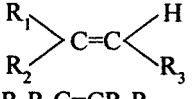
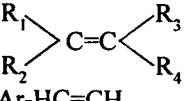
1255-1200	7.97-833	s., d.	Alkanes, tert. butyl	Skeletal str.
1240-1190	8.06-8.40	v.	Aromatic phosphorus comp.	P–O str.
1230-1150	8.13-8.70	s.	Sulfites	S=O str.
1210-1150	8.27-8.70	s.	Sulfonic acids	S=O str.
1220-1020	8.20-9.80	w.	Aliphatic amines	C–N vib.
ca. 1200	ca. 8.33	s.	Phenols	C–O str.
1200-1050	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 benzens	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.
1000-501				
995-985	10.05-10.15	s.	Monosubstituted alkenes ($RCH=CH_2$)	C–H def.
970-960	10.31-10.42	s.	Disubstituted alkenes ($R_1CH=CHR_2$) 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.	Trisubstitutated 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 ($R_1CH=CHR_2$) 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	

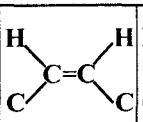
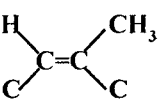
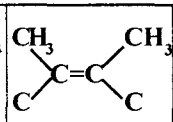
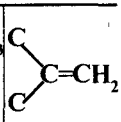
Table 2.2a: Infrarred absorption frequencies of alkenes

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
	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
$R_1CH=CHR_2$(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
$R_1CH=CHR_2$ (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
$R_1R_2C=CH_2$ (Vinylidine)				
	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
$R_1R_2C=CHR_3$	C–H str.	3040-3010	3.29-3.32	m
(Trisubstituted)	C=C str.	1675-1665	5.97-6.01	v
	C–H o–o–p def.	840-790	11.90-12.66	m
$R_1R_2C=CR_3R_4$				
(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 = mediurn, 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: Absorotion frequencies typical of aromatic homocyclic compounds:

Arormatic compound	Vibration mode	Frequency, cm^{-1}	Wave-length, μ	Relative Intensity
Monsubstituted	=C–H str. (Multiple bands)	3080-3030	3.24-3.33	w-m
(five adjacent	C=C str. (ring	1604 ± 3	6.25-6.22	v
hydrogen atoms)	stretching)	1585 ± 3	6.31-6.30	v
		1510→1480*	6.62 →6.75	v
		1452 ± 4	6.87-6.91	v
	C–H i–p def.	1177 ± 6(2,5 vs 3,6)	8.45-8.54	w
		1156 ± 5(3,5 vs 4)	8.61-8.69	w
		1073 ± 4(2,6 vs 3,4,5)	9.28-9.36	
		1027 ± 3(2,3 vs 5,6)	9.71-9 77	w
	C–H o–o–p def.	751 ± 15	13.06-13.58	s
		697 ± 11	14 1-14 58	s
1, 2-Disubstituted	=C–H str (multiple	3080-3030	3 24-3.33	w-m
(four adjacent	bands)	1607 ± 9	6.26-6 19	v
hydrogen atoms)	C=C str. (ring	1577 ± 4	6 33-6 36	v
	stretching)	1510 → 1460	6.85-6 62	v
		1447 ± 10	6.87-6 96	v
	C–H i–p def.	1269 ± 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	=C–H str.	3080-3030	3 24-3.33	w-m
(three adjacent	(multiple bands)			
hydrogen atoms)	C=C str	1600 → 1620	6 25 → 6.17	v
	(ring stretching)	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	=C–H str (multiple	3080-3030	3.24-3.33	w-m
(two adjacent	bands)	1606 ± 6	6.20-6.25	v
hydrogen atoms)	C=C str. (ring	1579 ± 6	6 31-6.36	v
	stretching)	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.	3080-3030	3.24-3.33	w-m
	(multiple bands)			
	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	3080-3030	3 24-3 33	w-m
	bands)			
	C=C str (ring	1616 ± 8	6 15-6.22	v
	stretching)	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 151 0 → 1480 indicates the range, in cm^{-1}, of absorption of radiation. Usually an electron donor substitutent causes absorption near 1510 cm^{-1}, while an electron acceptor substitutent 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 = 0 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		1830-1780	5.47-5-62
and aryl, acyclic		1770-1720	5.65-5-81
	Benzoic anhydride ($CHCl_3$)	1818 and 1740	5.50 and 5.75
d. α, β- Unsaturated,		1850-1800	5.41-5.56
5 membered ring		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		1715-1690	5.83-5.92
aliphatic			
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		1685-1665	5.94-6.01
	Methyl vinyl ketone (CCl_4)	1686	5.93
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		1700-1680	5.88-5.95
	propiophenone (CCl_4)	1686	5.93
g. Diaryl		1670-1660	5.99-6.02
	Benzophenone ($CHCl_3$)	1669	5.99
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)	1675and shoulder at 1705	5.97and 5.86 (sh.)
c. Tertiary, solid and all solutions		1670-1630	5.99-6.14
	N, N–dimethyl–(CCl_4) acetamide	1660 and shoulder at 1710	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
1. 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,	~1730	~5.78
6-membered ring	~1670	~5.99
p. Imides, cyclic,	~1770	~5.65
5-membered ring	~1700	~5.88
q. Imides, cyclic, α, β-	~1790	~5.59
unsaturated, 5-membered ring	~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**	**Substract cm^{-1}**
Basic value in CCl_4	1720	Neat solid or liquid state	10
Solvent			
Hydrocarbon solvents	7	$CHCl_3$, $CHBr_3$, CH_3CN (partially polar)	15
Ring strain		Ring strain	
Angle decreases 6 → 5 ring	35	Angle increases 6 → 7 to 10 ring	10

Bridged systems	15
Substitution on α-carbon (Field and inductive effects)	
Substituent cis oriented and Coplanar	
–Cl, –Br, –OR	20
–OH, and –OAC	
Substituent trans and nonplanar	Nil
Alkyl group substituted by electronegative atoms or groups	
–H (aldehyde)	10
–OR (ester)	25
–OH (monomeric acid)	40
–O–C=C (vinyl ester)	50
–Cl (acid chloride)	90
–OCOR (anhydrides)	100

Substitution on α-carbon	
Each alkyl group	5
Alkyl groups substituted by amine	
$-NH_2$ (amide)	5
–NHMe (monosubstituted amide)	30
$-NMe_2$ (disubstituted amide)	55
Intramolecular hydrogen bonding	
Weak: α or β-OH ketone	10
Medium: o–OH arylketone	40
Strong : β-diketone	100
Intermolecular hydrogen bonding	
Weak: ROH.....O=C<	15
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	C-N	C=O	C–O	Other vibrations
	asym	sym	deformation	stretching	stretching	stretching	and remarks
Primary amines	3550-3350 (2.82-2.99μ)	3450-3250 (2.90-3.08μ)	1650-1580 (6.06-6.33μ)	1220-1020 (ali) (8.2-9.8μ) 1340-1250 (aro) (7.46-8.0μ)			Shoulder at 3200 (3.12μ), overtone of 1610 (6.21μ) band N–H wagging strong band at 850-750 (11.76-13.34μ)
Scondary amines	3550-3350 (2.82-2.99μ)		1650-1550 (6.06-6.45μ)	1350-1280 aro (7.41-7.81μ)			N–H wagging strong band at 750-700 (13.34-14.29μ) –N–H def. band often masked by aromatic band in aromatic compounds
Tertiary amines				1380-1260 aro (7.24-7.94μ)			N–Me band in secondary and tertiary. amines. observed at 2820-2760 (3.54-3.62μ)
Amine hydrochloride chloride	About 3380, (2.96μ) NH^{+}_{3} str.		About 1600 (6.25μ) asym.				

Compound	N-H stretching asym	N-H stretching sym	N-H deformation	C-N stretching	C=O stretching	C–O stretching	Other vibrations and remarks
Charged amine derivatives	About 3280, (3.05μ) NH^+_3 str. 3350-3150, NH^+_3 str. (2.99-3.17μ) (12.5μ) NH^+_3 solid phase		About 1300 (7.7μ) sym. About 800 rock				
Primary amino acids	3125-3030 (3.2-3.3μ)		1660-1610 band I (6.02-6.21μ)		1600-1560 ionized (6.25-6.41μ) carboxyl str.		Weak band at 2760-2530 (3.62-3.96μ)
			1550-1485 band II (6.45-6.74μ)				Medium band at 1300 (7.69μ)
Dicarboxylic amino acids					1755-1720 (5.7-5.81μ) unionised carboxyl str.		
Amino acid hydrochlorides	3130-3030 (3.2-3.3μ)		1610-1590 band I (6.21-6.29μ)		1755-1730 (5.7-5.78μ)	1230-1215 (8.13-8.23μ)	Series of bands between 3030 and 2500 (3.3 and 4.0μ)
			1550-1480 band II (6.45-6.75μ)		Unionised carboxyl str.		
Amino acid sodium salts	3400-3200 (2.94-3.13μ) Two bands				1600-1560 (6.25-6.14μ) 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 CgH_7N 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)

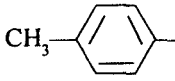
* [For a molecule (CwHxNyOz, the total number of rings and double bonds is obtained by the formula R = 1/2 (2w –x + y + 2)

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≡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

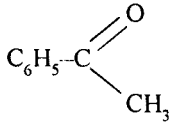


p–toluonitrile

(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}.

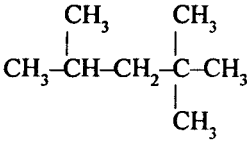
(3) Deduce the structure:

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

$[(CH_3)_2CH]$ $[C(CH_3)_3]CH_2$

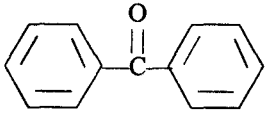
Therefore, the compound is



2,2,4–trimethylpentane

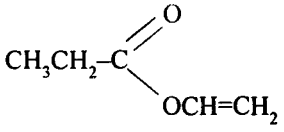
(4) From the following examples, we can readily see the usefulness of **Table 2.5** in predicting the values of C=O absorption bands. The wavenumbers for C=O stretching vibrations for a number of compounds are calculated as follows:

a. Benzophenone in chloroform



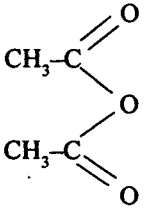
Basic value for C=O absorption	1720 cm^{-1}
Shift due to benzene rings 2 × 20	– 40 cm^{-1}
Shift due to solvent $CHCl_3$	– 15 cm^{-1}
Calculated	1665 cm^{-1}
Observed	1669 cm^{-1}

b. Vinyl propionate in CCl_4



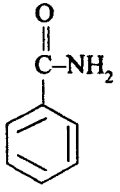
Basic value for C=O absorption	1720 cm^{-1}
Vinyl ester (–O–C=C) shift	+ 50 cm^{-1}
Alkyl group on a carbon	– 5 cm^{-1}
Calculated	1765 cm^{-1}
Observed	1760 cm^{-1}

c. Acetic anhydride in CCl_4



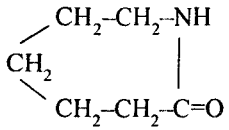
Basic value for C=O absorption	1720 cm^{-1}
Anhydride (–O–COR)	+ 100 cm^{-1}
Calculated	1820 cm^{-1}
Observed	1825 cm^{-1}

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 $C_4H_6O_2$. 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 CCl_4 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 $RHC{=}CH_2$ (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 $C_4H_6O_2$, only two structures with an –ene and an ester carbonyl group can be written.

(a) $CH_2 = CH - C(=O)-O-CH_3$ methyl acrylate (an α, β-unsaturated ester)

(b) $CH_3 - C(=O)-O\cdot CH = CH_2$ vinyl acetate

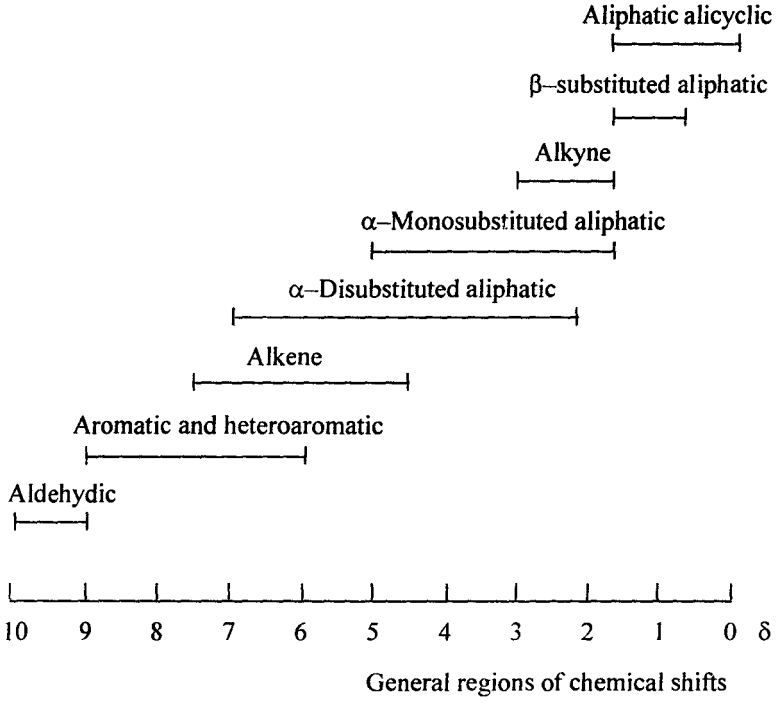
The two structures can be distinguished on the basis of their C=O stretching frequencies. We can calculate C=O stretching frequency in each case

a)	Basic value	1720 cm^{1}	since the observed value is
	OR (ester)	+ 25 cm^{1}	1765 cm^{-1} the compound is (b)
	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	$-CH_2X$	–CHX
H	0.23	0.90	1.25
CH_3or CH_2–	0.86	1.2	1.55
C=C–	1.6	2.1	
C≡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
C–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
C≡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_3X	$-CH_2X$	$-CHX$
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_2R		3.1	
SO_3R	3.0		
PR_2		2.4	
P^+Cl_3	3.32	3.4	
POR_2		2.4	
PSR_2		2.8	

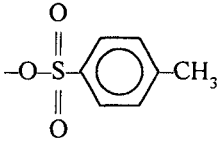
OTs is 

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

Functional group X	CH_3–C–X	$-CH_2$–C–X	–CH–C–X
CH_2–	0.86	1.2	1.55
C=C–	1.0	1.36	1.76
C≡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
C≡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:

(Y–CH_2–Z and Y–CH–Z)
|
W

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

$$\therefore \quad \delta = 0.23 + \Sigma\sigma i$$

Thus, to calculate the shift for the –CH_2– protons of $C_6H_5CH_2Br$

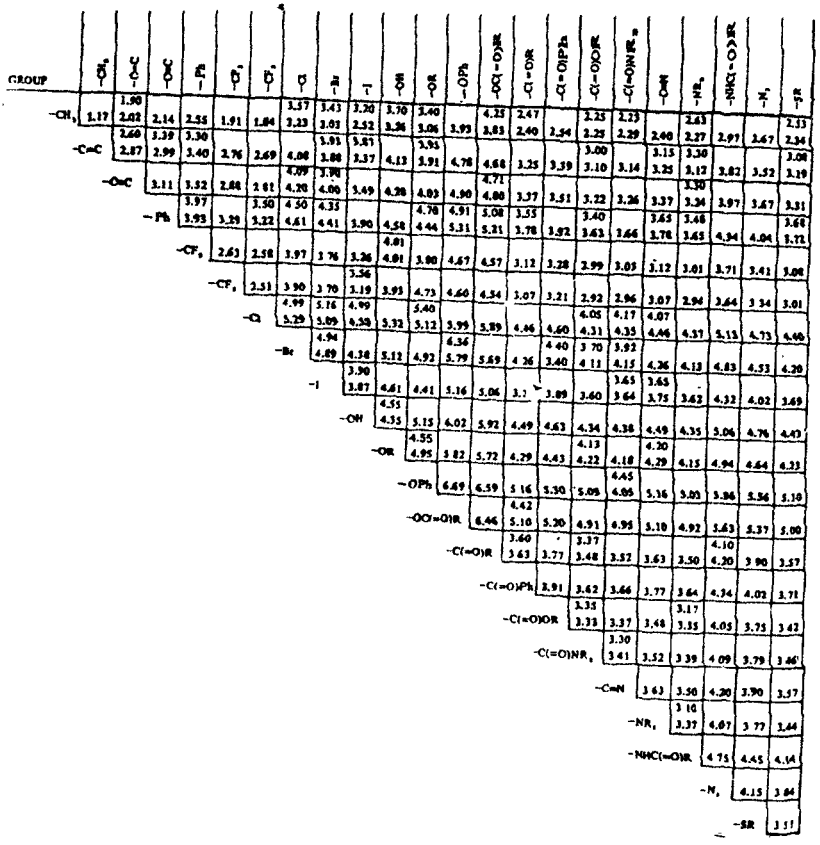
C_6H_5	=	1.85
Br	=	2.33
		4.18
add CH_4		**0.23**
		4.41

Table 3.3: Shielding constants

Functional group Y or Z	Shielding Constants σi
CH_3	0.47
C=C	1.32
C≡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
C≡N	1.70

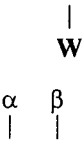
Functional group Y or Z	Shielding Constants σi
NR_2	1.57
NO_2	4.44
N=C=S	2.90
C≡C–Ar	1.70
NHCOR	2.27
N_3	1.97
SR	1.64
OSO_2R	3.13

The shielding constants were used to prepare the following chart 3.3.1.



This chart can be used to find the shift position of a methylene –roup 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 $BrCH_2CH_2OCH_2CH_2$ Br can be calculated.

CH_2 No. 1	
CH_2 (Table 3, 4, footnote a)	1.20
α–OR	2.35
β–Br	0.60
	4.15
CH_2 No. 2	
CH_2	1.20
α–Br	2.18
β–OR	0.15
	3.53

Determined: CH_2 No. 1 at ~δ 3.80;
CH_2 No. 2 at ~δ 3.40

Table 3.4: Substitutent 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
–C=C–C–R ‖ X	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	
O O ‖ ‖ –O–C–R, –O–C–OR	CH_3	2.88	0.38
–OAr	CH_2	2.98	0.43
	CH	3.43 (esters only)	
O ‖ –CR, Where R is alkyl,	CH_3	1.23	0.18
aryl, OH, OR', H, CO, or N	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 CH_3, δ 0.87; CH_2, δ 1.20; CH, δ 1.55.

3.3: Chemical Shifts in Alicyclic and Heterocyclic Rings

Table 3.5: Chemical shifts in Alicyclic Rings

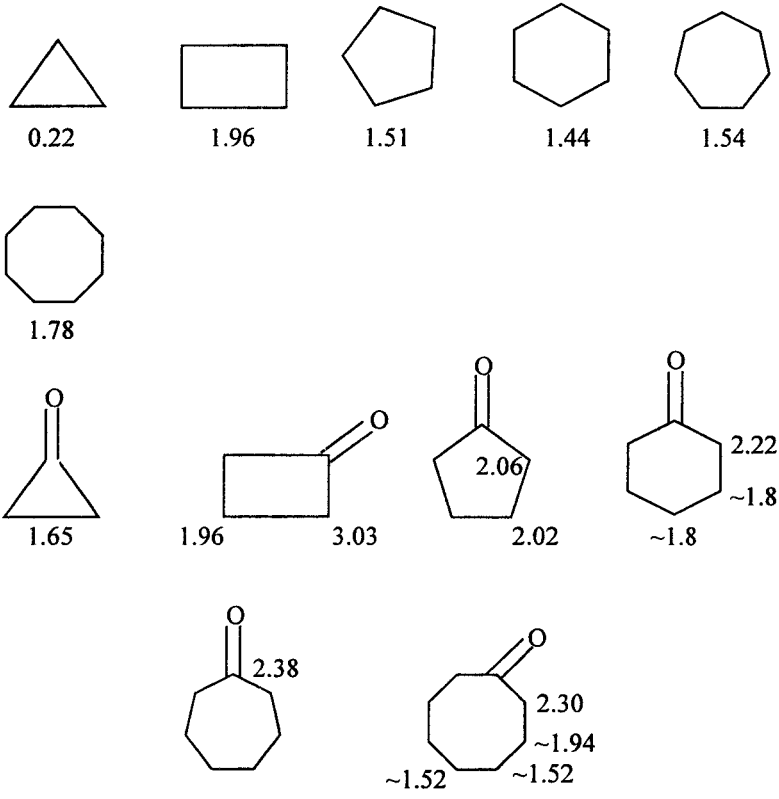
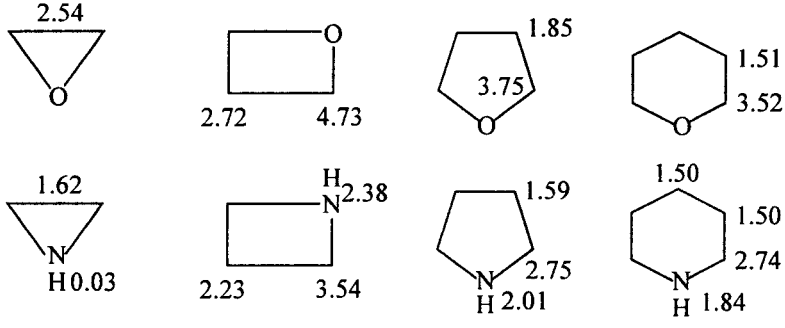
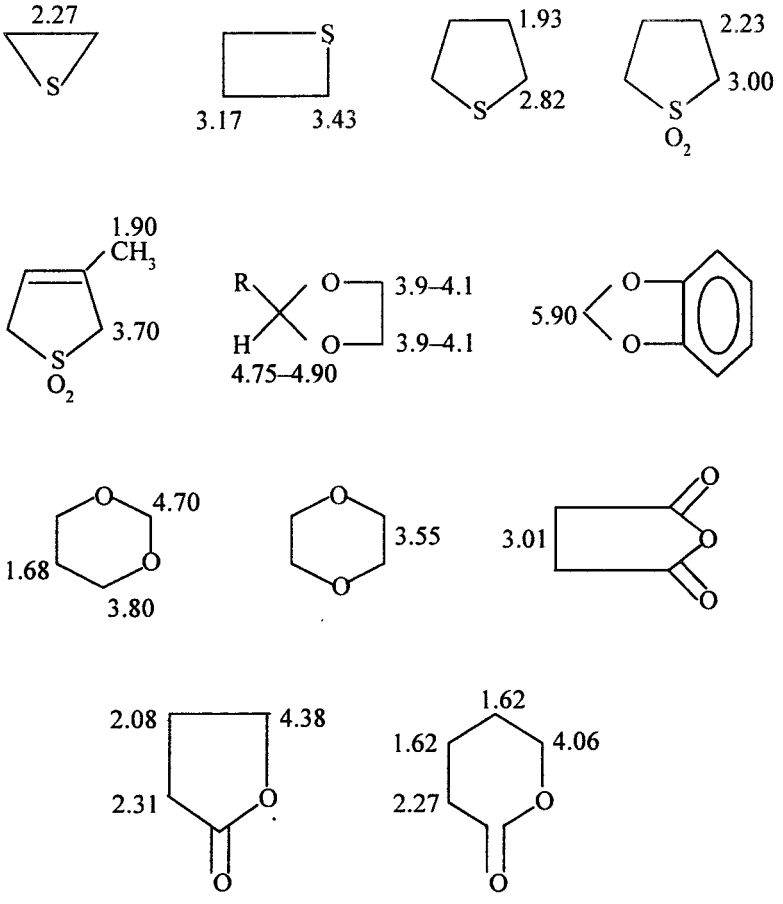
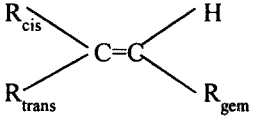


Table 3.6: Chemical Shifts in Heterocyclic Rings





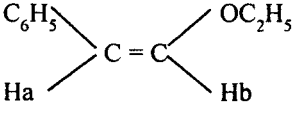
3.4: Chemical Shifts in Unsaturated and Aromatic Systems



$\delta H = 5.25 + \Sigma zi$

i.e. 5.25 + Zgem + Zcis + Ztrans

For example, the chemical shifts of the alkene protons in

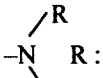
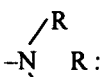


are calculated

Ha	C_6H_5 gem	1.35	5.25
	OR trans	–1.28	0.07
		0.07	δ,5.32
Hb	ORgem	1.18	5.25
	C_6H_5 trans	–0.10	1.08
		1.08	δ 6.33

Table 3.7: Substituent Constants (Z) for chemical shifts of substituted Ethylenes (in CCl_4)

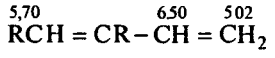
Substituent R	Z		
	gem	cis	trans
–H	0	0	0
–Alkyl	0.44	–0.26	–0.29
–Alkyl ring[a]	0.71	–0.33	–0.30
$-CH_2O$, $-CH_2I$	0.67	–0.02	–0.07
$-CH_2S$	0.53	–0.15	–0.15
$-CH_2Cl$, $-CH_2Br$	0.72	0.12	0.07
$-CH_2N$	0.66	–0.05	–0.23
–C≡C	0.50	0.35	0.10
–C≡N	0.23	0.78	0.58
–C=C	0.98	–0.04	–0.21
–C=C conj[b]	1.26	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
$-C(H)=O$	1.03	0.97	1.21
$-C(N)=O$	1.37	0.93	0.35
$-C(Cl)=O$	1.10	1.41	0.99
–OR, R: aliph	1.18	–1.06	–1.28

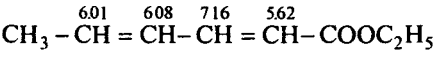
–OR, R: Conj[b]	1.14	–0.65	–1.05
–OCOR	2.09	–0.40	–0.67
–Aromatic	1.35	0.37	–0.10
–Cl	1.00	0.19	0.03
–Br	1.04	0.40	0.55
 R : aliph	0.69	–1.19	–1.31
 R : Conj[b]	2.30	–0.73	–0.81
–SR	1.00	–0.24	–0.04
$-SO_2$	1.58	1.15	0.95

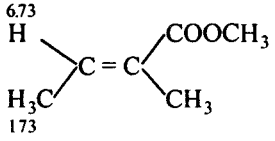
[a] Alkyl ring indicates that the double bond is part of the ring

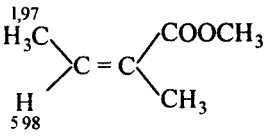
[b] The Z factor for the conjugated substitutent is used when either the substitutent or the double bond is further conjugated with other groups.

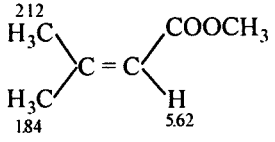
Table 3.8: Chemical Shifts of Miscellaneous Alkenes

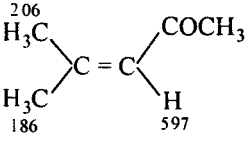


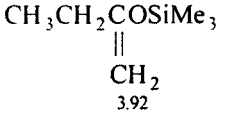


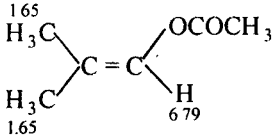


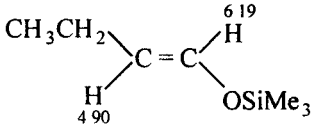


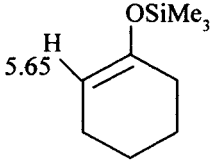


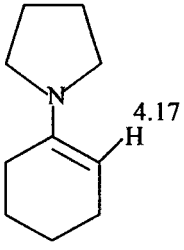


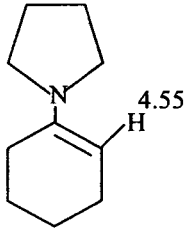

CH3CH2COSiMe3
CH2
3.92

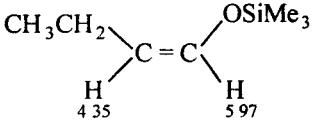

1.65
H3C
OCOCH3
C = C
H3C
H
6.79
1.65

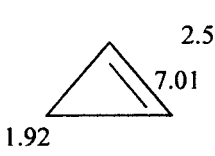

6.19
CH3CH2
H
C = C
H
OSiMe3
4.90

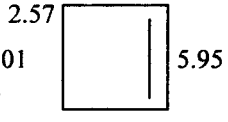

OSiMe3
H
5.65

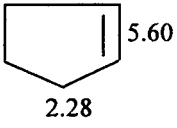

N
4.17
H

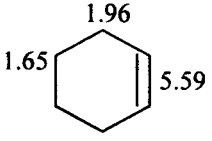

N
4.55
H

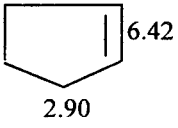

CH3CH2
OSiMe3
C = C
H
H
4.35
5.97

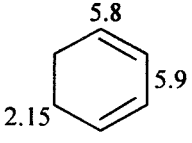

7.01
1.92

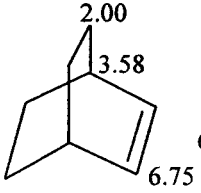

2.57
5.95

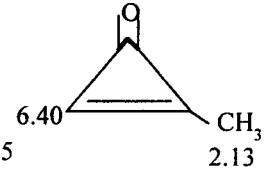

5.60
2.28

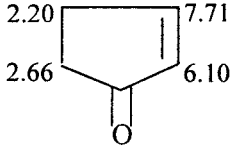

1.96
1.65
5.59

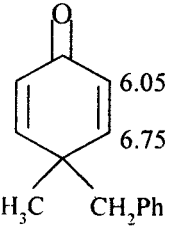

6.42
2.90

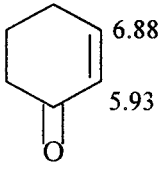

5.8
5.9
2.15

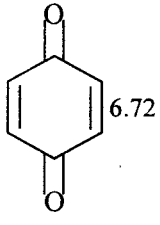

2.00
3.58
6.75


O
6.40
CH3
2.13


2.20
7.71
2.66
6.10
O


O
6.05
6.75
H3C
CH2Ph


6.88
5.93
O


O
6.72
O

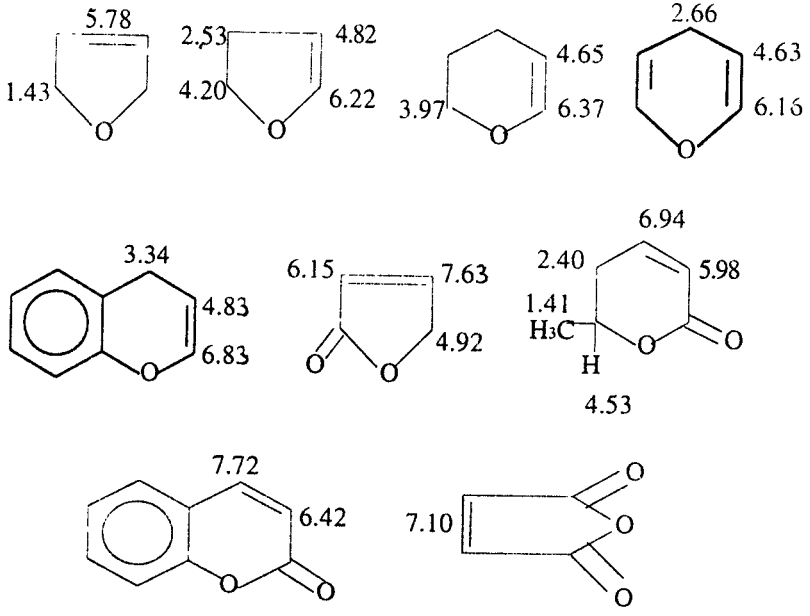


Table 3.9: Chemical Shifts of Alkyne Protons

HC≡CR	1.73–1.88
HC≡C–COH	2.23
HC≡C–C≡CR	1.95
HC≡CH	1.80
HC≡CAr	2.71–3.37
HC≡C–C≡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_3 CH_2 (omp)	7.16
$(CH_3)_2CH$ (omp)	7.16
$(CH_3)_3$ C (o, m, p)	7.32, 7.17, 7.04
C = CH_2 (omp)	7.25
C≡CH o, (mp)	7.44, 7.25
Phenyl o, m, p	7.44, 7.25, 7.16
CF_3 (omp)	7.50
CH_2 Cl (omp)	7.25
$CHCl_2$ (omp)	7.36
CCl_3 o, (mp)	8.10, 7.50

CH_2 OH (omp)	7.16
CH_2OR (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

[a]OTs = p – Toluenesulfonyloxy group

Table 3.11: Chemical shifts of protons on fused aromatic rings

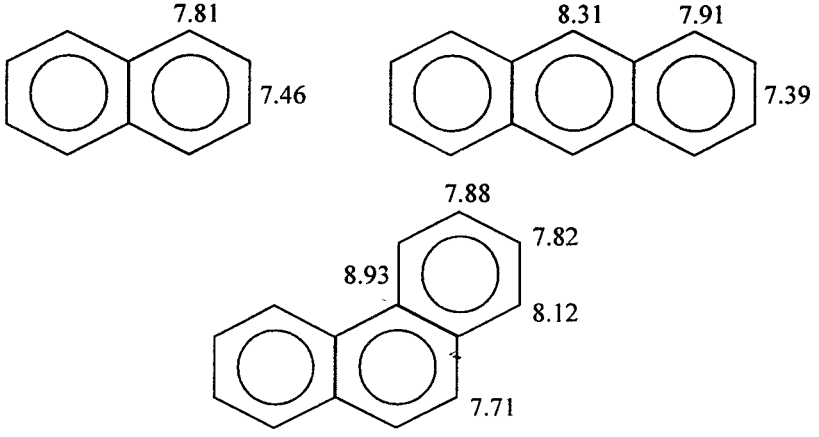


Table 3.12: Chemical shifts of protons on Heteroaromatic Rings

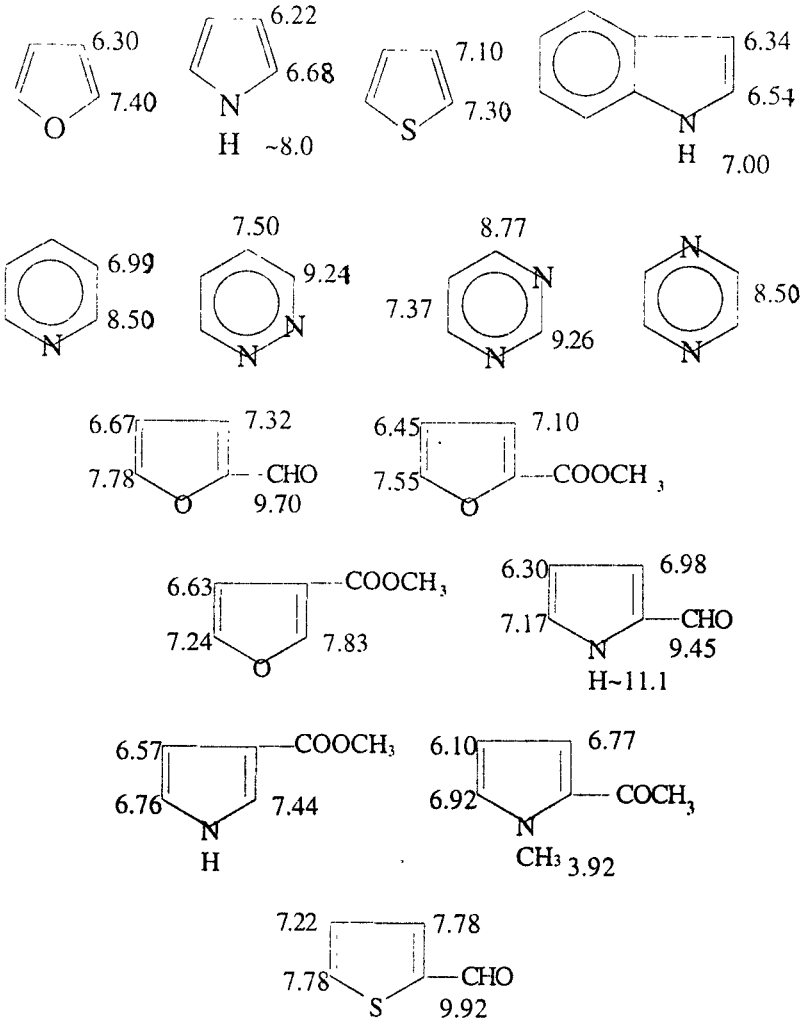
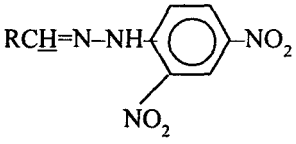


Table 3.13: Chemical Shifts of HC=O, HC=N, (also HC(=O)–O) Protons

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
	6.05

3.5: Protons on Heteroatoms

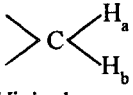
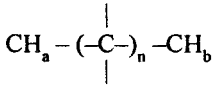
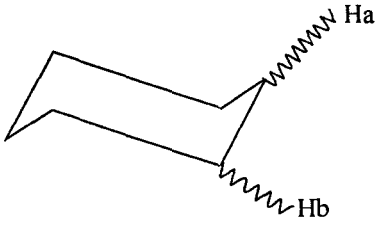
Table 3.14: Protons subject to Hydrogen. Bonding Effects (protons on Heteroatoms)[a]

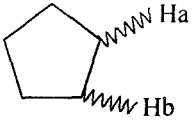
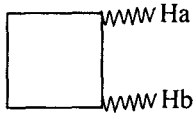
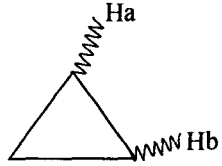
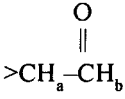
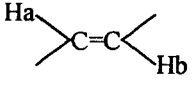
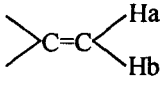
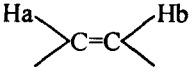
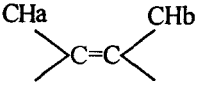
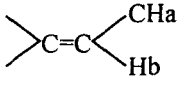
Proton	Class	δ
OH	Carboxylic acids	~13.2– ~10.0
	Sulfonic acids	12.0–10.0
	Phenols	~7.5– ~4.0
	Phenols (intramolecular H bond)	12.5–5.5
	Alcohols	4.0–0.5
	In DMSO	6.2–4.2
	Enols (cyclic α– diketones)	6.9–6.0
	Enols (β– diketones)	16.5–14.5
	Enols (β– ketoesters)	10.6–9.6
	Water (Bulk water as suspended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

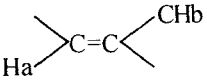
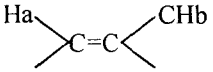
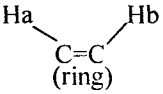
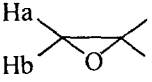
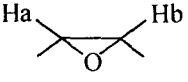
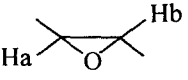
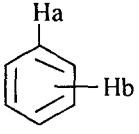
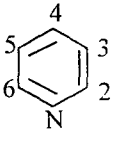
Proton	Class	δ
NH_2 and NHR	Alkyl and cyclic amines	3.0–0.5
	Aryl amines	5.0–3.0
	Amides	8.7–5.0
	Urethanes	7.6–4.6
	Amines in trifluoroacetic acid	8.7–6.0
SH	Aliphatic mercaptans	1.7–1.3
	Thiophenols	3.6–2.8

[a] Solvent $CDCl_3$. 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)

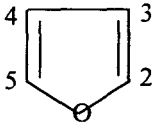
3.6: Proton Spin Coupling Constants

Type	Jab (Hz)	Jab Typical
Geminal		
	0–30	12–15
Vicinal		
$CH_a - CH_b$ (free rotation)	6–8	7
	0–1	0
		
ax–ax	6–14	8–10
ax–eq	0–5	2–3
eq–eq	0–5	2–3

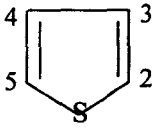
	cis 5–10	
(cis or trans)	trans 5–10	
	cis 4–12	
(cis or trans)	trans 2–10	
	cis 7–13	
(cis or trans)	trans 4–9	
$CH_a–OH_b$ (no exchange)	4–10	5
	1–3	2–3
	5–8	6
	12–18	17
	0–3	0–2
	6–12	10
	0–3	1–2
	4–10	7

	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≡CHb	9.5–9.8	9.1
CHa–C≡CHb	2–3	
–CHa–C≡C–CHb	2–3	
		6
		4
		2.5
	J (ortho)	6–10
	J (meta)	1–3
	J (para)	0–1
	J (2–3)	5–6
	J (3–4)	7–9
	J (2–4)	1–2
	J (3–5)	1–2
	J (2–5)	0–1
	J (2–6)	0–1

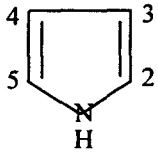
	9
	3
	~0
	5
	8
	1.5
	1.5
	1
	~0



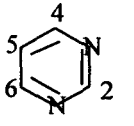
J (2–3)	1.3–2.0	1.8
J (3–4)	3.1–3.8	3.6
J (2–4)	0–1	~0
J (2–5)	1–2	1.5



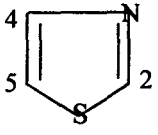
J (2–3)	4.9–6.2	5.4
J (3–4)	3.4–5.0	4.0
J (2–4)	1.2–1.7	1.5
J (2–5)	3.2–3.7	3.4



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

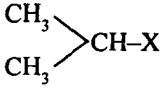


J (4–5)	4–6
J (2–5)	1–2
J (2–4)	0–1
J (4–6)	2–3



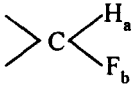
J (4–5)	3–4
J (2–5)	1–2
J (2–4)	~0

6.5–7.5

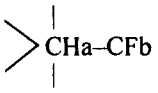


5.5–7.0

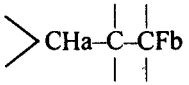
Proton Fluorine



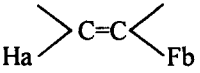
44–81



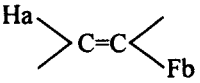
3–25



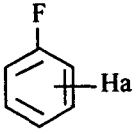
0–4



1–8

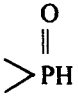


12–40



o–6–10
m–5–6
p–2

Proton Phosphorus



630–707

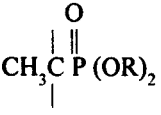
$(CH_3)_3$ P — 2.7

$(CH_3)_3P{=}O$ — 13.4

$(CH_3CH_2)_3P$ — 13.7 (HCCP) 0.5 (HCP)

$(CH_3CH_2)_3$ P=O — 16.3 (HCCP) 11.9 (HCP)

10–13



15–20

$CH_3OP(OR)_2$ — 10.5–12

$P[N(CH_3)_2]_3$ — 8.8

$O{=}P\ [N(CH_3)_2]_3$ — 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	11.53(l)	2
64.078	2.03 (5)	
Acetone – d_6	2.04(5)	2.2
64.117		
Acetonitrile – d_3	1.93 (5)	2.5
44.071		
Benzene – d_6	7.15 (br)	
84.152		
Chloroform – d	7.24(l)	
120.384		
Cyclohexane – d_{12}	1.38 (br)	
96.236		
Deuterium oxide	4.63	
20.028	(DSS)[b]	
	4.67	
	(TSP)[b]	
1,2 – Dichloroethane–d_4	3.72 (br)	
102.985		
Diethyl–d_{10} ether	3.34 (m)	
84.185	1.07 (m)	
Diglyme –d_{14}	3.49 (br)	
148.263	3.40 (br)	
	3.22 (5)	1.5
N, N –Dimethylformamide –d_7	8.01 (br)	
80.138	2.91(5)	2
	2.74 (5)	2
Dimethyl – d_6 sulphoxide	2.49 (5)	1.7
84.170		

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	5.26 (1)		
deuterate, 198.067			
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(l)	
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–d_4. Both are reference standards used in aqueous solutions.

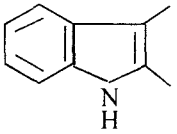
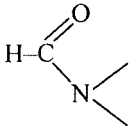
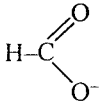
NMR table showing correlations of chemical shifts of protons

	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	0.95–0.85
		(8.7–9.3)	(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.		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.	$-CH_2-C-CO-R$	8.10–8.40	1.9–1.4
20.	$CH_3-C{=}C$	8.1–8.4	1.9–1.4
21.	$CH_3-C{=}C-$ with O–CO–R on the first C	8.09–8.13	1.91–1.87
22.	$-CH_2-C{=}C-O-R$	8.07	1.93
23.	$-CH_2-C-Cl$	8.04–8.40	1.96–1.60
24.	$CH_3-C{=}C-$ with COOR or CN on the first C	7.97–8.06	2.03–1.94
25.	$-CH_2-C-Br$	7.97–8.32	2.03–1.68
26.	$CH_3-C{=}C-CO-R$	7.94–8.07	2.06–1.93
27.	$-CH_2-C-NO_2$	7.93	2.07
28.	$-CH_2-C-SO_2-R$	7.84	2.16
29.	–C–O with both C and O bonded to CH (ring)	7.71	2.29
30.	$-CH_2-C{=}C$	7.69–8.17	2.31–1.83
31.	CH_3-N-N-	7.67	2.33
32.	$-CH_2-CO-R$	7.61–7.98[b]	2.39–2.02
33.	CH_3-SO-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.	$-CH_2-S-R$	7.47–7.61	2.53–2.39
36.	$CH_3-CO-SR$	7.46–7.67	2.54–2.33
37.	$-CH_2-C{\equiv}N$	7.42	2.58
38.	$CH_3-C{=}O$	7.4–7.9 (7.4–8.1)	2.6–2.1 (2.6–1.9)
39.	$CH_3-S-C{\equiv}N$	7.37	2.63
40.	$CH_3-CO-C = C$ or $CH_3-CO-Ar$	7.32–8.17	2.68–1.83
41.	$CH_3-CO-Cl$ or Br	7.19–7.34	2.81–2.66
42.	CH_3-S-	7.2–7.9	2.8–2.1
43.	CH_3-N	7.0–7.9	3.0–2.1
44.	$-C{=}C-C{\equiv}C-H$	7.13	2.87

45.	$-CH_2-SO_2-R$	7.08	2.92
46.	$-C\equiv C-H$, nonconjugated	7.35–7.55	2.65–2.45
47.	$-C\equiv C-H$, conjugated	6.9–7.2	3.1–2.8
48.	$Ar-C=C-H$	6.95	3.05
49.	$-CH_2(C=C-)_2$	6.95–7.10	3.05–2.9
50.	$-CH_2-Ar$	6.94–7.47	3.06–2.53
51.	$-CH_2-I$	6.80–6.97	3.2–3.03
52.	$-CH_2-SO_2F$	6.72	3.28
53.	$Ar-CH_2-N$	6.68	3.32
54.	$-CH_2-N-Ar$	6.63–6.72	3.37–3.28
55.	$Ar-CH_2-C=C-$	6.62–6.82	3.38–3.18
56.	$-CH_2-N^+-$	6.60	3.40
57.	$-CH_2-Cl$	6.43–6.65	3.57–3.35
58.	$-CH_2-O-R$	6.42–7.69	3.58–2.31
59.	CH_3-O-	6.2–6.5	3.8–3.5
		(6.0–6.7)	(4.0–3.3)
60.	$-CH_2-Br$	6.42–6.75	3.58–3.25
61.	$CH_3-O-SO-OR$	6.42	3.58
62.	$-CH_2-N=C=S$	6.39	3.61
63.	CH_3-SO_2-Cl	6.36	3.64
64.	$Br-CH_2-C\equiv N$	6.30	3.70
65.	$-C\equiv C-CH_2-Br$	6.18	3.82
66.	$Ar-CH_2-Ar$	6.08–6.19	3.92–3.81
67.	$Ar-NH^a_2$, $Ar-NH-R^a$,	6.0–6.6	4.0–3.4
	and $Ar-NH-Ar^a$	(5.7–6.7)	(4.3–3.3)
68.	CH_3-O-SO_2-OR	6.06	3.94
69.	$-C=C-CH_2-O-R$	6.03–6.10	3.97–3.90
70.	$-C=C-CH_2-Cl$	5.96–6.04	4.04–3.96
71.	$Cl-CH_2-C\equiv N$	5.93	4.07
72.	$H_2-C=C-O-CH_2-C=C$	5.87–6.17	4.13–3.83
73.	$-C\equiv C-CH_2-Cl$	5.84–5.91	4.16–4.09
74.	$-C=C-CH_2-OR$	5.82	4.18
75.	$-CH_2-O-CO-R$ or	5.71–6.02	4.29–3.98
	$-CH_2-O-Ar$		

76.	$-CH_2-NO_2$	5.62	4.38
77.	$Ar-CH_2-Br$	5.57–5.59	4.43–4.41
78.	$Ar-CH_2-OR$	5.51–5.64	4.49–4.36
79.	$Ar-CH_2-Cl$	5.50	4.50
80.	$-C=CH_2$	5.37	4.63
81.	–C=CH–, acyclic, nonconjugated	4.3–4.9 (4.1–4.9)	5.7–5 (5.9–5 1)
82.	–C=CH–, Cyclic, nonconjugated	4.3–4.8	5.7–5.2
83.	$-C=CH_2$	4.3–4.7 (3.75–4.8)	5.7–5.3 (6.25–5.2)
84.	$-CH(OR)_2$	4.80–5.20	5.20–4.80
85.	$Ar-CH_2-O-CO-R$	4.74	5.26
86.	R–O–H (conc. less than one mole in inert solvent)	4.8–7.0[a]	5.2–3.0[a]
87.	Ar–C=CH–	4.60–4.72	5.40–5.28
88.	–CH=C–O–R	4.45–5.46	5.55–4.54
89.	–CH=C–C≡N	4.25	5.75
90.	–C=CH–CO–R	3.95–4.32	6.05–5.68
91.	R–CO–CH=C–CO–R	3.87–3.97	6.13–6.03
92.	Ar–CH=C–	3.72–3.77	6.28–6.23
93.	–C=C–H, conjugated	3.3–4.5 (2.2–4.7)	6.7–5.5 (7.8–5.3)
94.	–C=C–H, acyclic, conjugated	3.5–4.0 (2.9–4.5)	6.5–6.0 (7.1–5.5)
95.	H–C = C– | | H CO–R	3.60–3.70	6.40–6.30
96.	–C=CH–O–R	3.55–3.78	6.45–6.22
97.	Br–CH=C–	3.00–3.38	7.00–6.62
98.	–CH=C–CO–R	2.96–4.53	7.04–5.47
99.	$-C=Ch-O-CO-CH_3$	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.	$-SO_3H$	–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.

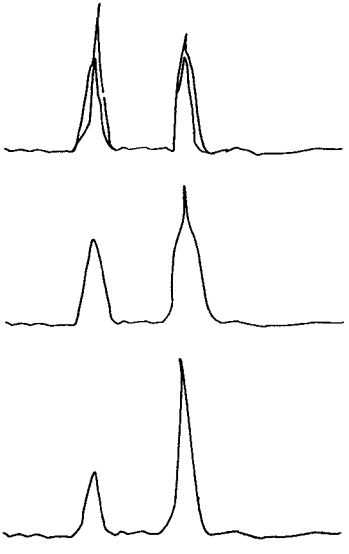
[b] In these compounds R=H, alkyl, aryl, OH, OR or NH_2.

Exercises and Problems:

Problem 1. The compounds $CHCl_2$–$CHCl_2$ (δ=6 ppm) and CCl_3–CH_2Cl (δ=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.

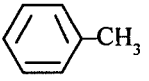
Answer: Halogens shift the proton signal downfield and the shift is the larger, the larger the number of halogen atoms.

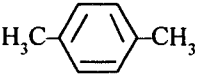
Problem 2. Toluene, p–xylene and mesitylene have two peaks each in their NMR spectra. Assign the spectra shows in fig. shown below (1, 2 and 3) to these compounds.



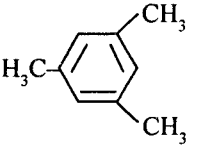
Alkyl Aromalic

3:5





3:2



3:1

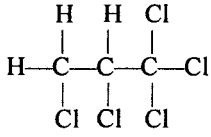
Answer: The signal with δ=2 ppm is produced by the protons of the methyl group and the signal at about 7 ppm by the aromatic protons. As the lines have approximately the same width, the ratios of the peak areas are 3:5, 3:2 and 3:1 in the first, second and third spectra, respectively. Hence, the spectra 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:

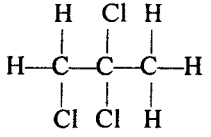
(1) Triplet (δ=4.52 ppm) and doublet (δ=6.07 ppm) with the peak area ratio of 1:2

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

Answer: The triplet with δ=4.52 ppm and the doublet with δ=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:

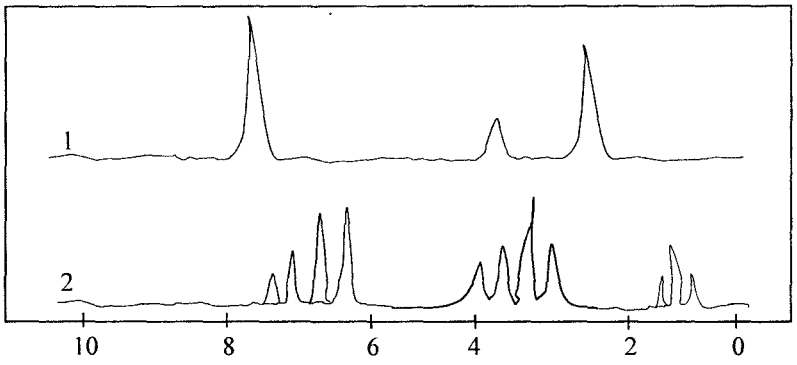


Problem 4. Fig. shown below gives two spectra for the compounds with the same empirical formula $C_8H_{10}O$. Determine the structure and explain the differences in the chemical shifts.

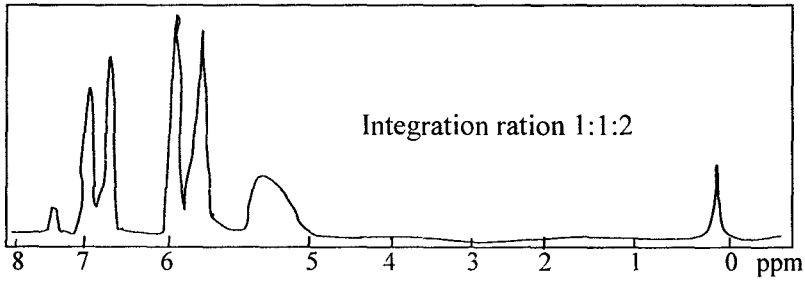
Answer: 1. C_6H_5–CH_2–O–CH_3 2. C_6H_5–O–CH_2–CH_3

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 $C_3H_4N_2S$



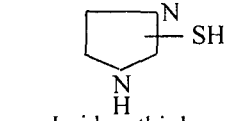
Answer: $C_3H_4N_2S$ Index = 3

doublet δ7.08 (1H) J = 5Hz

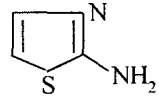
doublet δ6.48 (1H) J = 5Hz

very broad δ5.61 (2H)

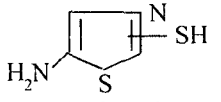
The two non–equivalent protons, which are coupled to each other are in the aromatic region. With an index value of 3 and only $3C^1$ atoms, only imidazole and thiazole are the possible aromatic compounds. But the former, imidazole – thiol has four non–equivalent protons as against three observed. So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



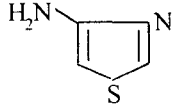
Imidazothiol



2–Aminothiazole



5–Aminothiazole



4–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 ($\because \upsilon = \gamma Ho/2\pi$) 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 (υ_{sample}) and the resonance frequency of the protons in the standard ($\upsilon_{standard}$)

$(\upsilon_{sample} - \upsilon_{TMS})$

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 [$(CD_3)_2SO$] are often employed.

The internal standard used to locate the resonance frequency of most protons is tetramethyl silane (TMS) [$(CH_3)_4$ 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.

$$(CH_3)_3\ SiCH_2CH_2CH_2SO_3Na$$

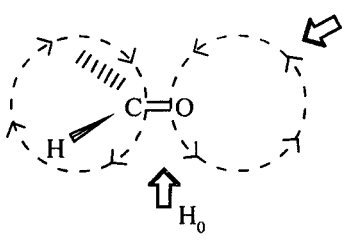
The methyl groups in this compound provide a suitable reference peak.

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.



applied magnetic field

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:

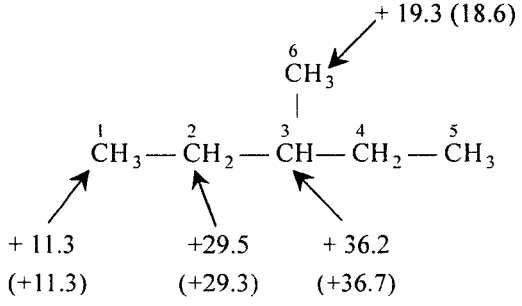
Alkane groups unsubstituted by heteroatoms absorb downfield from TMS to about 60 ppm. (Methane absorbs at 2.5 ppm upfield from TMS.) Within this range we can predict the chemical shifts of individual ^{13}C atoms in a straight chain or branched chain hydrocarbon from the data in Table 4.1 and the formula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

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 1α, 1β–, 2γ and 1δ–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°(3°) = – 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° (2°) = –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, 1α–, 2β–, and 2γ carbon atoms, and it is a 1° atom with a 3° atom attached [1° (3°) = –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 culculations be structurally similar to thecompound 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
∈	+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

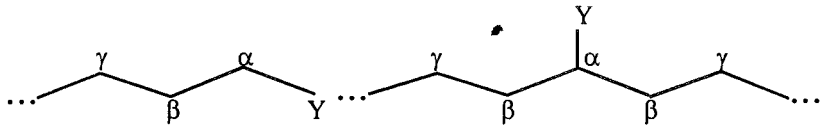
[a] The notations 1° (3°) and 1° (4°) denote a CH_3 group bound to a R_2CH group and to a R_3C group, respectively. The notation 2° (3°) denotes a RCH_2 group bound to a R_2CH group, and so on.

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)

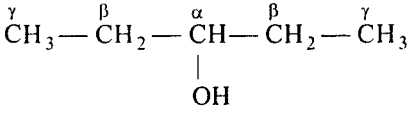


	Terminal		Internal		
Y	**α**		**β**		**γ**
	Terminal	**Internal**	**Terminal**	**Internal**	
CH_3	+9	+6	+10	+8	–2
$CH{=}CH_2$	+20		+6		–0.5
C≡CH	+4.5		+5.5		–3.5
COOH	+21	+16	+3	+2	–2
COO^-	+25	+20	+5	+3	–2
COOR	+20	+17	+3	+2	–2
COCl	+33	+28		+2	
$CONH_2$	+22		+2.5		–0.5
COR	+30	+24	+1	+ 1	–2
CHO	+31		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:



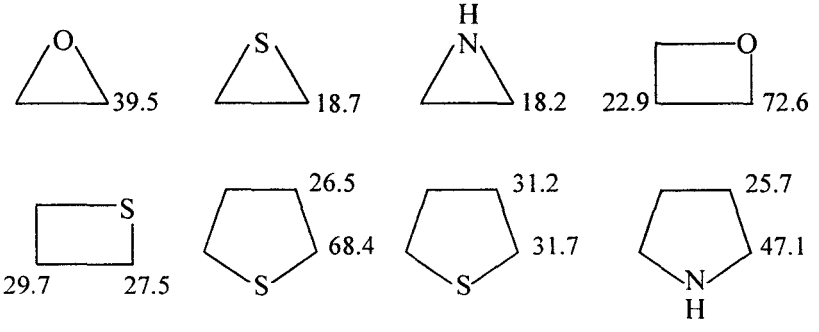
	Calculated	Found
Cα	34.7 + 41 = 75.8	73.8
Cβ	22.8 + 8 = 30.8	30.0
Cγ	13.9 – 5 = 8.9	10.1

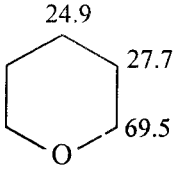
The chemical shifts of the CH_2 groups in monocyclic alkanes are given in Table 4.4. Each ring skeleton has its own set of shfit parameters. Rough estimates for substituted rings can be made with the substitution increments in Table 4.3. Table 4.5 presents chemical shifts for several saturated heterocyclics.

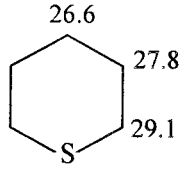
Table 4.4: Chemical shifts of Cycloalkanes (ppm from TMS)

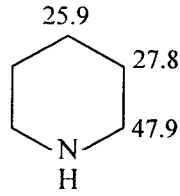
C_3H_6	–2.9
C_4H_8	22.4
C_5H_{10}	25.6
C_6H_{12}	26.9
C_7H_{14}	28.4
C_8H_{16}	26.9
C_9H_{18}	26.1
$C_{10}H_{20}$	25.3

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

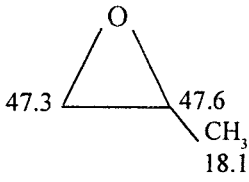


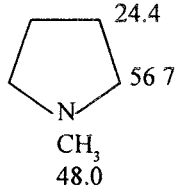






Substituted



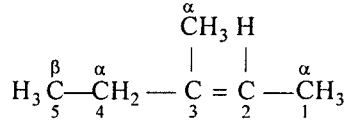


4.2 Alkenes and Alkynes

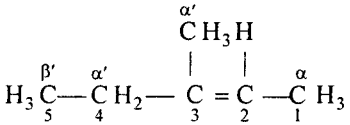
The sp^2 carbon atoms of alkenes substituted only by alkyl groups, absorb in the range of about 110–150 ppm downfield from TMS. The double bond has a rather small effect on the shift of the sp^3 carbon in the molecule. Calculation of approximate shifts can be made from the following parameters where (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:



$\delta_{C-3} = 123.3 + (2 \times 10.6) + (1 \times 7.2) + (1 \times -7.9) - 1.1 = 142.7$ ppm.



$\delta_{C-2} = 123.3 + (1 \times 10.6) + (2 \times -7.9) + (1 \times 1.8) - 1.1 = 115.2$ ppm.

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

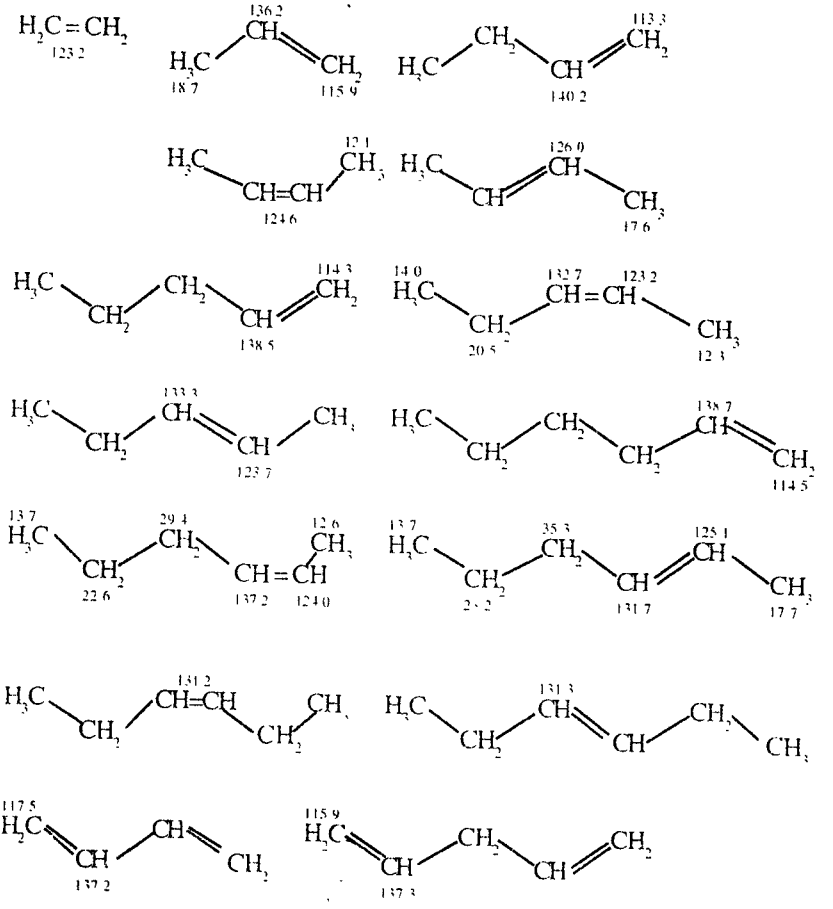
an (E) alkene by about 4–6 ppm. Alkene carbon atoms in polyenes are treated as though they were alkane carbon substituents on one of the double bonds. Thus in calculating the shift of C–2 in 1,4–pentadiene, C–4 is treated like a β–sp^3 carbon atom.

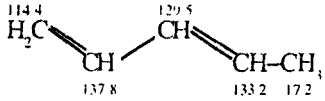
Representative alkenes are presented in Table 4.6.

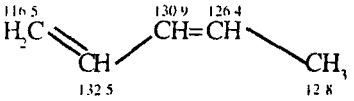
There are no simple rules to handle polar substituents on an alkene carbon. Shifts for several substituted alkenes are presented in Table 4.7.

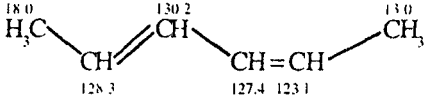
The central carbon atom (=C=) of alkyl substituted allenes absorbs far downfield in the range of about 200–215 ppm, whereas the terminal atoms (C=C=C) absorb upfield in the range of about 75–97 ppm.

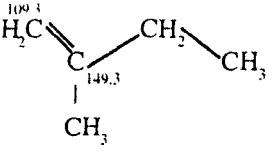
Table 4.6: Alkene and Cycloalkene Chemical shifts (ppm from TMS)

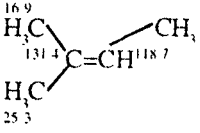


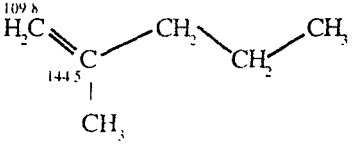

114.4
129.5
137.8
133.2
17.2

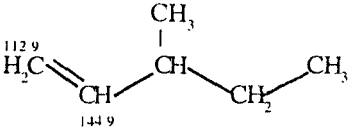

116.5
130.9
126.4
132.5
12.8

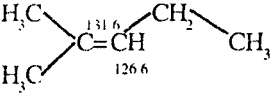

18.0
130.2
13.0
128.3
127.4
123.1

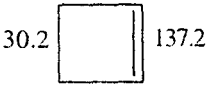

109.3
149.3

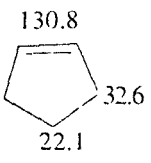

16.9
131.4
118.7
25.3

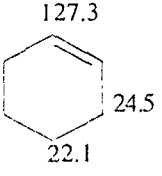

109.8
144.5

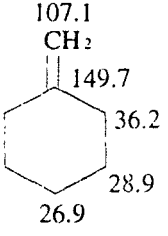

112.9
144.9

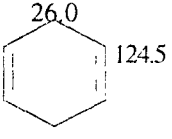

131.6
126.6

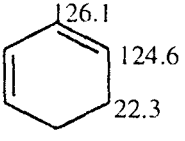

30.2
137.2


130.8
32.6
22.1


127.3
24.5
22.1


107.1
CH2
149.7
36.2
28.9
26.9


26.0
124.5


126.1
124.6
22.3

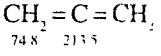
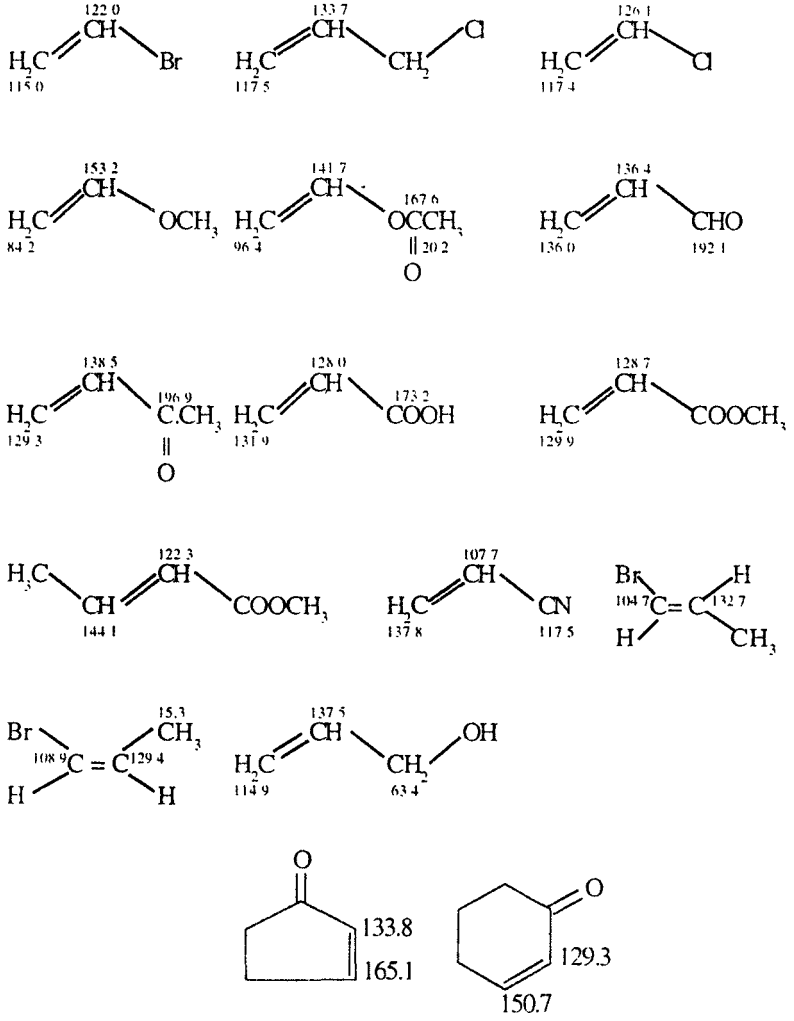

74.8
213.5

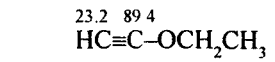
Table 4.7: Chemical Shifts of substituted Alkenes (ppm from TMS)

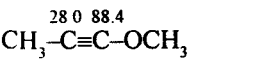


The sp carbon atoms of alkynes substituted only by alkyl groups absorb in the range of approximately 65–90 ppm (Table 4.8). The triple bond shifts the sp^3 carbon atoms directly attached about 5–15 ppm upfield relative to the corresponding alkane. The terminal ≡ CH absorbs upfield from the internal ≡CR. 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.

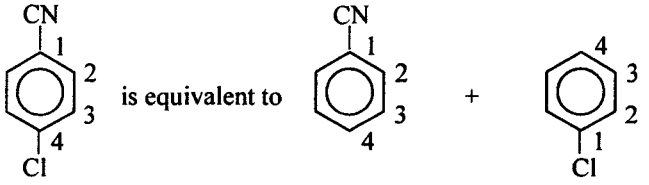
Table 4.9: Incremental shifts of the Aromatic Carbon Atoms of Monosubstituted Benzenes (ppm from Benzene at 128.5 ppm, +downfield, – upfield). Carbon Atom of substituents in parts per million from TMS

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)
$CH(CH_3)_2$	+20.1	–2.0	0.0	–2.5	34.4(CH), 24.1(CH_3)
$C(CH_3)_3$	+22.2	–3.4	–0.4	–3.1	34.5(C), 31.4(CH_3)
$CH{=}CH_2$	+9.1	–2.4	+0.2	–0.5	137.1(CH), 113.2(CH_2)
C≡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

CH_2OC-CH_3 (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	
$OCCH_3$ (O)	+22.4	–7.1	–0.4	–3.2	23.9(CH_3), 169.7 (C=O)
CH (O)	+8.2	+1.2	+0.6	+5.8	192.0
CCH_3 (O)	+7.8	–0.4	–0.4	+2.8	24.6(CH_3), 195.7 (C=O)
CC_6H_5 (O)	+9.1	+1.5	–0.2	+3.8	196.4 (C=O)
CCF_3 (O)	–5.6	+1.8	+0.7	+6.7	
COH (O)	+2.9	+1.3	+0.4	+4.3	168.0
$COCH_3$ (O)	+2.0	+1.2	–0.1	+4.8	51.0(CH_3), 166.8 (C=O)
CCl (O)	+4.6	+2.9	+0.6	+7.0	168.5
C≡N	–16.0	+3.6	+0.6	+4.3	119.5
NH_2	+19.2	–12.4	+1.3	–9.5	
$N(CH_3)_2$	+22.4	–15.7	+0.8	–11.8	40.3
$NHCCH_3$ (O)	+11.1	–9.9	+0.2	–5.6	
NO_2	+19.6	–5.3	+0.9	+6.0	
N=C=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_2NH_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):



I II III

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=0), 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	

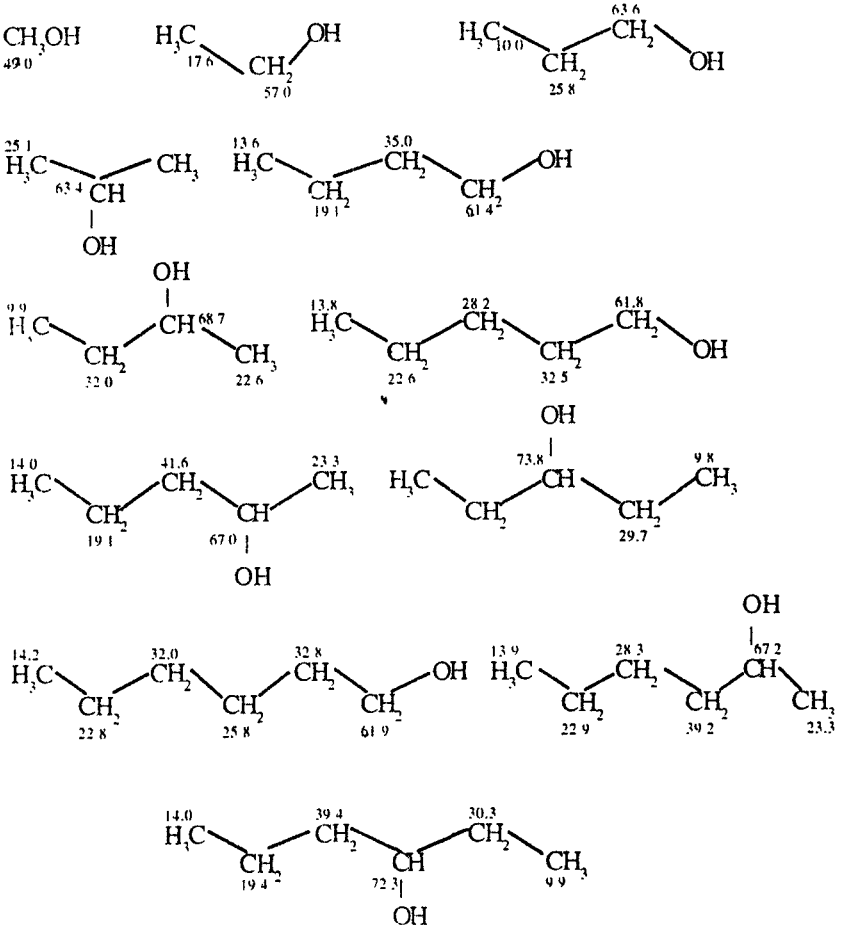
Pyrazine	145.6				
2–Methylpyrazine	154.0	141.8[a]	143.8[a]	144.7[a]	21.6
Pyridazine		152.8	127.6		

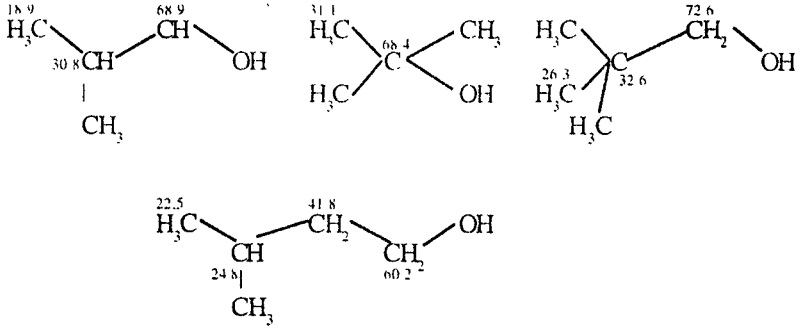
[a] Assignment not certain

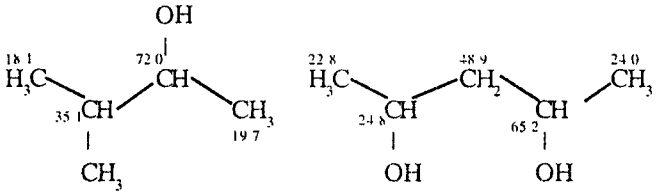
4.4: Alcohols

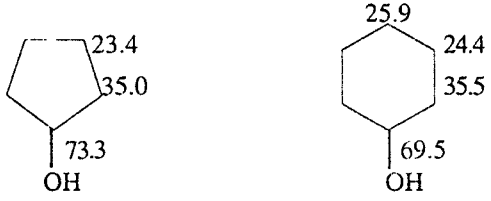
Substitution of H in an alkane by an OH group causes down field shifts of 35–52 ppm for C–1, 5–12 ppm for C–2, and upfield shift of about 0–6 ppm for C–3. Shifts for several acyclic and alicyclic alcohols are given in Table 4.11.

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



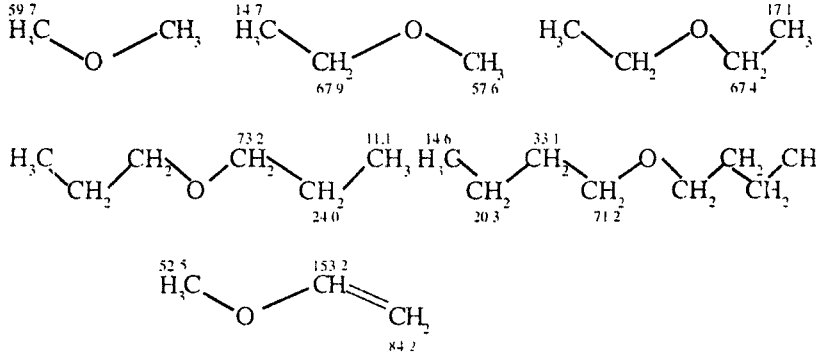


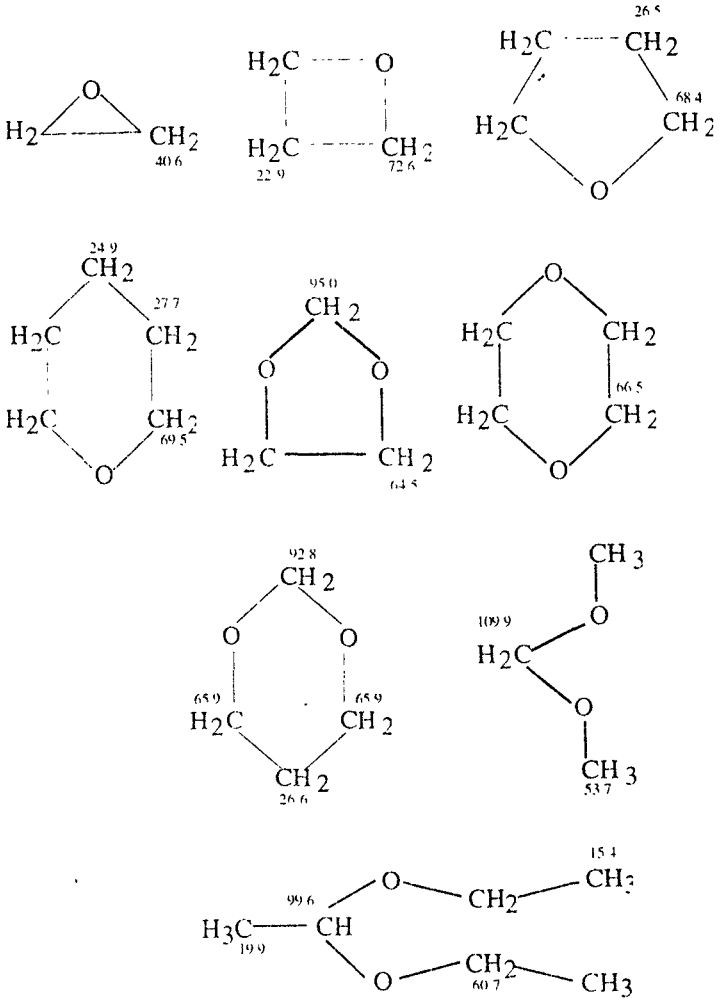




4.5 Ethers, Acetals, and Epoxides :

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		
CH_3CH_2F	79.3	14.6	
CH_3CH_2Cl	39.9	18.7	
CH_3CH_2Br	28.3	20.3	
CH_3CH_2I	–0.2	21.6	
$CH_3CH_2CH_2Cl$	46.7	26.5	11.5
$CH_3CH_2CH_2Br$	35.7	26.8	13.2
$CH_3CH_2CH_2I$	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			
$CH_3CH_2NH_2$	35.9	17.7		
$CH_3CH_2CH_2NH_2$	44.9	27.3	11.2	
$CH_3CH_2CH_2CH_2NH_2$	42.3	36.7	20.4	14.0
$(CH_3)_3N$	47.5			
$CH_3CH_2N(CH_3)_2$	58.2	13.8		
Cyclohexylamine	504	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		
CH_3CH_2SH	19.8	17.3	
$CH_3CH_2CH_2SH$	26.4	27.6	12.6
$CH_3CH_2CH_2CH_2SH$	23.7	35.7	21.0
$(CH_3)_2S$	19.3		
$(CH_3CH_2)_2S$	25.5	14.8	
$(CH_3CH_2CH_2)_2S$	34.3	23.2	13.7
$(CH_3CH_2CH_2CH_2)_2S$	34.1	31.4	22.0
CH_3SCH_3	22.0		
$(CH_3CH_2SSCH_2CH_3$	32.8	14.5	

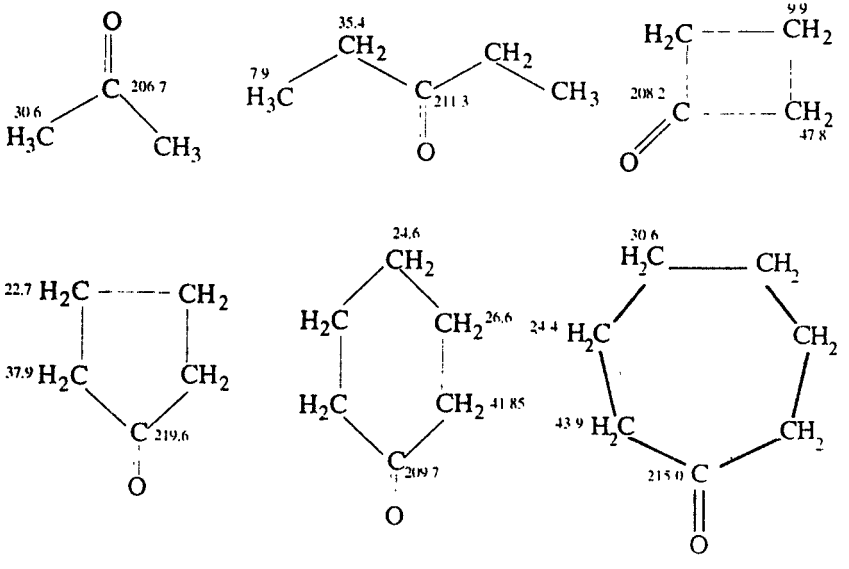
4.9: Functional Groups Containing Carbon

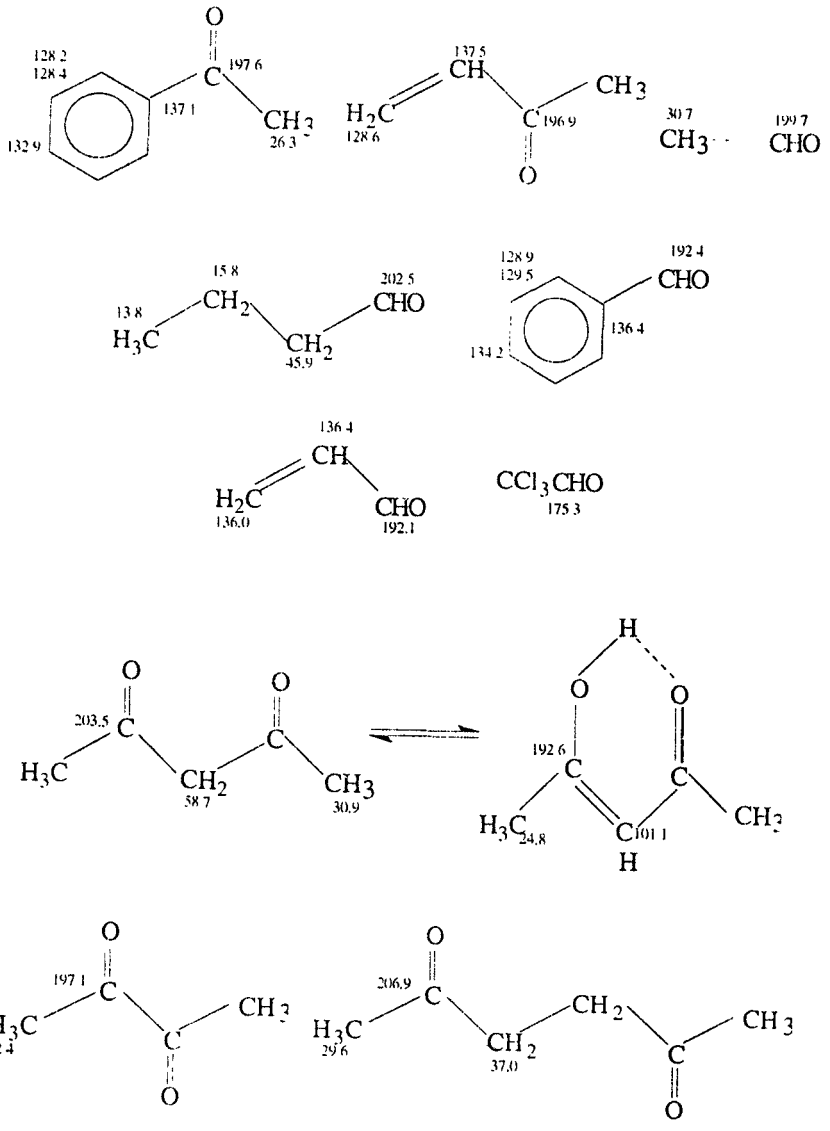
Carbon–^{13}C NMR spectrometry permits direct observation of carbon containing functional groups. With the exception of CH=O, the presence of these groups could not be directly ascertained by ^{1}H NMR.

4.9.1. Ketones and Aldehyde:

Table 4.15 presents chemical shifts of the C=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 C=O Group and Other carbon Atoms of Ketones and Aldehydes (ppm from TMS)

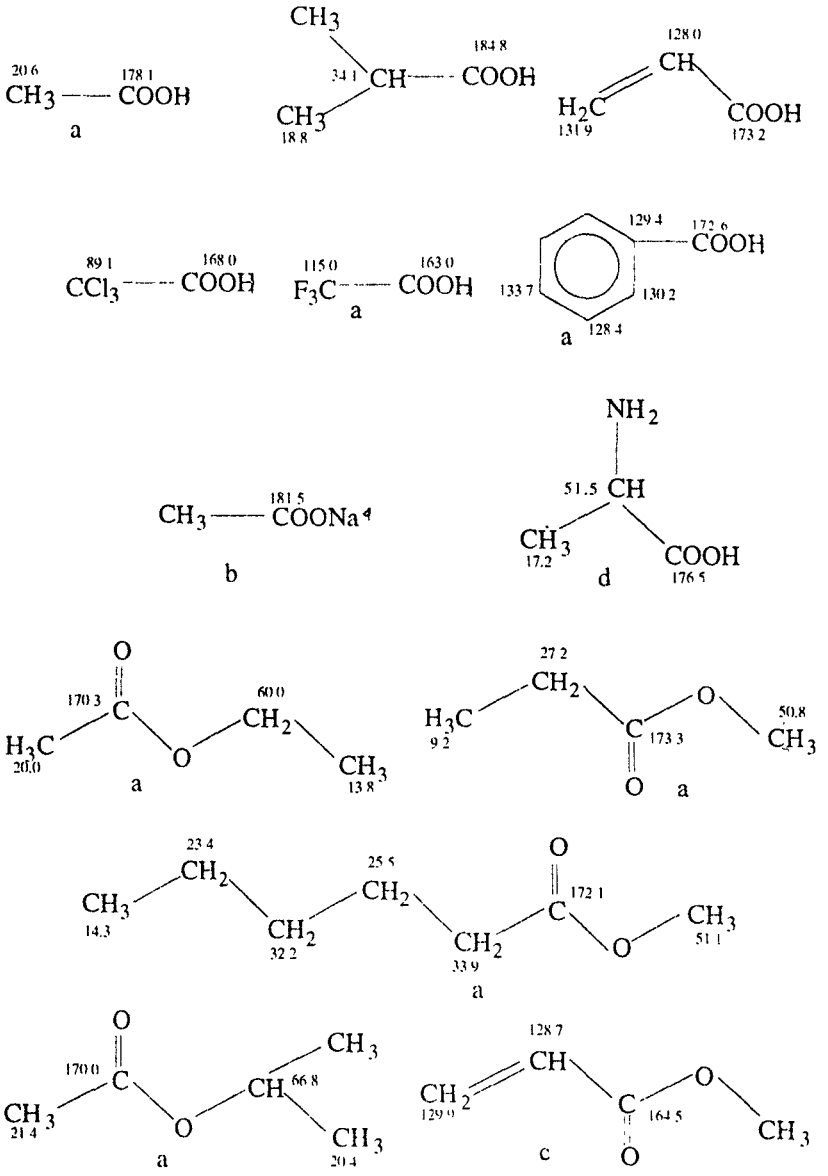


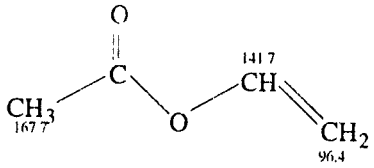


4.9.2. Carboxylic Acids, Ester, Chlorides Anhydrides, Amides and Nitriles:

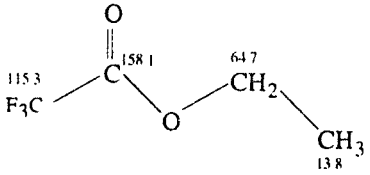
The C=O groups of carboxylic acids and derivatives are in the range of 150–185 ppm. Nitriles absorb in the range of 115–125 ppm.

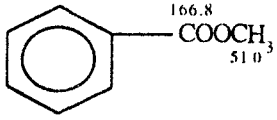
Table 4.16: Shift Positions for the C=O group and other carbon atoms of carboxylic acids, esters, Icatones, chlorides, anhydrides, amides, carbamates, and nitriles (ppm from TMS)

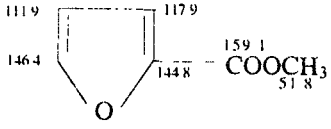


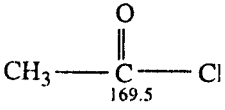

O
C
141.7
CH
CH3
167.7
O
CH2
96.4

c

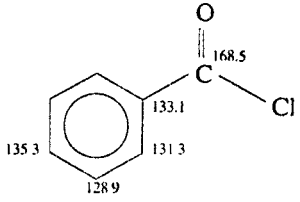

O
158.1
115.3
C
64.7
F3C
CH2
O
CH3
13.8


166.8
COOCH3
51.0

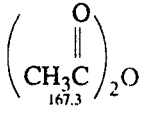

111.9
117.9
146.4
144.8
159.1
COOCH3
51.8
O


O
CH3
C
Cl
169.5

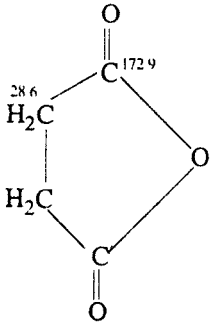
c

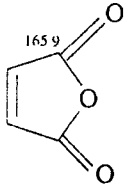

O
168.5
C
Cl
133.1
135.3
131.3
128.9

a

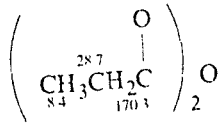

O
CH3C
2O
167.3

c

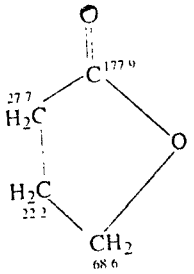

O
172.9
28.6
H2C
O
H2C
C
O


165.9
O
O
O

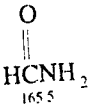
a



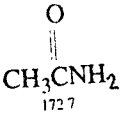
a



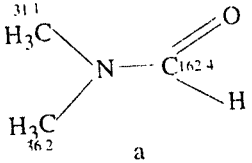
a



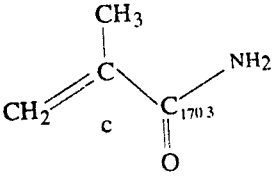
c



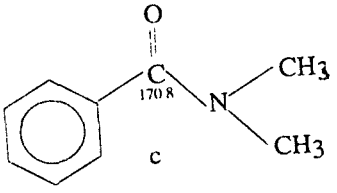
c



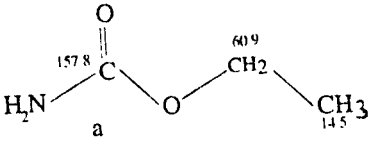
a



c



c



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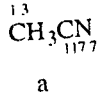
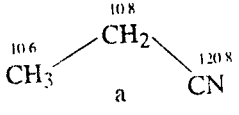
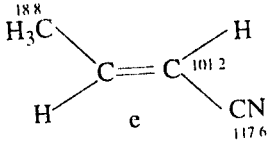


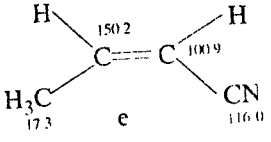
a



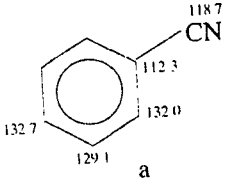
a



e



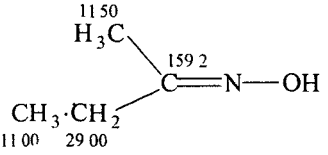
e



a

a. In $CHCl_3$ (~50%)
b. Saturated aqueous solution of CH_3COONa
c. Neat or saturated solution
d. In H2O
e. In DMSO
f. 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 $^{13}C^1$ atoms in a molecule. One bond ^{13}C–H coupling ($^1J_{CH}$) 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 ($^nJ_{CH}$). Table 4.17 gives some representative ($^1J_{CH}$) values. Table 4.18 gives some representative ($^2J_{CH}$) values, which range from about –5 to 60 Hz.

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

Compound	J(Hz)
SP^3	
CH_3CH_3	124.9
$CH_3CH_2CH_3$	119.2
$(CH_3)_3CH$	114.2
CH_3NH_2	133.0
CH_3OH	141.0
CH_3Cl	150.0
CH_2Cl_2	178.0
$CHCl_3$	209.0

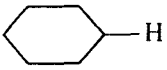
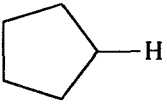
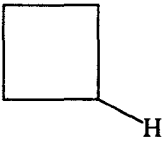
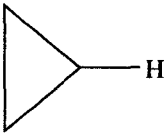
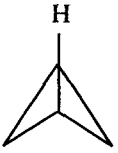
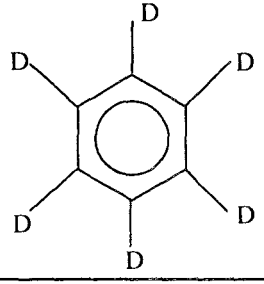
	123.0
	128.0
	134.0
	161.0
	205.0
sp^2	
$CH_2=CH_2$	156.2
$CH_3\underline{C}H=C(CH_3)_2$	148.4
$CH_3\underline{C}H=O$	172.4
$NH_2\underline{C}H=O$	188.3
C_6H_6	159.0
sp	
CH≡CH	249.0
$C_6H_5C\equiv CH$	251.0
HC≡N	269.0

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

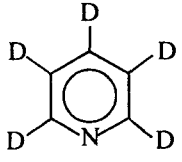
Compound	J(HZ)
sp^3	
$C\underline{H}_3\underline{C}H_3$	–4.5
$C\underline{H}_3\underline{C}Cl_3$	5.9

$\underline{C}H_3\underline{C}H{=}O$	26.7
sp^2	
$\underline{C}H_2{=}\underline{C}H_2$	-2.4
$(\underline{C}H_3)_2\underline{C}{=}O$	5.5
$CH_2{=}\underline{C}H\underline{C}H{=}O$	26.9
C_6H_6	1.0
s p	
$\underline{C}H{\equiv}\underline{C}H$	49.3
$C_6H_5O\underline{C}{\equiv}\underline{C}H$	61.0

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

Compound	^1J(HZ)	^2J(HZ)	^3J(HZ)
CH_3CF_3	271		
CF_2H_2	235		
CF_3CO_2H	284	43.7	
C_6H_5F	245	21.0	
$(CH_3CH_2)_3P$	5.4	10.0	
$(CH_3CH_2)_4P^+Br^-$	49	4.3	
$(C_6H_5)_3P^+CH_3I$	88($CH_3$52)	10.9	
$CH_3CH_2P(OCH_2CH_3)_2$ ‖ O	143	7.1(j_{COP}6.9)	J_{CCOP} 6–2
$CDCl_3$	31.5		
CD_3CCD_3 ‖ O	19.5		
$(CD_3)_2SO$	22.0		
	25.5		

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

Structure	Name	δ(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
$DCN(CD_3)_2$	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
$D_2C(CD_2)_2O$	THF–d_8	25.2	20.5	Quintet
		67.4	22	Quintet
$D_2C(CD_2)_2OCD_2O$	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
CD_3CCD_3	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_3CD_2OD	Ethanol–d_6	15.8(C–2)	19.5	Septet
		55.4(C–1)	22	Quintet
$(CD_3CD_2)_2O$	Ether–d_{10}	13.4 (C–2)	19	Septet
		64.3(C–1)	21	Quintet
$[(CD_3)_2N]_3$ P=O	HMPA–d_{18}	35.8	21	Septet
CD_3CO_2D	Acetic acid–d_4	20.0(C–2)	20	Septet
		178.4(C–1)	<1	Septet[b]
CD_2Cl_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 ^{13}C Correlation Table for Chemical Classes

R = H or alkyl substituents

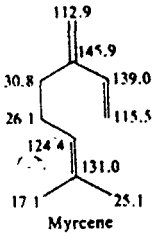
Y = Polar substituents

Types and group	δ(ppm)
Acyclic hydrocarbons	
$-CH_3$	8–30
$-CH_2-$	14–55
$-CH<$	24–59
$-C(<)(<)-$	30–40
Aticyclic hydrocarbons	
C_3H_6	15–19
C_4H_8 to $C_{10}H_{20}$	21–29
Alkenes	
$H_2C=C-R$	102–121 ($H_2C=$) 109–150 (=C–R)
$H_2C=C-Y$	80–170
$C=C-C=C-R$	109–151

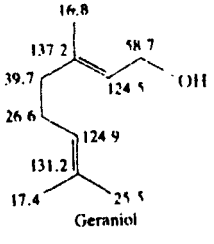
Allenes	
C=C=C	70–97 (=C)
	200–214 (=C=)
Alkynes	
C≡C–R	63–73 (HC≡)
	71–89 (≡C–R)
C≡C–Y	20–94
Aromatics	
Ar–R	120–150
Ar–Y	94–158
Heteroaromatics	100–166
Alcohols C–OH	44–86
Ethers C–O–C	54–86
Acetals, Ketals O–C–O	8–12
Halides	
$C–F_{1-3}$	72–134
$C–Cl_{1-4}$	20–98
$C–Br_{1-4}$	–28.5–+33
$C–I_{1-4}$	–292.5–+42
Amines $C–NR_2$	20–70
Nitro $C–NO_2$	60–78
Mercaptans, Sulfides C–S–R	5.5–46
Sulfoxides, Sulfones	
C–SO–R, $C–SO_2–R$	36–54
Aldehydes, Sat. R–CHO	197–220
Aldehydes, α, β– unsat. R–C=C–CH=O	176–194
Ketones, Sat. $R_2C=O$	195–220
Ketones, α, β unsat.	
R–C=C–C=O	182–212
Carboxylic acids, sat.	
R–COOH	166–186
Salts 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 $(RCO)_2O$	148–174
Amides $RCONH_2$	150—177
Nitriles RC≡N	108–124
Oximes R_2C=NOH	144–166
Carbamates	
R_2NCOOR^1	151–160
Isocyanates	
R–N=C=O	111–134
Cyanates R–O–C≡N	104–120
Isothiocyanates	
R–N=C=S	116–141
Thiocyanates	
R–S–C≡N	98–118

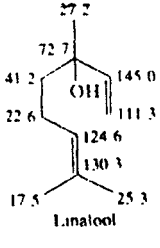
^{13}C NMR data for several natural products (δ)



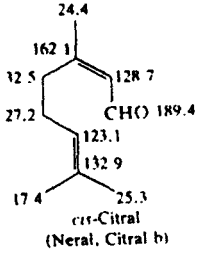
Myrcene



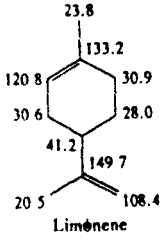
Geraniol



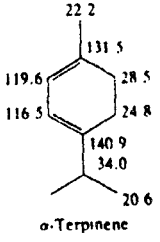
Linalool



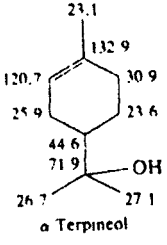
cis-Citral
(Neral, Citral b)



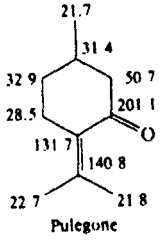
Limonene



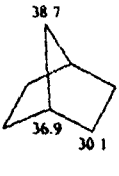
α-Terpinene



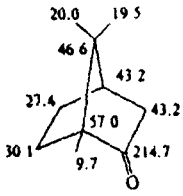
α Terpineol



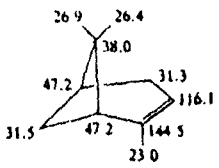
Pulegone



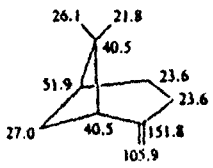
Norbornane



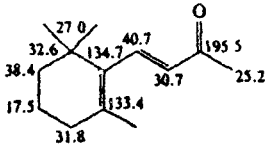
Camphor



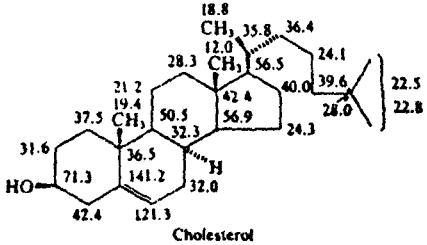
α-Pinene



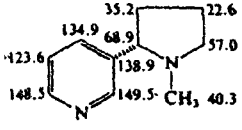
β-Pinene



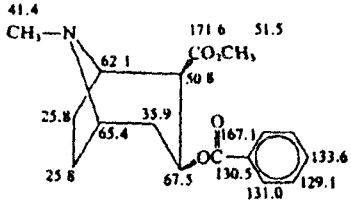
β-Ionone



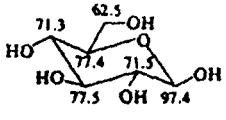
Cholesterol



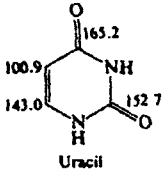
Nicotine



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 $\left(M_{+}^{\bullet}\right)$. The symbol $^{\bullet}_{+}$ indicates that the molecule has lost an electron, it has unpaired electron and is positively charged.

$$\underset{\text{Molecule}}{M} \xrightarrow{70\ eV} \underset{\text{Molecular ion}}{M_{+}^{\bullet}} + e^{-}$$

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:

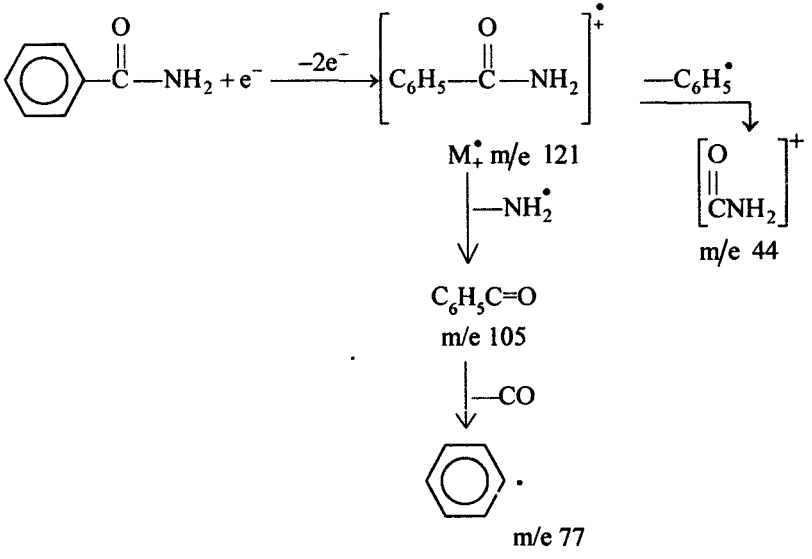


Table 5.1: Exact Masses of Isotopes

Element	Atomic Weight	Nuclide	Mass
Hydrogen	1.00794	^{1}H	1.00783
		D(^{2}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
BroTnitfe	79.9094	^{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

$$CH_3CH_2CH_2CH_2CH_3 \xrightarrow{70\ eV} [CH_3(CH_2)_3CH_3]^{+\bullet} + e^-$$

Molecular ion

m/z = 72

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 occuring 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 $(M^{+\bullet} + 2)$ 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 occuring 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 and 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 F = 19 of 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 (–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.

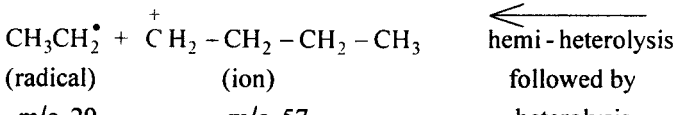
* Molecular ion peaks are more abundant in cycloparaffins than in straight chain paraffins containing the same number of carbon atoms, although the cyclic compounds tend to lose their side chains.

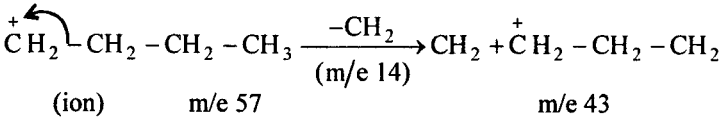
If the ring undergoes fragmentation, it loses two carbon atoms simultaneously, thus producing an abundance of $^+C_2H_4$ (m/e 28), $^+C_2H_5$ (m/e 29), and M-28, M-29 ions in the spectrum. Due to this tendency to lose ethylene C_2H_4 and other even-mass number fragments, the percentage of fragments having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

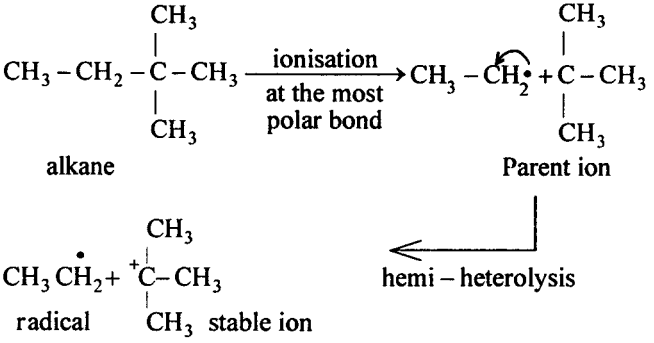
(i) Straight chain alkanes

$$\underset{\text{alkane}}{CH_3CH_2CH_2CH_2CH_2CH_3} \xrightarrow[-e]{\text{ionisation}} \underset{\text{(Parent ion)}}{CH_3\overset{\curvearrowleft}{C}H_2^{\bullet}} + CH_2CH_2CH_2CH_3$$

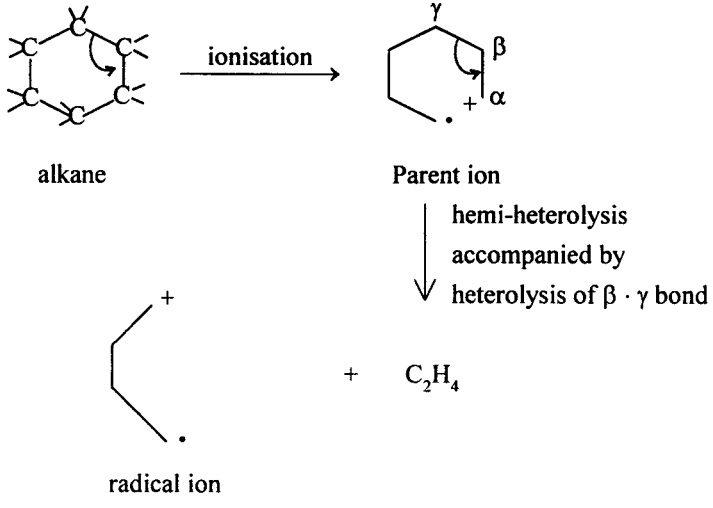




(ii) Branched chain alkanes



(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.

$$H_2C = CH - CH_2 - R \xrightarrow{-e} H_2C \overset{+\cdot}{} CH \underset{\alpha}{} CH_2 \underset{\beta}{} R$$

$$\downarrow$$

$$H_2\overset{+}{C} - CH = CH_2 + R^{\cdot}$$

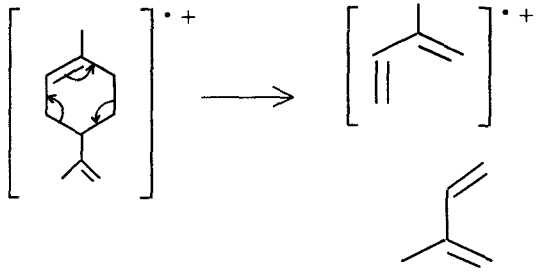
m/e 41

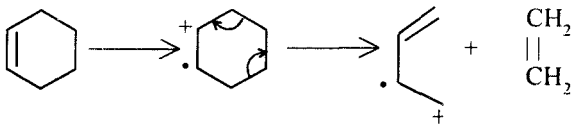
The natural outcome of allylic cleavage is a series of fragments at masses 41, 55, 69, 83, etc., with the general formula C_nH_{2n-1} (allyl carbonium ions)

* McLafferty rearrangements are also common in these ions. These rearrangments produce ions of the general formula C_nH_{2n}.

* Cyclic alkenes usually show a distinct molecular ion peak. A unique mode of cleavage is the retro-Diels-Alder reaction shown by limonene:

(i)

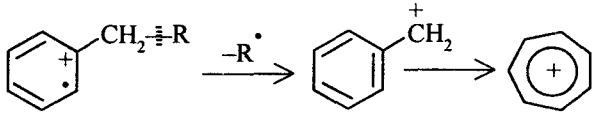


(ii) 

(c) Aromatic hydro carbons

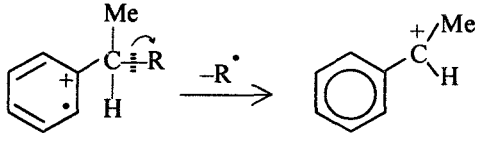
* An aromatic ring in a molecule stabilises the molecular ion peak, which is usually sufficiently large that accurate intensity measurements can be made on the M+1 and M+2 peaks.

* 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.

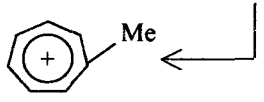


m/e = 91

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

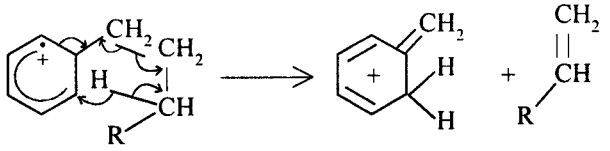


m/e 105



m/e = 105

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.



m/e = 92

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

m/e = 39 m/e = 91 m/e = 65

Cyclopropenium ion Cyclopentylcation

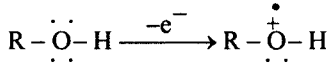
A characteristic cluster of ions resulting from an α cleavage and hydrogen migration in monoallcylbenzenes appears at m/e 77 ($C_6H_5^+$), 78 ($C_6H_6^+$) and 79 ($C_6H_7^+$).

(2) Hydroxy compounds

(a) Alcohols:

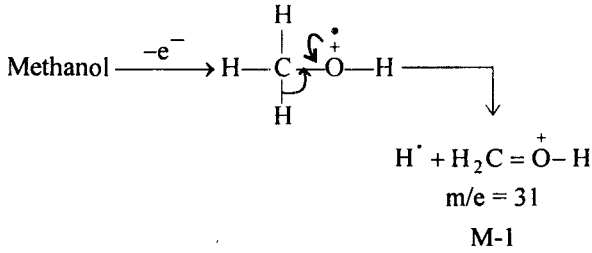
* In the spectra of alcohols, the molecular ion peak M is usually either very small or totally absent. It is somewhat more abundant in the spectra of secondary than in those of primary and tertiary alcohols.

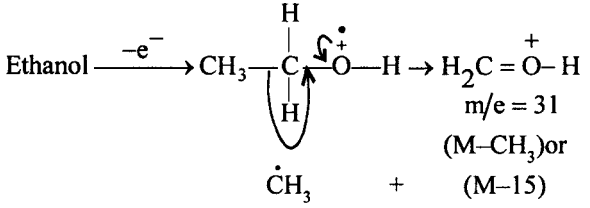
The odd-electron molecular ion is produced initially by the removal of an n-electron from oxygen:



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

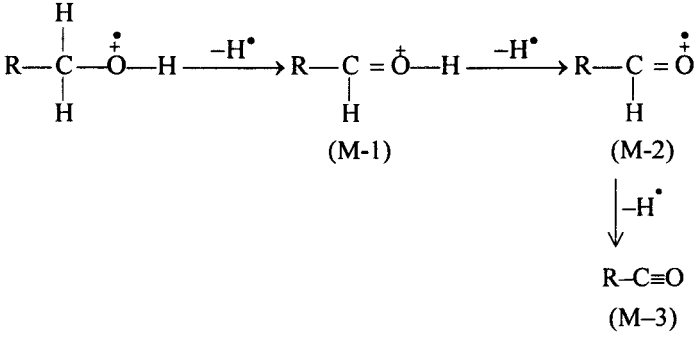
One such decomposition involves energetically favoured α-cleavage. This cleavage leads to more stable, even-electron, oxonium ions.



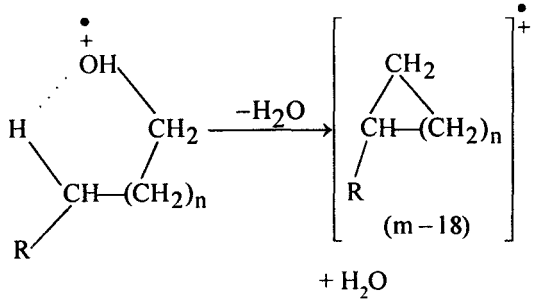


Although ethanol shows an M-1 peak at m/e = 45 by α-elimination of a hydrogen radical, the M-15 peak is more intense because α-elimination of a larger substituent is always favoured.

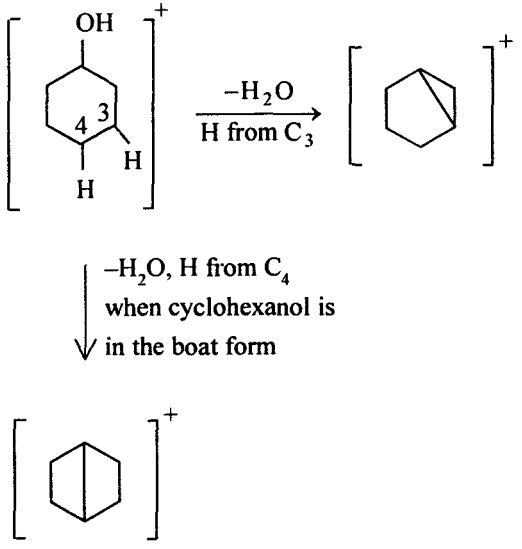
* In the spectra of primary alcohols, in addition to the M-1 peak, very low intensity M-2 and M-3 peaks are also observed.



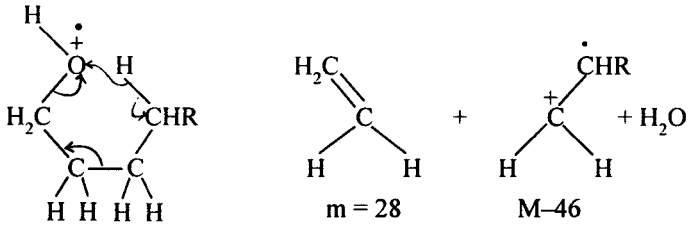
* All primary alcohols (except methanol) and high molecular-weight secondary and tertiary alcohols display peaks at M-18 due to the loss of H_2O through a cyclic mechanism.



* In cyclic alcohols, the principal dehydration process involves loss of a hydroxyl group together with a hydrogen atom from either C_3 or C_4 to produce bicyclo ions.

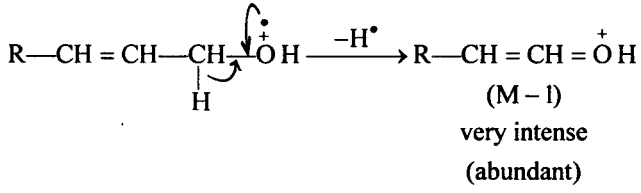


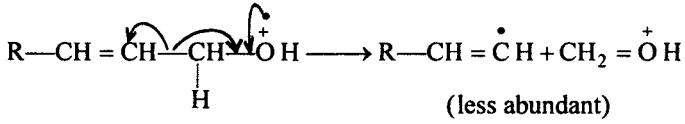
* Butanol & longer-chain primary alcohols often suffer double elimination. That is, they lose one molecule of water and one of ethylene simultaneously through a six-numbered cyclic mechanism, thus displaying an M-46 peak



* 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 $(CH_2OH)^+$ in the spectra of primary alcohols, while secondary and tertiary alcohols display analogous peaks at m/e = 45 $(MeCHOH)^+$ and m/e = 59 $[(CH_3)_2COH]^+$.

* 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.

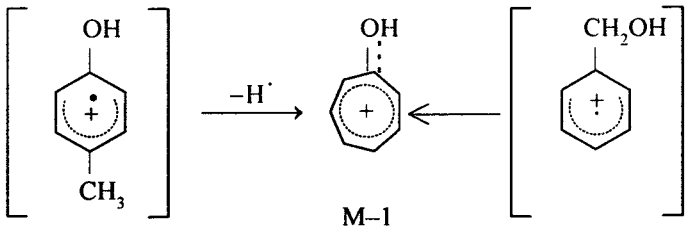




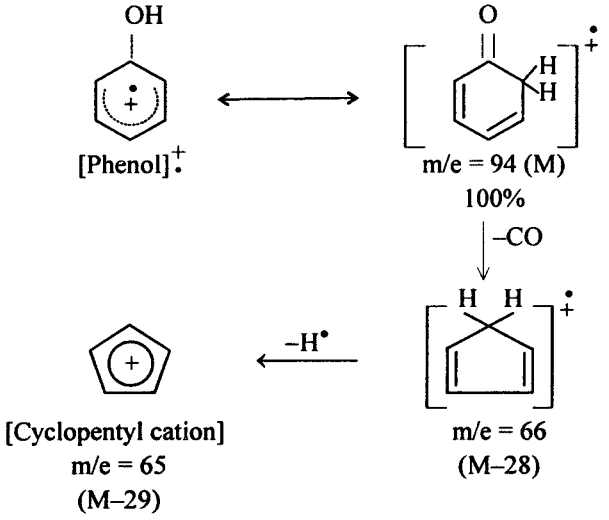
(b) Phenols and other aromatic alcohols:

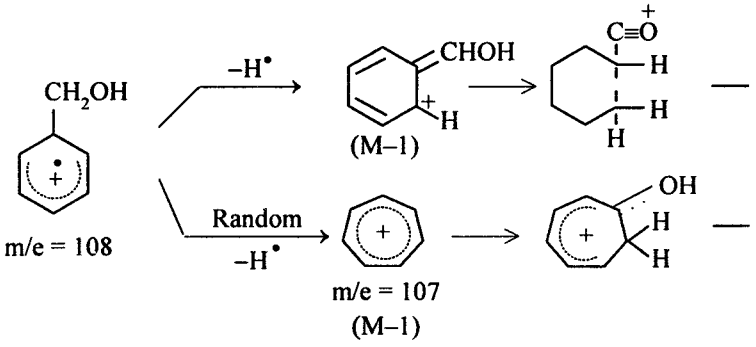
* As in all aromatic compounds, the molecular-ion peak M in phenol and aromatic alcohols is strong. In phenols it forms the base peak.

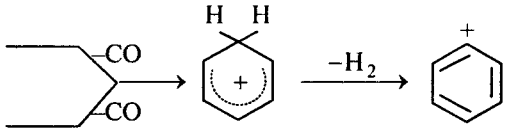
* The M-1 peak due to the loss of hydrogen is small in phenol, but is very strong in cresols and benzyl alcohols. The production of M-1 ions is due to the random abstraction of hydrogen bonded to any of the carbon atoms to produce a resonance-stabilised. π complex system such as hydroxy tropyllium ions.



* 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.



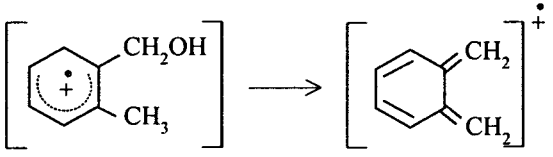




m/e = 79 (M-29) m/e = 77 (M-31)

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

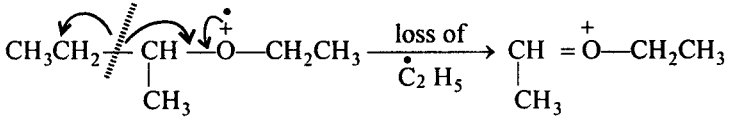
  The dehydration is more pronounced if the substituents are ortho to each other.



(M) (M-18, 100%)

Ethers:

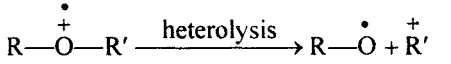
A molecular ion of ether is formed by the removal of one of the nonbonded electrons on oxygen, and, just as with alcohols, the molecular ions of ethers are unstable and readily undergo α-cleavage. (cleavage of a bond β to oxygen).



(m/e = 73)

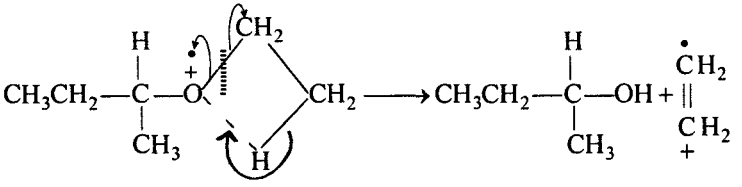
This type of cleavage usually accounts for the base peak and some strong peaks at 45, 59, 73 etc.

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



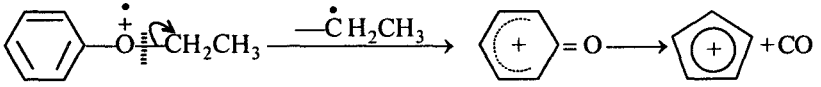
In such a cleavage, the alkyl portion carries the charge and accounts for hydrocarbon peaks at m/e = 29, 43, 57, 71 etc.

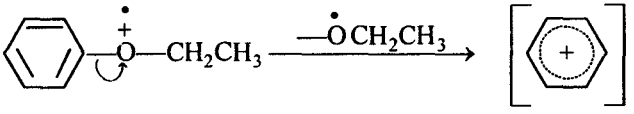
* Homolytic fission of bonds α to oxygen may often be accompanied by rearrangement of one hydrogen atom to eliminate an olefin.



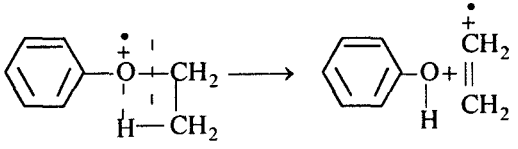
* Aromatic ethers display a somewhat stronger M peak, and show a fragmentation behaviour similar to that of aliphatic ethers.

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





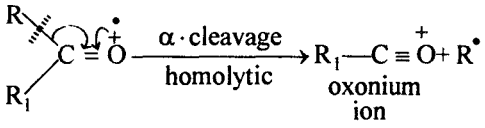
(ii) Cleavage of bond α to oxygen with rearrangement of hydrogen to eliminate an alkene.



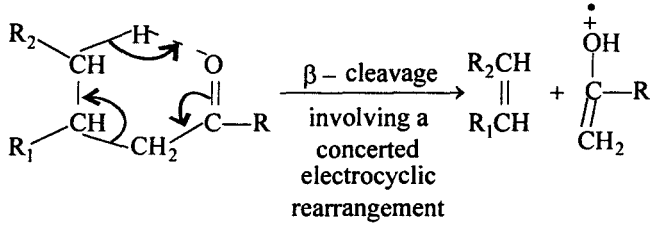
Aldehydes and Ketones:

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.



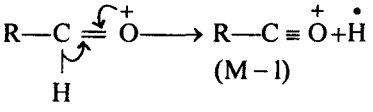
When a γ hydrogen is available for migration, β-cleavage results in the formation of an olefin and a charged enol through the McLafferty rearrangement.



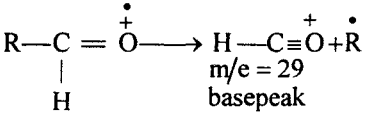
(a) Aldehydes:

* 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.

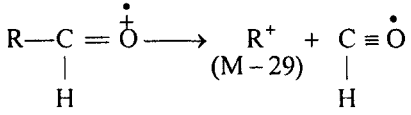
* In aldehydes, the M-1 peak is usually as intense as the M peak. The peak results from the loss of hydrogen through homolytic α-cleavage.



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

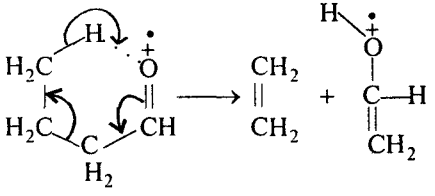


However, with straight chain aldehydes of higher molecular weight, this peak is approximately 40% of the base peak which may be displayed at M-29 due to ions produced through heterolytic cleavage as:



* 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.

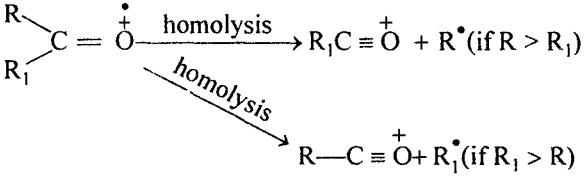


[n-butyraldehyde]$^{+\bullet}$ m/e = 44

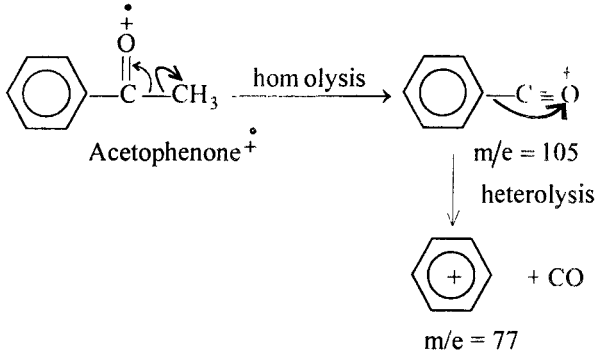
(b) Ketones:

* 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 R–C≡O^{+} ions.

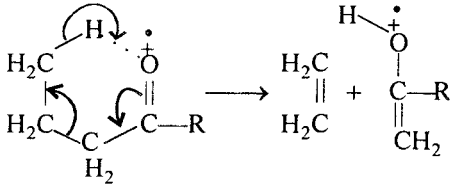


m/e = 43, 57, 71 etc.



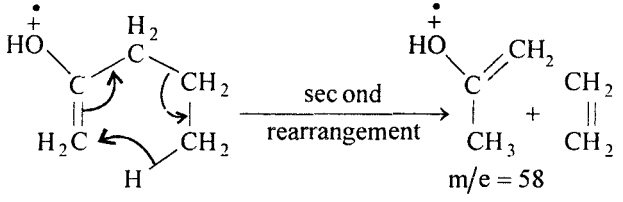
* McLafferty rearrangements (β-cleavage with migration of γ-hydrogen) are common in ketones containing a chain of three or more carbon atoms attached to the carbonyl group. However, complications arise due to the following facts:

(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.



m/e = 58, 72, 86 etc.

(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.

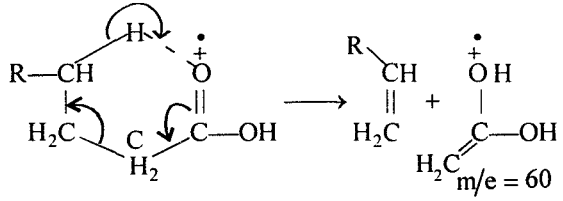
Carboxylic acids and esters

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

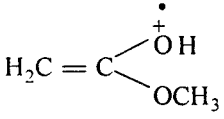
  Aromatic monocarboxylic acids and esters, like other aromatic compounds, display a strong M peak.

* 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



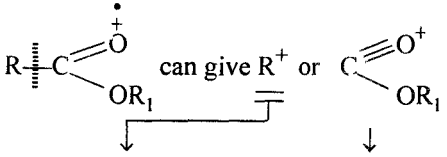
A corresponding β-cleavage peak in methyl esters appears at m/e = 74 due to (II).



II

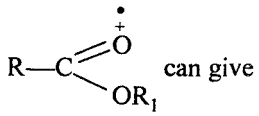
Analogous peaks in ethyl and butyl esters appear at 88 and 116, respectively.

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

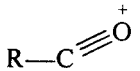


m/e = 15, 29, 43, 57 (M–45, M–59 etc.)

m/e = 45, 59, 73, 87 etc. (M–15, M-29, M–43 etc.)



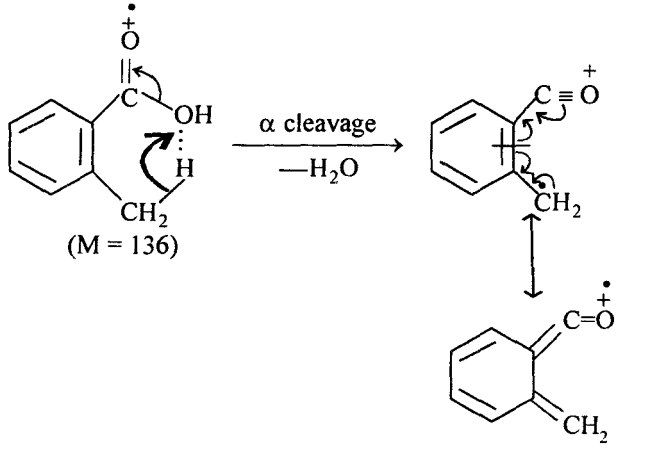
or



m/e = 17, 31, 45, 59 etc. (M–43, M–47 etc.)

m/e = 43, 57, 71 etc. (M–17, M–31, M–45 etc.)

* 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.



(M = 136)

m/e = 118 (M–18)

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

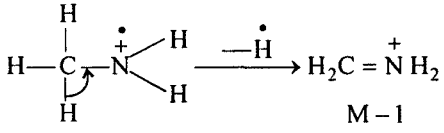
Amines

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.

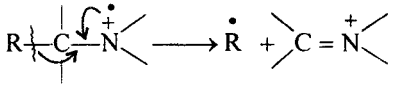
* The molecular-ion peak M is weak to absent in high-molecular weight aliphatic open-chain amines, but strong in aromatic and cyclic amines.

* 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.

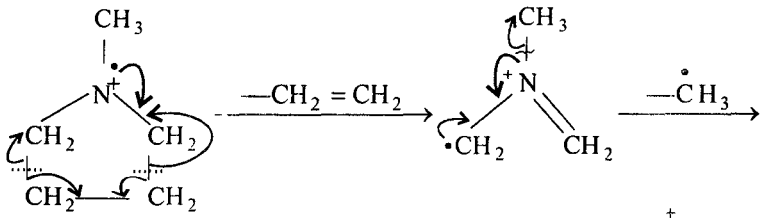


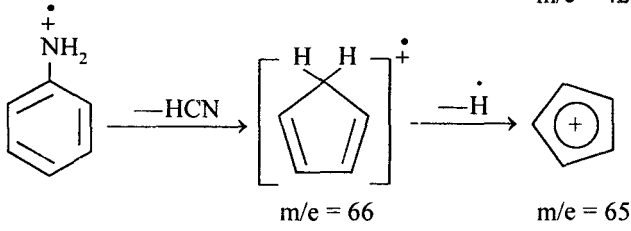
* In amines, as in alcohols, the most important fragmentation is that of the bond β to nitrogen. In many amines this fragmentation is responsible for the base peak.



m/e = 30, 44, 58, 72, 86 etc.

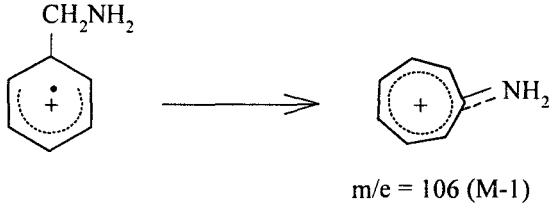
* In cyclic and aromatic amines, both bonds β to nitrogen can rupture.



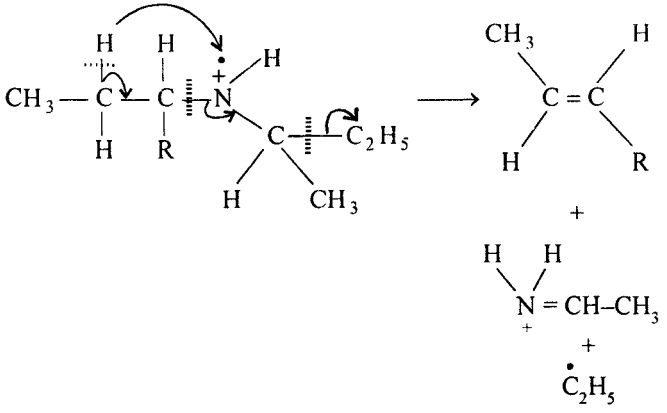


The loss of HCN and H_2CN from aniline is similar to the elimination of CO and CHO from phenol.

* 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 aminotropyllium 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,

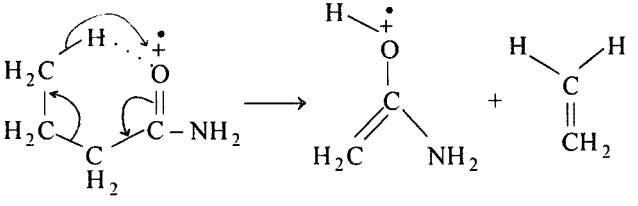


Amides

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.



m/e = 59

* In the case of long-chain primary amides cleavage of the bond γ to carbonyl can also take place, giving minor peaksat 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.

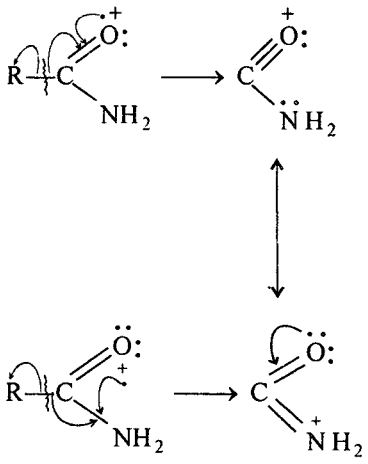


Table 5.3: Masses and Isotopic Abundance Ratios for Various Combinations of Carbon, Hydrogen, Nitrogen and Oxygen[a]

	FM		FM		FM
		16		**25**	
12		O	15.9949	C_2H	25.0078
C	12.0000	H_2N	16.0187	**26**	
13		CH_4	16.0313	CN	26.0031
CH	13.0078	**17**		C_2H_2	26.0157
14		HO	17.0027	**27**	
N	14.0031	H_3N	17.0266	CHN	27.0109
CH_2	14.0157	**18**		C_2H_3	27.0235
15		H_2O	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_2N	28.0187	**38**		H_2N_3	44.0249
C_2H_4	28.0313	C_2N	38.0031	CO_2	43.9898
29		C_3H_2	38.0157	CH_2NO	44.0136
HN_2	29.0266	**39**		CH_4N_2	44.0375
CHO	29.0027	C_2HN	39.0109	C_2H_4O	44.0262
CH_3N	29.0140	C_3H_3	39.0235	C_2H_6N	44.0501
C_2H_5	29.0391	**40**		C_3H_8	44.0626
30		CN_2	40.0062	**45**	
NO	29.9980	C_2O	39.9949	HN_2O	45.0089
H_2N_2	30.0218	C_2H_2N	40.0187	H_3N_3	45.0328
CH_2O	30.0106	C_3H_4	40.0313	CHO_2	44.9976
CH_4N	30.0344	**41**		CH_3NO	45.0215
C_2H_6	30.0470	CHN_2	41.0140	CH_5N_2	45.0453
31		C_2HO	41.0027	C_2H_5O	45.0340
HNO	31.0058	C_2H_3N	41.0266	C_2H_7N	45.0579
H_3N_2	31.0297	C_3H_5	41.0391	**46**	
CH_3O	31.0184	**42**		NO_2	45.9929
CH_5N	31.0422	N_3	42.0093	H_2N_2O	46.0167
32		CNO	41.9980	H_4N_3	46.0406
O_2	31.9898	CH_2N_2	42.0218	CH_2O_2	46.0054
H_2NO	32.0136	C_2H_2O	42.0106	CH_4NO	46.0293
H_4N_2	32.0375	C_2H_4N	42.0344	CH_6N_2	46.0532
CH_4O	32.0262	C_3H_6	42.0470	C_2H_6O	46.0419
33		**43**		**47**	
HO_2	32.9976	HN_3	43.0171	HNO_2	47.0007
H_3NO	33.0215	CHNO	43.0058	H_3N_2O	47.0246
34		CH_3N_2	43.0297	H_5N_3	47.0484
H_2O_2	34.0054	C_2H_3O	43.0184	CH_3O_2	47.0133
36		C_2H_5N	43.0422	CH_5NO	47.0371
C_3	36.0000	C_3H_7	43.0548	**48**	
37		**44**		O_3	47.9847
C_3H	37.0078	N_2O	44.0011	H_2NO_2	48.0085

	FM		FM		FM
H_4N_2O	48.0324	C_2HNO	55.0058	C_2H_4NO	58.0293
CH_4O_2	48.0211	$C_2H_3N_2$	55.0297	$C_2H_6N_2$	58.0532
C_4	48.0000	C_3H_3O	55.0184	C_3H_6O	58.0419
49		C_3H_5N	55.0422	C_3H_8N	58.0657
HO_3	48.9925	C_4H_7	55.0548	C_4H_{10}	58.0783
H_3NO_2	49.0164	**56**		**59**	
C_4H	49.0078	N_4	56.0124	HN_3O	59.0120
50		CN_2O	56.0011	H_3N_4	59.0359
H_2O_3	50.0003	CH_2N_3	56.0249	$CHNO_2$	59.0007
C_3N	50.0031	C_2O_2	55.9898	CH_3N_2O	59.0246
C_4H_2	50.0157	C_2H_2NO	56.0136	CH_5N_3	59.0484
51		$C_2H_4N_2$	56.0375	$C_2H_3O_2$	59.0133
C_3HN	51.0109	C_3H_4O	56.0262	C_2H_5NO	59.0371
C_4H_3	51.0235	C_3H_6N	56.0501	$C_2H_7N_2$	59.0610
52		C_4H_8	56.0626	C_3H_7O	59.0497
C_2N_2	52.0062	**57**		C_3H_9N	59.0736
C_3O	51.9949	HN_4	57.0202	**60**	
C_3H_2N	52.0187	CHN_2O	57.0089	N_2O_2	59.9960
C_4H_4	52.0313	CH_3N_3	57.0328	H_2N_3O	60.0198
53		C_2HO_2	56.9976	H_4N_4	60.0437
C_2HN_2	53.0140	C_2H_3NO	57.0215	CO_3	59.9847
C_3HO	53.0027	$C_2H_5N_2$	57.0453	CH_2NO_2	60.0085
C_3H_3N	53.0266	C_3H_5O	57.0340	CH_4N_2O	60.0324
C_4H_5	53.0391	C_3H_7N	57.0579	CH_6N_3	60.0563
54		C_4H_9	57.0705	$C_2H_4O_2$	60.0211
CN_3	54.0093	**58**		C_2H_6NO	60.0449
C_2NO	53.9980	N_3O	58.0042	$C_2H_8N_2$	60.0688
$C_2H_2N_2$	54.0218	H_2N_4	58.0280	C_3H_8O	60.0575
C_3H_2O	54.0106	CNO_2	57.9929	C_5	60.0000
C_3H_4N	54.0344	CH_2N_2O	58.0167	**61**	
C_4H_6	54.0470	CH_4N_3	58.0406	HN_2O_2	61.0038
55		$C_2H_2O_2$	58.0054	H_3N_3O	61.0277
CHN_3	55.0171				

	FM		FM		FM
H_5N_4	61.0515	C_3N_2	64.0062	$C_3H_4N_2$	68.0375
CHO_3	60.9925	C_4O	63.9949	C_4H_4O	68.0262
CH_3NO_2	61.0164	C_4H_2N	64.0187	C_4H_6N	68.0501
CH_5N_2O	61.0402	C_5H_4	64.0313	C_5H_8	68.0626
CH_7N_3	61.0641	**65**		**69**	
$C_2H_5O_2$	61.0289	HO_4	64.9874	CHN_4	69.0202
C_2H_7NO	61.0528	H_3NO_3	65.0113	C_2HN_2O	69.0089
C_5H	61.0078	C_3HN_2	65.0140	$C_2H_3N_3$	69.0328
62		C_4HO	65.0027	C_3HO_2	68.9976
NO_3	61.9878	C_4H_3N	65.0266	C_3H_3NO	69.0215
$H_2N_2O_2$	62.0016	C_5H_5	65.0391	$C_3H_5N_2$	69.0453
H_4N_3O	62.0355	**66**		C_4H_5O	69.0340
H_6N_4	62.0594	H_2O_4	65.9953	C_4H_7N	69.0579
CH_2O_3	62.0003	C_2N_3	66.0093	C_5H_9	69.0705
CH_4NO_2	62.0242	C_3NO	65.9980	**70**	
CH_6N_2O	62.0480	$C_3H_2N_2$	66.0218	CN_3O	70.0042
$C_2H_6O_2$	62.0368	C_4H_2O	66.0106	CH_2N_4	70.0280
C_4N	62.0031	C_4H_4N	66.0344	C_2NO_2	69.9929
C_5H_2	62.0157	C_5H_6	66.0470	$C_2H_2N_2O$	70.0167
63		**67**		$C_2H_4N_3$	70.0406
HNO_3	62.9956	C_2HN_3	67.0171	$C_3H_2O_2$	70.0054
$H_3N_2O_2$	63.0195	C_3HNO	67.0058	C_3H_4NO	70.0293
H_5N_3O	63.0433	$C_3H_3N_2$	67.0297	$C_3H_6N_2$	70.0532
CH_3O_3	63.0082	C_4H_3O	67.0184	C_4H_6O	70.0419
CH_5NO_2	63.0320	C_4H_5N	67.0422	C_4H_8N	70.0657
C_4HN	63.0109	C_5H_7	67.0548	C_5H_{10}	70.0783
C_5H_3	63.0235	**68**		**71**	
64		CN_4	68.0124	CHN_3O	71.0120
O_4	63.9796	C_2N_2O	68.0011	CH_3N_4	71.0359
H_2NO_3	64.0034	$C_2H_2N_3$	68.0249	C_2HNO_2	71.0007
$H_4N_2O_2$	64.0273	C_3O_2	67.9598	$C_2H_3N_2O$	71.0246
CH_4O_3	64.0160	C_3H_2NO	68.0136	$C_2H_5N_3$	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_4HN_2	77.0140	$H_4N_2O_3$	80.0222	C_5H_8N	82.0657
C_5HO	77.0027	CH_4O_4	80.0109	C_6H_{10}	82.0783
C_5H_3N	77.0266	C_2N_4	80.0124	**83**	
C_6H_5	77.0391	C_3N_2O	80.0011	C_2HN_3O	83.0120
78		$C_3H_2N_3$	80.0249	$C_2H_3N_4$	83.0359
NO_4	77.9827	C_4O_2	79.9898	C_3HNO_2	83.0007
$H_2N_2O_3$	78.0065	C_4H_2NO	80.0136	$C_3H_3N_2O$	83.0246
$H_4N_3O_2$	78.0304	$C_4H_4N_2$	80.0375	$C_3H_5N_3$	83.0484
H_6N_4O	78.0542	C_5H_4O	80.0262	$C_4H_3O_2$	83.0133
CH_2O_4	77.9953	C_5H_6N	80.0501	C_4H_5NO	83.0371
CH_4NO_3	78.0191	C_6H_8	80.0626	$C_4H_7N_2$	83.0610
$C_2H_6O_3$	78.0317	**81**		C_5H_7O	83.0497
$CH_6N_2O_2$	78.0429	H_3NO_4	81.0062	C_5H_9N	83.0736
C_3N_3	78.0093	C_2HN_4	81.0202	C_6H_{11}	83.0861
C_4NO	77.9980	C_2HN_2O	81.0089	**84**	
$C_4H_2N_2$	78.0218	$C_3H_3N_3$	81.0328	CN_4O	84.0073
C_5H_2O	78.0106	C_4HO_2	80.9976	$C_2N_2O_2$	83.9960
C_5H_4N	78.0344	C_4H_3NO	81.0215	$C_2H_2N_3O$	84.0198
C_6H_6	78.0740	$C_4H_5N_2$	81.0453	$C_2H_4N_4$	84.0437
79		C_5H_5O	81.0340	C_3O_3	83.9847
HNO_4	78.9905	C_5H_7N	81.0579	$C_3H_2NO_2$	84.0085
$H_3N_2O_3$	79.0144	C_6H_8	81.0705	$C_3H_4N_2O$	84.0324
$H_5N_3O_2$	79.0382	**82**		$C_3H_6N_3$	84.0563
CH_3O_4	79.0031	C_2N_3O	82.0042	$C_4H_4O_2$	84.0211
CH_5NO_3	79.0269	$C_2H_2N_4$	82.0280	C_4H_6NO	84.0449
C_3HN_3	79.0171	C_3NO_2	81.9929	$C_4H_8N_2$	84.0688
C_4HNO	79.0058	$C_3H_2N_2O$	82.0167	C_5H_8O	84.0575
$C_4H_3N_2$	79.0297	$C_3H_4N_3$	82.0406	$C_5H_{10}N$	84.0814
C_5H_3O	79.0184	$C_4H_2O_2$	82.0054	C_6H_{12}	84.0939
C_5H_5N	79.0422	C_4H_4NO	82.0293	C_7	84.0000
C_6H_7	79.0548	$C_4H_6N_2$	82.0532	**85**	
80		C_5H_6O	82.0419	CHN_4O	85.0151
H_2NO_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_4HN_3	91.0171	$CH_5N_2O_3$	93.0300
$CH_2N_2O_3$	90.0065	C_5HNO	91.0058	$CH_7N_3O_2$	93.0539
$CH_4N_3O_2$	90.0304	$C_5H_3N_2$	91.0297	$C_2H_5O_4$	93.0187
CH_6N_4O	90.0542	C_6H_3O	91.0184	$C_2H_7NO_3$	93.0426
$C_2H_2O_4$	89.9953	C_6H_5N	91.0422	C_3HN_4	93.0202
$C_2H_4NO_3$	90.0191	C_7H_7	91.0548	C_4HN_2O	93.0089
$C_2H_6N_2O_2$	90.0429	**92**		$C_4H_3N_3$	93.0328
$C_2H_8N_3O$	90.0668	N_2O_4	91.9858	C_5HO_2	92.9976
$C_2H_{10}N_4$	90.0907	$H_2N_3O_3$	92.0096	C_5H_3NO	93.0215
$C_3H_6O_3$	90.0317	$H_4N_4O_2$	92.0335	$C_5H_5N_2$	93.0453
$C_3H_8NO_2$	90.0555	CH_2NO_4	91.9983	C_6H_5O	93.0340
$C_3H_{10}N_2O$	90.0794	$CH_4N_2O_3$	92.0222	C_6H_7N	93.0579
$C_4H_{10}O_2$	90.0681	$CH_6N_3O_2$	92.0460	C_7H_9	93.0705
C_4N_3	90.0093	CH_8N_4O	92.0699	**94**	
C_5NO	89.9980	$C_2H_4O_4$	92.0109	$H_2N_2O_4$	94.0014
$C_5H_2N_2$	90.0218	$C_2H_6NO_3$	92.0348	$H_4N_3O_3$	94.0253
C_6H_2O	90.0106	$C_2H_8N_2O_2$	92.0586	$H_6N_4O_2$	94.0491
C_6H_4N	90.0344	$C_3H_8O_3$	92.0473	CH_4NO_4	94.0140
C_7H_6	90.0470	C_3N_4	92.0124	$CH_6N_2O_3$	94.0379
91		C_4N_2O	92.0011	$C_2H_6O_4$	94.0266
HN_3O_3	91.0018	$C_4H_2N_3$	92.0249	C_3N_3O	94.0042
$H_3N_4O_2$	91.0257	C_5O_2	91.9898	$C_3H_2N_4$	94.0280
$CHNO_4$	90.9905	C_5H_2NO	92.0136	C_4NO_2	93.9929
$CH_3N_2O_3$	91.0144	$C_5H_4N_2$	92.0375	$C_4H_2N_2O$	94.0167
$CH_5N_3O_2$	91.0382	C_6H_4O	92.0262	$C_4H_4N_3$	94.0406
CH_7N_4O	91.0621	C_6H_6N	92.0501	$C_5H_2O_2$	94.0054
$C_2H_3O_4$	91.0031	C_7H_8	92.0626	C_5H_4NO	94.0293
$C_2H_5NO_3$	91.0269	**93**		$C_5H_6N_2$	94.0532
$C_2H_7N_2O_2$	01.0508	HN_2O_4	92.9936	C_6H_6O	94.0419
$C_2H_9N_3O$	91.0746	$H_3N_3O_3$	93.0175	C_6H_8N	94.0657
$C_3H_7O_3$	91.0395	$H_5N_4O_2$	93.0413	C_7H_{10}	94.0783
$C_3H_9NO_2$	91.0634	CH_3NO_4	93.0062	**95**	
				$H_3N_2O_4$	95.0093

	FM		FM		FM
$H_5N_3O_3$	95.0331	$C_3HN_2O_2$	97.0038	C_8H_2	98.0157
CH_5NO_4	95.0218	$C_3H_3N_3O$	97.0277	**99**	
C_3HN_3O	95.0120	$C_3H_5N_4$	97.0515	$C_2HN_3O_2$	99.0069
$C_3H_3N_4$	95.0359	C_4HO_3	96.9925	$C_2H_3N_4O$	99.0308
C_4HNO_2	95.0007	$C_4H_3NO_2$	97.0164	C_3HNO_3	98.9956
$C_4H_3N_2O$	95.0246	$C_4H_5N_2O$	97.0402	$C_3H_3N_2O_2$	99.0195
$C_4H_5N_3$	95.0484	$C_4H_7N_3$	97.0641	$C_3H_5N_3O$	99.0433
$C_5H_3O_2$	95.0133	$C_5H_5O_2$	97.0289	$C_3H_7N_4$	99.0672
C_5H_5NO	95.0371	C_5H_7NO	97.0528	$C_4H_3O_3$	99.0082
$C_5H_7N_2$	95.0610	$C_5H_9N_2$	97.0767	$C_4H_5NO_2$	99.0320
C_6H_7O	95.0497	C_6H_9O	97.0653	$C_4H_7N_2O$	99.0559
C_6H_9N	95.0736	$C_6H_{11}N$	97.0892	$C_4H_9N_3$	99.0798
C_7H_{11}	95.0861	C_7H_{13}	97.1018	$C_5H_7O_2$	99.0446
96		C_8H	97.0078	C_5H_9NO	99.0684
$H_4N_2O_4$	96.0171	**98**		$C_5H_{11}N_2$	99.0923
C_2N_4O	96.0073	$C_2N_3O_2$	97.9991	$C_6H_{11}O$	99.0810
$C_3N_2O_2$	95.9960	$C_2H_2N_4O$	98.0229	$C_6H_{13}N$	99.1049
$C_3H_2N_3O$	96.0198	C_3NO_3	97.9878	C_7H_{15}	99.1174
$C_3H_4N_4$	96.0437	$C_3H_2N_2O_2$	98.0116	C_7HN	99.0109
C_4O_3	95.9847	$C_3H_4N_3O$	98.0355	C_8H_3	99.0235
$C_4H_2NO_2$	96.0085	$C_3H_6N_4$	98.0594	**100**	
$C_4H_4N_2O$	96.0324	$C_4H_2O_3$	98.0003	CN_4O_2	100.0022
$C_4H_6N_3$	96.0563	$C_4H_4NO_2$	98.0242	$C_2N_2O_3$	99.9909
$C_5H_4O_2$	96.0211	$C_4H_6N_2O$	98.0480	$C_2H_2N_3O_2$	100.0147
C_5H_6NO	96.0449	$C_4H_8N_3$	98.0719	$C_2H_4N_4O$	100.0386
$C_5H_8N_2$	96.0688	$C_5H_6O_2$	98.0368	C_3O_4	99.9796
C_6H_8O	96.0575	C_5H_8NO	98.0606	$C_3H_2NO_3$	100.0034
$C_6H_{10}N$	96.0814	$C_5H_{10}N_2$	98.0845	$C_3H_4N_2O_2$	100.0273
C_7H_{12}	96.0939	$C_6H_{10}O$	98.0732	$C_3H_6N_3O$	100.0511
C_8	96.0000	$C_6H_{12}N$	98.0970	$C_3H_8N_4$	100.0750
97		C_7H_{14}	98.1096	$C_4H_4O_3$	100.0160
C_2HN_4O	97.0151	C_7N	98.0031	$C_4H_6NO_2$	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
$C_7O^{\cdot}$	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	$C_3H_8N_2O_2$	104.0586

	FM		FM		FM
$C_3H_{10}N_3O$	104.0825	C_6HO_2	104.9976	$CH_7N_4O_2$	107.0570
$C_3H_{12}N_4$	104.1063	C_6H_3NO	105.0215	$C_2H_5NO_4$	107.0218
$C_4H_8O_3$	104.0473	$C_6H_5N_2$	105.0453	$C_2H_7N_2O_3$	107.0457
$C_4H_{10}NO_2$	104.0712	C_7H_5O	105.0340	$C_2H_9N_3O_2$	107.0695
$C_4H_{12}N_2O$	104.0950	C_7H_7N	105.0579	$C_3H_7O_4$	107.0344
C_4N_4	104.0124	C_8H_9	105.0705	$C_3H_9NO_3$	107.0583
$C_5H_{12}O_2$	104.0837	**106**		C_4HN_3O	107.0120
C_5N_2O	104.0011	$CH_2N_2O_4$	106.0014	$C_4H_3N_4$	107.0359
$C_5H_2N_3$	104.0249	$CH_4N_3O_3$	106.0253	C_5HNO_2	107.0007
C_6O_2	103.9898	$CH_6N_4O_2$	106.0491	$C_5H_3N_2O$	107.0246
C_6H_2NO	104.0136	$C_2H_4NO_4$	106.0140	$C_5H_5N_3$	107.0484
$C_6H_4N_2$	104.0375	$C_2H_6N_2O_3$	106.0379	$C_6H_3O_2$	107.0133
C_7H_4O	104.0262	$C_2H_8N_3O_2$	106.0617	C_6H_5NO	107.0371
C_7H_6N	104.0501	$C_2H_{10}N_4O$	106.0856	$C_6H_7N_2$	107.0610
C_8H_8	104.0626	$C_3H_6O_4$	106.0266	C_7H_7O	107.0497
105		$C_3H_8NO_3$	106.0504	C_7H_9N	107.0736
CHN_2O_4	104.9936	$C_3H_{10}N_2O_2$	106.0743	C_8H_{11}	107.0861
$CH_3N_3O_3$	105.0175	$C_4H_{10}O_3$	106.0630	**108**	
$CH_5N_4O_2$	105.0413	C_4N_3O	106.0042	$CH_4N_2O_4$	108.0171
$C_2H_3NO_4$	105.0062	$C_4H_2N_4$	106.0280	$CH_6N_3O_3$	108.0410
$C_2H_5N_2O_3$	105.0300	C_5NO_2	105.9929	$CH_8N_4O_2$	108.0648
$C_2H_7N_3O_2$	105.0539	$C_5H_2N_2O$	106.0167	$C_2H_6NO_4$	108.0297
$C_2H_9N_4O$	105.0777	$C_5H_4N_3$	106.0406	$C_2H_8N_2O_3$	108.0535
$C_3H_5O_4$	105.0187	$C_6H_2O_2$	106.0054	$C_3H_8O_4$	108.0422
$C_3H_7NO_3$	105.0426	C_6H_4NO	106.0293	C_3N_4O	108.0073
$C_3H_9N_2O_2$	105.0664	$C_6H_6N_2$	106.0532	$C_4N_2O_2$	107.9960
$C_3H_{11}N_3O$	105.0903	C_7H_6O	106.0419	$C_4H_2N_3O$	108.0198
$C_4H_9O_3$	105.0552	C_7H_8N	106.0657	$C_4H_4N_4$	108.0437
$C_4H_{11}NO_2$	105.0790	C_8H_{10}	106.0783	C_5O_3	107.9847
C_4HN_4	105.0202	**107**		$C_5H_2NO_2$	108.0085
C_5HN_2O	105.0089	$CH_3N_2O_4$	107.0093	$C_5H_4N_2O$	108.0324
$C_5H_3N_3$	105.0328	$CH_5N_3O_3$	107.0331	$C_5H_6N_3$	108.0563

	FM		FM		FM
$C_6H_4O_2$	108.0211	$C_4H_4N_3O$	110.0355	C_9H_3	111.0235
C_6H_6NO	108.0449	$C_4H_6N_4$	110.0594	**112**	
$C_6H_8N_2$	108.0688	$C_5H_2O_3$	110.0003	$C_2N_4O_2$	112.0022
C_7H_8O	108.0575	$C_5H_4NO_2$	110.0242	$C_3N_2O_3$	111.9909
$C_7H_{10}N$	108.0814	$C_5H_6N_2O$	110.0480	$C_3H_2N_3O_2$	112.0147
C_8H_{12}	108.0939	$C_5H_8N_3$	110.0719	$C_3H_4N_4O$	112.0386
C_9	108.0000	$C_6H_6O_2$	110.0368	C_4O_4	111.9796
109		C_6H_8NO	110.0606	$C_4H_2NO_3$	112.0034
$CH_5N_2O_4$	109.0249	$C_6H_{10}N_2$	110.0845	$C_4H_4N_2O_2$	112.0273
$CH_8N_3O_3$	109.0488	$C_7H_{10}O$	110.0732	$C_4H_6N_3O$	112.0511
$C_2H_7NO_4$	109.0375	$C_7H_{12}N$	110.0970	$C_4H_8N_4$	112.0750
C_3HN_4O	109.0151	C_8H_{14}	110.1096	$C_5H_4O_3$	112.0160
$C_4HN_2O_2$	109.0038	C_8N	110.0031	$C_5H_6NO_2$	112.0399
$C_4H_3N_3O$	109.0277	C_9H_2	110.0157	$C_5H_8N_2O$	112.0637
$C_4H_5N_4$	109.0515	**111**		$C_5H_{10}N_3$	112.0876
C_5HO_3	108.9925	$C_3HN_3O_2$	111.0069	$C_6H_8O_2$	112.0524
$C_5H_3NO_2$	109,0164	$C_3H_3N_4O$	111.0308	$C_6H_{10}NO$	112.0763
$C_5H_5N_2O$	109.0402	C_4HNO_3	110.9956	$C_6H_{12}N_2$	112.1001
$C_5H_7N_3$	109.0641	$C_4H_3N_2O_2$	111.0195	$C_7H_{12}O$	112.0888
$C_6H_5O_2$	109.0289	$C_4H_5N_3O$	111.0433	$C_7H_{14}N$	112.1127
C_6H_7NO	109.0528	$C_4H_7N_4$	111.0672	C_7N_2	112.0062
$C_6H_9N_2$	109.0767	$C_5H_3O_3$	111.0082	C_8H_{16}	112.1253
C_7H_9O	109.0653	$C_5H_5NO_2$	111.0320	C_8O	111.9949
$C_7H_{11}N$	109.0892	$C_5H_7N_2O$	111.0559	C_8H_2N	112.0187
C_8H_{13}	109.1018	$C_5H_9N_3$	111.0798	C_9H_4	112.0313
C_9H	109.0078	$C_6H_7O_2$	111.0446	**113**	
110		C_6H_9NO	111.0684	$C_2HN_4O_2$	113.0100
$CH_6N_2O_4$	110.0328	$C_6H_{11}N_2$	111.0923	$C_3HN_2O_3$	112.9987
$C_3N_3O_2$	109.9991	$C_7H_{11}O$	111.0810	$C_3H_3N_3O_2$	113.0226
$C_3H_2N_4O$	110.0229	$C_7H_{13}N$	111.1049	$C_3H_5N_4O$	113.0464
C_4NO_3	109.9878	C_8H_{15}	111.1174	C_4HO_4	112.9874
$C_4H_2N_2O_2$	110.0116	C_8HN	111.0109	$C_4H_3NO_3$	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_7O_2	115.9898	C_8H_7N	117.0579	$C_2H_5N_3O_3$	119.0331
C_7H_2NO	116.0136	C_9H_9	117.0705	$C_2H_7N_4O_2$	119.0570
$C_7H_4N_2$	116.0375	**118**		$C_3H_5NO_4$	119.0218
C_8H_4O	116.0262	$C_2H_2N_2O_4$	118.0014	$C_3H_7N_2O_3$	119.0457
C_8H_6N	116.0501	$C_2H_4N_3O_3$	118.0253	$C_3H_9N_3O_2$	119.0695
C_9H_8	116.0626	$C_2H_6N_4O_2$	118.0491	$C_3H_{11}N_4O$	119.0934
117		$C_3H_4NO_4$	118.0140	$C_4H_7O_4$	119.0344
$C_2HN_2O_4$	116.9936	$C_3H_6N_2O_3$	118.0379	$C_4H_9NO_3$	119.0583
$C_2H_3N_3O_3$	117.0175	$C_3H_8N_3O_2$	118.0617	$C_4H_{11}N_2O_2$	119.0821
$C_2H_5N_4O_2$	117.0413	$C_3H_{10}N_4O$	118.0856	$C_4H_{13}N_3O$	119.1060
$C_3H_3NO_4$	117.0062	$C_4H_6O_4$	118.0266	$C_5H_{11}O_3$	119.0708
$C_3H_5N_2O_3$	117.0300	$C_4H_8NO_3$	118.0504	$C_5H_{13}NO_2$	119.0947
$C_3H_7N_3O_2$	117.0539	$C_4H_{10}N_2O_2$	118.0743	C_5HN_3O	119.0120
$C_3H_9N_4O$	117.0777	$C_4H_{12}N_3O$	118.0981	$C_5H_3N_4$	119.0359
$C_4H_5O_4$	117.0187	$C_4H_{14}N_4$	118.1220	C_6HNO_2	119.0007
$C_4H_7NO_3$	117.0426	$C_5H_{10}O_3$	118.0630	$C_6H_3N_2O$	119.0246
$C_4H_9N_2O_2$	117.0664	$C_5H_{12}NO_2$	118.0868	$C_6H_5N_3$	119.0484
$C_4H_{11}N_3O$	117.0903	$C_5H_{14}N_2O$	118.1107	$C_7H_3O_2$	119.0133
$C_4H_{13}N_4$	117.1142	C_5N_3O	118.0042	C_7H_5NO	119.0371
$C_5H_9O_3$	117.0552	$C_5H_2N_4$	118.0280	$C_7H_7N_2$	119.0610
$C_5H_{11}NO_2$	117.0790	$C_6H_{14}O_2$	118.0994	C_8H_7O	119.0497
$C_5H_{13}N_2O$	117.1029	C_6NO_2	117.9929	C_8H_9N	119.0736
$C_5H_{15}N_3$	117.1267	$C_6H_2N_2O$	118.0167	C_9H_{11}	119.0861
C_5HN_4	117.0202	$C_6H_4N_3$	118.0406	**120**	
$C_6H_{13}O_2$	117.0916	$C_7H_2O_2$	118.0054	$C_2H_4N_2O_4$	120.0171
$C_6H_{15}NO$	117.1154	C_7H_4NO	118.0293	$C_2H_6N_3O_3$	120.0410
C_6HN_2O	117.0089	$C_7H_6N_2$	118.0532	$C_2H_8N_4O_2$	120.0648
$C_6H_3N_3$	117.0328	C_8H_6O	118.0419	$C_3H_6NO_4$	120.0297
C_7HO_2	116.9976	C_8H_8N	118.0657	$C_3H_8N_2O_3$	120.0535
C_7H_3NO	117.0215	C_9H_{10}	118.0783	$C_3H_{10}N_3O_2$	120.0774
$C_7H_5N_2$	117.0453	**119**		$C_3H_{12}N_4O$	120.1012
C_8H_5O	117.0340	$C_2H_3N_2O_4$	119.0093	$C_4H_8O_4$	120.0422

	FM		FM		FM
$C_4H_{10}NO_3$	120.0661	$C_6H_3NO_2$	121.0164	C_9H_{14}	122.1096
$C_4H_{12}N_2O_2$	120.0899	$C_6H_5N_2O$	121.0402	C_9N	122.0031
C_4N_4O	120.0073	$C_6H_7N_3$	121.0641	$C_{10}H_2$	122.0157
$C_5H_{12}O_3$	120.0786	$C_7H_5O_2$	121.0289	**123**	
$C_5N_2O_2$	119.9960	C_7H_7NO	121.0528	$C_2H_7N_2O_4$	123.0406
$C_5H_2N_3O$	120.0198	$C_7H_9N_2$	121.0767	$C_2H_9N_3O_3$	123.0644
$C_5H_4N_4$	120.0437	C_8H_9O	121.0653	$C_3H_9NO_4$	123.0532
C_6O_3	119.9847	$C_8H_{11}N$	121.0892	$C_4HN_3O_2$	123.0069
$C_6H_2NO_2$	120.0085	C_9H_{13}	121.1018	$C_4H_3N_4O$	123.0308
$C_6H_4N_2O$	120.0324	$C_{10}H$	121.0078	C_5HNO_3	122.9956
$C_6H_6N_3$	120.0563	**122**		$C_5H_3N_2O_2$	123.0195
$C_7H_4O_2$	120.0211	$C_2H_6N_2O_4$	122.0328	$C_5H_5N_3O$	123.0433
C_7H_6NO	120.0449	$C_2H_8N_3O_3$	122.0566	$C_5H_7N_4$	123.0672
$C_7H_8N_2$	120.0688	$C_2H_{10}N_4O_2$	122.0805	$C_6H_3O_3$	123.0082
C_8H_8O	120.0575	$C_3H_8NO_4$	122.0453	$C_6H_5NO_2$	123.0320
$C_8H_{10}N$	120.0814	$C_3H_{10}N_2O_3$	122.0692	$C_6H_7N_2O$	123.0559
C_9H_{12}	120.0939	$C_4H_{10}O_4$	122.0579	$C_6H_9N_3$	123.0798
C_{10}	120.0000	$C_4N_3O_2$	121.9991	$C_7H_7O_2$	123.0446
121		$C_4H_2N_4O$	122.0229	C_7H_9NO	123.0684
$C_2H_5N_2O_4$	121.0249	C_5NO_3	121.9878	$C_7H_{11}N_2$	123.0923
$C_2H_7N_3O_3$	121.0488	$C_5H_2N_2O_2$	122.0116	$C_8H_{11}O$	123.0810
$C_2H_9N_4O_2$	121.0726	$C_5H_4N_3O$	122.0355	$C_8H_{13}N$	123.1049
$C_3H_7NO_4$	121.0375	$C_5H_6N_4$	122.0594	C_9H_{15}	123.1174
$C_3H_9N_2O_3$	121.0614	$C_6H_2O_3$	122.0003	C_9HN	123.0109
$C_3H_{11}N_3O_2$	121.0852	$C_6H_4NO_2$	122.0242	$C_{10}H_3$	123.0235
$C_4H_9O_4$	121.0501	$C_6H_6N_2O$	122.0480	**124**	
$C_4H_{11}NO_3$	121.0739	$C_6H_8N_3$	122.0719	$C_2H_8N_2O_4$	124.0484
C_4HN_4O	121.0151	$C_7H_6O_2$	122.0368	$C_3N_4O_2$	124.0022
$C_5HN_2O_2$	121.0038	C_7H_8NO	122.0606	$C_4N_2O_3$	123.9909
$C_5H_3N_3O$	121.0277	$C_7H_{10}N_2$	122.0845	$C_4H_2N_3O_2$	124.0147
$C_5H_5N_4$	121.0515	$C_8H_{10}O$	122.0732	$C_4H_4N_4O$	124.0386
C_6HO_3	120.9925	$C_8H_{12}N$	122.0970	C_5O_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
$C_4H_{12}N_5O_2$	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_9H_2NO	140.0136	C_9H_3NO	141.0215	$C_9H_2O_2$	142.0054
$C_9H_4N_2$	140.0375	$C_9H_5N_2$	141.0453	$C_9H_{20}N$	142.1597
$C_{10}H_{20}$	140.1566	$C_{10}H_{21}$	141.1644	C_9H_4NO	142.0293
$C_{10}H_4O$	140.0262	$C_{10}H_5O$	141.0340	$C_9H_6N_2$	142.0532
$C_{10}H_6N$	140.0501	$C_{10}H_7N$	141.0579	$C_{10}H_{22}$	142.1722
$C_{11}H_8$	140.0626	$C_{11}H_9$	141.0705	$C_{10}H_6O$	142.0419
141		**142**		$C_{10}H_8N$	142.0657
$C_4HN_2O_4$	140.9936	$C_4H_2N_2O_4$	142.0014	$C_{11}H_{10}$	142.0783
$C_4H_3N_3O_3$	141.0175	$C_4H_4N_3O_3$	142.0253	**143**	
$C_4H_5N_4O_2$	141.0413	$C_4H_6N_4O_2$	142.0491	$C_4H_3N_2O_4$	143.0093
$C_5H_3NO_4$	141.0062	$C_5H_4NO_4$	142.0140	$C_4H_5N_3O_3$	143.0331
$C_5H_5N_2O_3$	141.0300	$C_5H_6N_2O_3$	142.0379	$C_4H_7N_4O_2$	143.0570
$C_5H_7N_3O_2$	141.0539	$C_5H_8N_3O_2$	142.0617	$C_5H_5NO_4$	143.0218
$C_5H_9N_4O$	141.0777	$C_5H_{10}N_4O$	142.0856	$C_5H_7N_2O_3$	143.0457
$C_6H_5O_4$	141.0187	$C_6H_6O_4$	142.0266	$C_5H_9N_3O_2$	143.0695
$C_6H_7NO_3$	141.0426	$C_6H_8NO_3$	142.0504	$C_5H_{11}N_4O$	143.0934
$C_6H_9N_2O_2$	141.0664	$C_6H_{10}N_2O_2$	142.0743	$C_6H_7O_4$	143.0344
$C_6H_{11}N_3O$	141.0903	$C_6H_{12}N_3O$	142.0981	$C_6H_9NO_3$	143.0583
$C_6H_{13}N_4$	141.1142	$C_6H_{14}N_4$	142.1220	$C_6H_{11}N_2O_2$	143.0821
$C_7H_9O_3$	141.0552	$C_7H_{10}O_3$	142.0630	$C_6H_{13}N_3O$	143.1060
$C_7H_{11}NO_2$	141.0790	$C_7H_{12}NO_2$	142.0868	$C_6H_{15}N_4$	143.1298
$C_7H_{13}N_2O$	141.1029	$C_7H_{14}N_2O$	142.1107	$C_7H_{11}O_3$	143.0708
$C_7H_{15}N_3$	141.1267	$C_7H_{16}N_3$	142.1346	$C_7H_{13}NO_2$	143.0947
C_7HN_4	141.0202	C_7N_3O	142.0042	$C_7H_{15}N_2O$	143.1185
$C_7H_{13}O_2$	141.0916	$C_7H_2N_4$	142.0280	$C_7H_{17}N_3$	143.1424
$C_8H_{15}NO$	141.1154	$C_8H_{14}O_2$	142.0994	C_7HN_3O	143.0120
$C_8H_{17}N_2$	141.1393	$C_8H_{16}NO$	142.1233	$C_7H_3N_4$	143.0359
C_8HN_2O	141.0089	C_8NO_2	141.9929	$C_8H_{15}O_2$	143.1072
$C_8H_3N_3$	141.0328	$C_8H_{18}N_2$	142.1471	$C_8H_{17}NO$	143.1311
$C_9H_{17}O$	141.1280	$C_8H_2N_2O$	142.0167	C_8HNO_2	143.0007
C_9HO_2	140.9976	$C_8H_4N_3$	142.0406	$C_8H_{19}N_2$	143.1549
$C_9H_{19}N$	141.1519	$C_9H_{18}O$	142.1358	$C_8H_3N_2O$	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	$C_8H_3O_3$	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	$C_9H_{13}N_2O$	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
$C_5HN_2O_4$	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	$C_6HN_4O_2$	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
$C_{12}H_2O$	162.0106	$C_{11}H_{17}N$	163.1362	$C_{10}H_{14}NO$	164.1076
$C_{12}H_4N$	162.0344	$C_{11}HNO$	163.0058	$C_{10}H_{16}N_2$	164.1315
$C_{13}H_6$	162.0470	$C_{11}H_3N_2$	163.0297	$C_{10}N_2O$	164.0011
163		$C_{12}H_{19}$	163.1488	$C_{10}H_2N_3$	164.0249
$C_5H_{11}N_2O_4$	163.0719	$C_{12}H_3O$	163.0184	$C_{11}H_{16}O$	164.1202
$C_5H_{13}N_3O_3$	163.0958	$C_{12}H_5N$	163.0422	$C_{11}O_2$	163.9898
$C_5H_{15}N_4O_2$	163.1196	$C_{13}H_7$	163.0548	$C_{11}H_{18}N$	164.1440
$C_6H_{13}NO_4$	163.0845	**164**		$C_{11}H_2NO$	164.0136
$C_6H_{15}N_2O_3$	163.1083	$C_5H_{12}N_2O_4$	164.0797	$C_{11}H_4N_2$	164.0375
$C_6H_{17}N_3O_2$	163.1322	$C_5H_{14}N_3O_3$	164.1036	$C_{12}H_{20}$	164.1566
$C_6HN_3O_3$	163.0018	$C_5H_{16}N_4O_2$	164.1275	$C_{12}H_4O$	164.0262
$C_6H_3N_4O_2$	163.0257	$C_6H_{14}NO_4$	164.0923	$C_{12}H_6N$	164.0501
$C_7H_{15}O_4$	163.0970	$C_6H_{16}N_2O_3$	164.1162	$C_{13}H_8$	164.0626
$C_7H_{17}NO_3$	163.1209	$C_6N_2O_4$	163.9858	**165**	
C_7HNO_4	161.9905	$C_6H_2N_3O_3$	164.0096	$C_5H_{13}N_2O_4$	165.0876
$C_7H_3N_2O_3$	163.0144	$C_6H_4N_4O_2$	164.0335	$C_5H_{15}N_3O_3$	165.1114
$C_7H_5N_3O_2$	163.0382	$C_7H_{16}O_4$	164.1049	$C_6H_{15}NO_4$	165.1001
$C_7H_7N_4O$	163.0621	$C_7H_2NO_4$	163.9983	$C_6HN_2O_4$	164.9936
$C_8H_3O_4$	163.0031	$C_7H_4N_2O_3$	164.0222	$C_6H_3N_3O_3$	165.0175
$C_8H_5NO_3$	163.0269	$C_7H_6N_3O_2$	164.0460	$C_6H_5N_4O_2$	165.0413
$C_8H_7N_2O_2$	163.0508	$C_7H_8N_4O$	164.0699	$C_7H_3NO_4$	165.0062
$C_8H_9N_3O$	163.0746	$C_8H_4O_4$	164.0109	$C_7H_5N_2O_3$	165.0300
$C_8H_{11}N_4$	163.0985	$C_8H_6NO_3$	164.0348	$C_7H_7N_3O_2$	165.0539
$C_9H_7O_3$	163.0395	$C_8H_8N_2O_2$	164.0586	$C_7H_9N_4O$	165.0777
$C_9H_9NO_2$	163.0634	$C_8H_{10}N_3O$	164.0825	$C_8H_5O_4$	165.0187
$C_9H_{11}N_2O$	163.0872	$C_8H_{12}N_4$	164.1063	$C_8H_7NO_3$	165.0426
$C_9H_{13}N_3$	163.1111	$C_9H_8O_3$	164.0473	$C_8H_9N_2O_2$	165.0664
$C_{10}H_{11}O_2$	163.0759	$C_9H_{10}NO_2$	164.0712	$C_8H_{11}N_3O$	165.0903
$C_{10}H_{13}NO$	163.0998	$C_9H_{12}N_2O$	164.0950	$C_8H_{13}N_4$	165.1142
$C_{10}H_{15}N_2$	163.1236	$C_9H_{14}N_3$	164.1189	$C_9H_9O_3$	165.0552
$C_{10}HN_3$	163.0171	C_9N_4	164.0124	$C_9H_{11}NO_2$	165.0790
$C_{11}H_{15}O$	163.1123	$C_{10}H_{12}O_2$	164.0837	$C_9H_{13}N_2O$	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	$C_8H_2N_2O_2$	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	$C_7H_{15}NO_4$	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	$C_{10}H_{16}N_3$	1781346	$C_9H_{13}N_3O$	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
$C_0H_7N_4O$	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	$C_9H_7N_4O_2$	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	$C_{12}H_2N_3O$	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
$C_{12}H_5N_4$	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
$C_{13}H_5N_2O$	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
$C_{14}H_5O_2$	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	$C_{12}H_5N_3O$	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	$C_{11}H_3N_3O_2$	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	$C_{13}H_{25}N_2$	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	$C_{15}H_{16}N$	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	$C_9H_{13}N_2O_4$	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	$C_{13}H_{16}N_3$	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
$C_{12}H_{13}N_3O$	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	$C_{13}H_5N_3O$	219.0433	$C_{11}H_{14}N_3O_2$	220.1087
$C_{17}N$	218.0031	$C_{13}H_7N_4$	219.0672	$C_{11}H_{16}N_4O$	220.1325
$C_{18}H_2$	218.0157	$C_{14}H_{19}O_2$	219.1385	$C_{11}N_4O_2$	220.0022
219		$C_{14}H_3O_3$	219.0082	$C_{12}H_{12}O_4$	220.0735
$C_9H_{19}N_2O_4$	219.1345	$C_{14}H_{21}NO$	219.1624	$C_{12}H_{14}NO_3$	220.0974
$C_9H_{21}N_3O_3$	219.1584	$C_{14}H_5NO_2$	219.0320	$C_{12}H_{16}N_2O_2$	220.1213
$C_9H_{23}N_4O_2$	219.1822	$C_{14}H_{23}N_2$	219.1863	$C_{12}N_2O_3$	219.9909
$C_{10}H_{21}NO_4$	219.1471	$C_{14}H_7N_2O$	219.0559	$C_{12}H_{18}N_3O$	220.1451
$C_{10}H_{23}N_2O_3$	219.1710	$C_{14}H_9N_3$	219.0798	$C_{12}H_2N_3O_2$	220.0147
$C_{10}H_7N_2O_4$	219.0406	$C_{15}H_{23}O$	219.1750	$C_{12}H_{20}N_4$	220.1690
$C_{10}H_{25}N_3O_2$	219.1948	$C_{15}H_7O_2$	219.0446	$C_{12}H_4N_4O$	220.0386
$C_{10}H_9N_3O_3$	219.0644	$C_{15}H_{25}N$	219.1988	$C_{13}H_{16}O_3$	220.1100
$C_{10}H_{11}N_4O_2$	219.0883	$C_{15}H_9NO$	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	$C_{13}H_2NO_3$	220.0034
$C_{11}H_9NO_4$	219.0532	$C_{16}H_{11}O$	219.0810	$C_{13}H_{20}N_2O$	220.1577
$C_{11}H_{11}N_2O_3$	219.0770	$C_{16}H_{13}N$	219.1049	$C_{13}H_4N_2O_2$	220.0273
$C_{11}H_{13}N_3O_2$	219.1009	$C_{17}H_{15}$	219.1174	$C_{13}H_{22}N_3$	220.1815
$C_{11}H_{15}N_4o$	219.1247	$C_{17}HN$	219.0109	$C_{13}H_6N_3O$	220.0511
$C_{12}H_{11}O_4$	219.0657	$C_{18}H_3$	219.0235	$C_{13}H_8N_4$	220.0750
$C_{12}H_{13}NO_3$	219.0896	**220**		$C_{14}H_{20}O_2$	220.1464
$C_{12}H_{15}N_2O_2$	219.1134	$C_9H_{20}N_2O_4$	220.1424	$C_{14}H_4O_3$	220.0160
$C_{12}H_{17}N_3O$	219.1373	$C_9H_{22}N_3O_3$	220.1662	$C_{14}H_{22}NO$	220.1702
$C_{12}HN_3O_2$	219.0069	$C_9H_{24}N_4O_2$	220.1901	$C_{14}H_6NO_2$	220.0399
$C_{12}H_9N_4$	219.1611	$C_{10}H_{22}NO_4$	220.1549	$C_{14}H_{24}N_2$	220.1941
$C_{12}H_3N_4O$	219.0308	$C_{10}H_{24}N_2O_3$	220.1788	$C_{14}H_8N_2O$	220.0637
$C_{13}H_{15}O_3$	219.1021	$C_{10}H_8N_2O_4$	220.0484	$C_{14}H_{10}N_3$	220.0876
$C_{13}H_{17}NO_2$	219.1260	$C_{10}H_{10}N_3O_3$	220.0723	$C_{15}H_{24}O$	220.1828
$C_{13}HNO_3$	218.9956	$C_{10}H_{12}N_4O_2$	220.0961	$C_{15}H_8O_2$	220.0524
$C_{13}H_{19}N_2O$	219.1498	$C_{11}H_{24}O_4$	220.1675	$C_{15}H_{26}N$	220.2067
$C_{13}H_3N_2O_2$	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	$C_{11}H_{12}N_2O_3$	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
$C_{15}H_{30}O$	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	$C_{16}H_3NO_2$	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	$C_{14}H_2N_4O$	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:

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

$\simeq 1.1 \times$ number of C atoms + $0.36 \times$ number of N atoms.

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

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

+ $0.20 \times$ 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 Ions*	**(Structural Inference)**
14	CH_2
15	CH_3
16	O
17	OH
18	H_2O, NH_4
19	F, H_3O
26	$C{\equiv}N$, C_2H_2
27	C_2H_3
28	C_2H_4, CO, N_2 (air), CH=NH
29	C_2H_5, CHO
30	$CH_2NH_2(RCH_2NH_2)$, NO
31	$CH_2OH(RCH_2OH)$, OCH_3
32	O_2(air)
33	SH, CH_2F

34 H_2S

35 Cl (^{37}Cl at 37)

36 HCl ($H^{37}Cl$ at 38)

39 C_3H_3

40 $CH_2C{=}N$, Ar (air)

41 C_3H_5, $CH_2C{=}N + H^a$, C_2H_2NH

42 C_3H_6, C_2H_2O

43 C_3H_7, $CH_3C{=}O$, $CH_3C{=}OG$, (G = R, Ar, NH_2, OR, OH), C_2H_5N

44 $CH_2\overset{H}{\underset{|}{C}}{=}O + H$ (Aldehydes, McLafferty Rearrangement), CH_3CHNH_2, CO_2, $NH_2C{=}O$ ($RC{=}ONH_2$), $(CH_3)_2N$

45 $\overset{CH_3}{\underset{|}{C}}HOH$, CH_2CH_2OH, CH_2OCH_3 (RCH_2OCH_3), $\overset{O}{\underset{\|}{C}}$–OH, CH_3CH–O+H(CH_3CHOHR)

46 NO_2

47 CH_2SH (RCH_2SH), CH_3S

48 CH_3S+H

49 CH_2Cl(CH_2 ^{37}Cl at 51)

51 CHF_2, C_4H_3

53 C_4H_5

54 $CH_2CH_2C{\equiv}N$

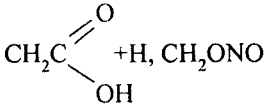
55 C_4H_7, $CH_2{=}CHC{=}O$

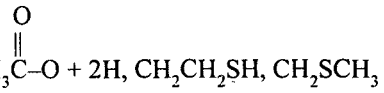
56 C_4H_8

57 C_4H_9, $C_2H_5C{=}O$

58 $CH_3{-}\overset{\overset{O}{\|}}{\underset{CH_2}{C}}$ + H, $C_2H_5CHNH_2$, $(CH_3)_2NCH_2$, $C_2H_5NHCH_2$, C_2H_2S

59 $(CH_3)_2COH$, $CH_2OC_2H_5$, $\overset{O}{\underset{\|}{C}}$–$OCH_3$ (RCO_2CH_3). $NH_2C{=}O$ + H, $CH_3O\overset{CH_2}{\underset{|}{C}}HCH_3$, CH_3CHCH_2OH, C_2H_5CHOH

60  +H, CH_2ONO

61 

65 C_5H_5

66  $\equiv C_5H_6, H_2S_2$ (RSSR)

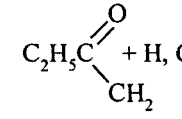
67 C_5H_7

68 $CH_2CH_2CH_2C{\equiv}N$

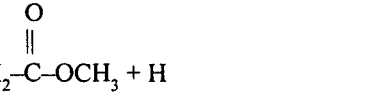
69 C_5H_9, CF_3, $CH_3CH{=}CHC{=}O$,
$CH_2{=}C(CH_3)C{=}O$

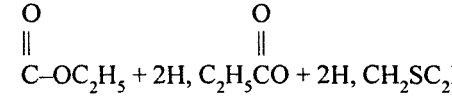
70 C_5H_{10}

71 C_5H_{11}, $C_3H_7C{=}O$

72  + H, $C_3H_7CHNH_2$, $(CH_3)_2N{=}C{=}O$,
$C_2H_5NHCHCH_3$ and isomers

73 Homologs of 59, $(CH_3)_3Si$

74 

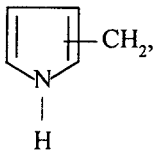
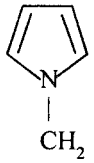
75 
$CH, (CH_3)_2SiOH$

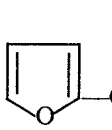
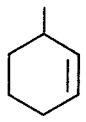
76 $C_6H_4(C_6H_5X, C_6H_4XY)$

77 C_6H_5 (C_6H_5X)

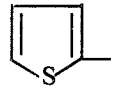
78 $C_6H_5 + H$

79 $C_6H_5 + 2H$, Br (^{81}Br at 81)

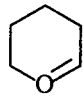
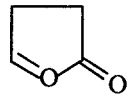
80   CH_3SS + H, HBr (H ^{81}Br at 82)

81  

82 $CH_2CH_2CH_2CH_2C{\equiv}N$, CCl_2($C^{35}Cl^{37}Cl$ at 84, $C^{37}Cl_2$ at 86), C_6H_{10}

83 C_6H_{11}, $CHCl_2$ ($CH^{35}Cl^{37}Cl$ at 85, $CH^{37}Cl_2$ at 87), 

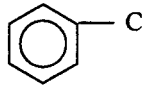
85 C_6H_{13}, $C_4H_9C=O$,

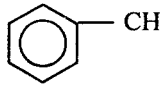
$CClF_2$ ($C^{37}ClF_2$ at 87),  

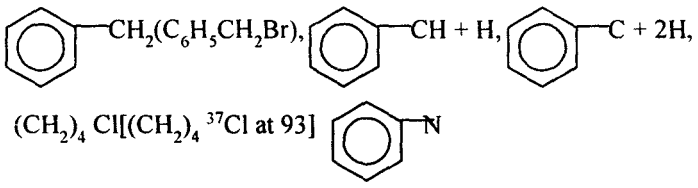
86 $C_3H_7C(=O)CH_2$ + H, $C_4H_9CHNH_2$ and isomers

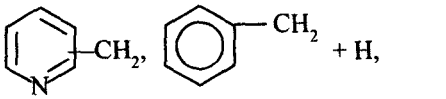
87 C_3H_7CO, homologs of 73, $CH_2CH_2COCH_3$ (O)

88 $CH_2(=O)C{-}OC_2H_5$ + H

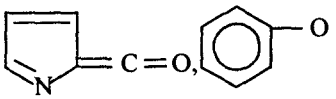
89 $C(=O){-}OC_3H_7$ + 2H, 

90 CH_3CHONO_2, 

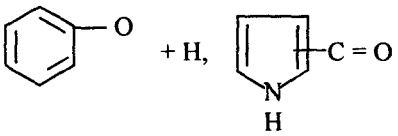
91 

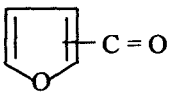
92 

93 $CH_2Br(CH_2\ ^{81}Br$ at 95, $RCH_2Br)$, C_7H_9,

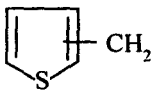


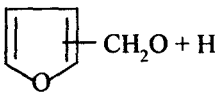
C_7H_9 (terpenes)

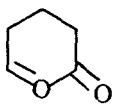
94 

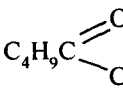
95 

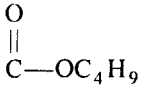
96 $CH_2CH_2CH_2CH_2CH_2C{\equiv}N$

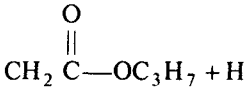
97 C_7H_{13}, 

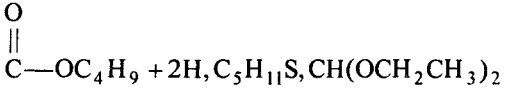
98 

99 C_7H_{15}, $C_6H_{11}O$, 

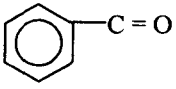
100 

101 

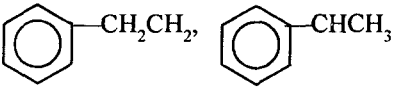
102 

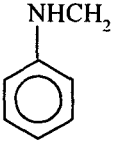
103 

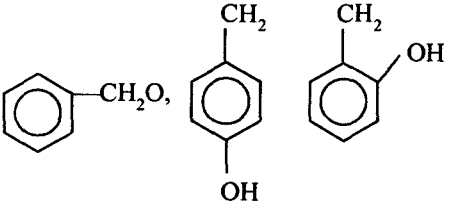
104

105 

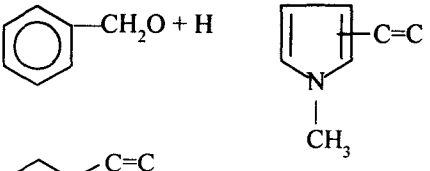
$[C_6H_5(C=O)G, G = OH, OR, OAr, halogen, NH_2]$,

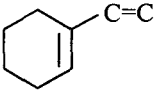


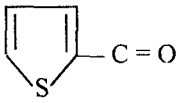
106 

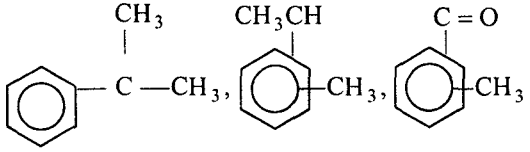
107 

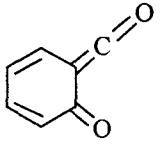
$C_2H_4Br(C_2H_4\ ^{81}Br$ at 109)

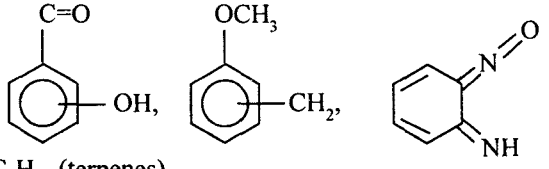
108 

109 

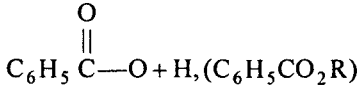
111 

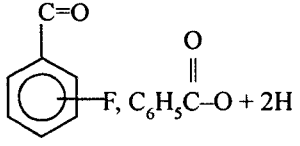
119 CF_3CF_2, 

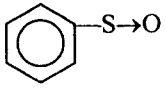
120 

121 

C_9H_{13} (terpenes)

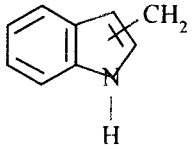
122 

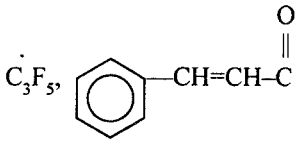
123 

125 

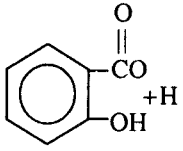
127 I

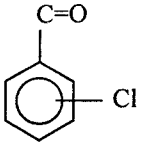
128 HI

130 

131 

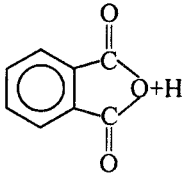
135 $(CH_2)_4Br[(CH_2)_4\ ^{81}Br$ at 137]

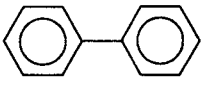
138 

139 

141 $CH_2I\ (RCH_2I)$

147 $(CH_3)_2Si = O - Si\ (CH_3)_3$

149 

154 

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[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	$H^{\bullet}$	
2	$2H^{\bullet}$	
15	$CH_3^{\bullet}$	
16	$O(ArNO_2$, amine oxides, sulfoxides); NH_2 (carboxamides, sulfonamides)	
17	$HO^{\bullet}$	
18	H_2O (alcohols, aldehydes, ketones)	
19	$F^{\bullet}$	
20	HF	
26	$CH{\equiv}CH, {}^{\bullet}CH{\equiv}N$	
27	$CH_2{=}CH^{\bullet}$, $HC{\equiv}N$ (aromatic nitrites, nitrogen heterocycles)	
28	$CH_2 = CH_2$, CO, (quinones) (HCN + H)	
29	$CH_3CH_2^{\bullet}$, (ethyl ketones, $ArCH_2CH_2CH_3$), ${}^{\bullet}CHO$	
30	$NH_2CH_2^{\bullet}$, $CH_2O(ArOCH_3)$, $NO(ArNO_2)$, C_2H_6	
31	${}^{\bullet}OCH_3$(methyl esters), ${}^{\bullet}CH_2OH$, CH_3NH_2	
32	CH_3OH, S	
33	$HS^{\bullet}$ (thiols), (${}^{\bullet}CH_3$ and H_2O)	
34	H_2S (thiols)	
35	$Cl^{\bullet}$	
36	HCl, $2H_2O$	
37	H_2Cl (or HCl + H)	
38	C_3H_2, C_2N, F_2	
39	C_3H_3, HC_2N	
40	$CH_3C{\equiv}CH$	
41	$CH_2{=}CHCH_2^{\bullet}$	

42 $CH_2{=}CHCH_3$, $CH_2{=}C{=}O$,  , NCO, $NCNH_2$

43 $C_3H_7^{\bullet}$ (propyl ketones, $ArCH_2{-}C_3H_7$), $CH_3{-}\overset{O}{\overset{\|}{C}}{}^{\bullet}$ (methyl ketones, CH_3CG, where G = various functional groups), $CH_2{=}CH{-}O^{\bullet}$, ($CH_3^{\bullet}$ and $CH_2{=}CH_2$), HCNO

44 $CH_2{=}CHOH$, CO_2 (esters, anhydrides), N_2O, $CONH_2$, $NHCH_2CH_3$

45 CH_3CHOH, $CH_3CH_2O^{\bullet}$ (ethyl esters), CO_2H, $CH_3CH_2NH_2$

46 (H_2O and $CH_2{=}CH_2$), CH_3CH_2OH, $^{\bullet}NO_2$ ($ArNO_2$)

47 $CH_3S^{\bullet}$

48 CH_3SH, SO(sulfoxides), O_3

49 $^{\bullet}CH_2Cl$

51 $^{\bullet}CHF_2$

52 C_4H_4, C_2N_2

53 C_4H_5

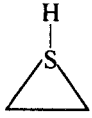
54 $CH_2{=}CH{-}CH{=}CH_2$

55 $CH_2{=}CHCHCH_3$

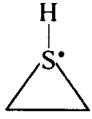
56 $CH_2{=}CHCH_2CH_3$, $CH_3CH{=}CHCH_3$, 2CO

57 $C_4H_9^{\bullet}$ (butyl ketones), C_2H_5CO (ethyl ketones, EtC = OG, G = various structural units)

58 $^{\bullet}NCS$, (NO + CO), CH_3COCH_3, C_4H_{10}

59 $CH_3O\overset{O}{\overset{\|}{C}}{}^{\bullet}$, $CH_3{-}\overset{O}{\overset{\|}{C}}{-}NH_2$, 

60 C_3H_7OH, $CH_2{=}C(OH)_2$ (acetate esters)[a]

61 $CH_3CH_2S^{\bullet}$, 

62 (H_2S and $CH_2{=}CH_2$)

63 $^{\bullet}CH_2CH_2Cl$

64	C_5H_4, S_2, SO_2
68	$CH_2{=}C(CH_3){-}CH{=}CH_2$
69	$CF_3^{\bullet}$, $C_5H_9^{\bullet}$
71	$C_5H_{11}^{\bullet}$
73	$CH_3CH_2OC^{\bullet}{=}O$
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	$^{\bullet}CCIF_2$
100	$CF_2{=}CF_2$
119	$CF_3{-}CF_2^{\bullet}$
122	C_6H_5COOH
127	$I^{\bullet}$
128	HI

[a]Mclafferty 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 $C_6H_{12}O$. Again replacing CH_4 by O gives $C_5H_8O_2$, and repeating the process a third time gives $C_4H_4O_3$. 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}, $C_5H_{10}O$, $C_4H_6O_2$, $C_3H_2O_3$

(b) C_9H_{20}, C_9H_4O, $C_{10}H_8$, $C_8H_{16}O$, $C_7H_{12}O_2$, $C_6H_8O_3$, $C_5H_4O_4$

(c) $C_{11}H_{24}$, $C_{12}H_{12}$, $C_{11}H_8O$, $C_{10}H_{20}O$, $C_{10}H_4O_2$, $C_9H_{16}O_2$, $C_8H_{12}O_3$, $C_7H_8O_4$, $C_6H_4O_5$

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

(a) Alpha cleavage of 2–pentanone ($CH_3COCH_2CH_2CH_3$)

Ans. 43, 71

(b) Dehydration of cyclohexanol (hydroxycyclohexane)

Ans. 82

(c) McLafferty rearrangement of 4–methyl–2–pentanone [$CH_3COCH_2CH(CH_3)_2$]

Ans. 58

(d) Aplha cleavage of triethylamine [$(CH_3CH_2)_3N$]

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 chomophores (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.	–OH; –COOH;
2.	$-NH_2$; –NH; $-CONH_2$; –CONH:
3.	C≡C; HC≡C; –CN; C=C=C;
4.	Aromatic rings, nature of substitution in the ring.
5.	Carbonyl functions.
6.	Enes and their cis–trans stereochemistry.

7. Alkyl units $-CH(CH_3)_2$; $CH(CH_3)_3$

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 ^{1}HNMR.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 fromula 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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