

## Table of Contents - Carbon NMR

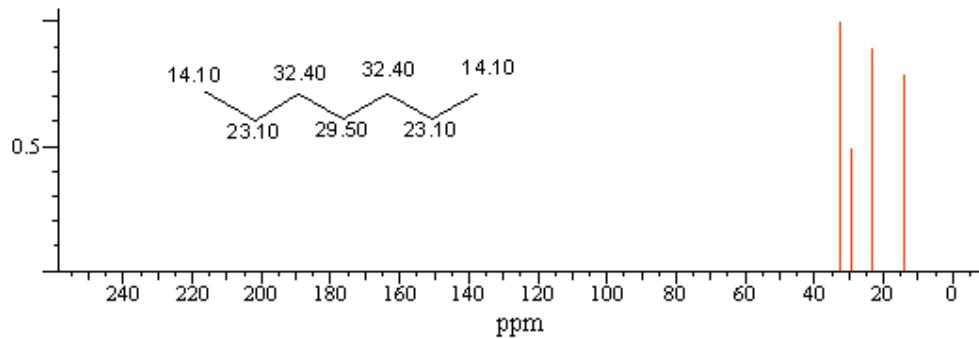
- I. [Hydrocarbons](#)
- II. [Halogenated Hydrocarbons](#)
- III. [Nitrogen Containing Compounds](#)
- IV. [Silicon Containing Compounds \(Except Si-O\)](#)
- V. [Phosphorus Containing Compounds \(Except P-O And P\(=O\)-O\)](#)
- VI. [Sulfur Containing Compounds](#)
- VII. [Oxygen Containing Compounds \(Except -C\(=O\)-\)](#)
- VIII. [Compounds Containing Carbon To Oxygen Double Bonds](#)

### I. Hydrocarbons

#### A. Saturated Hydrocarbons

##### 1. [Normal Alkanes](#)

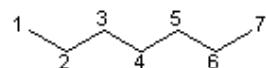
#### Normal Alkanes



This section contains the carbon-13 NMR chemical shifts of the straight chain alkanes.

The aliphatic additivity constants presented in many of the section heading discussions are usually very useful when utilized with these parent alkane chemical shifts in the calculation of theoretical chemical shifts for straight aliphatic compounds.

#### Alkanes

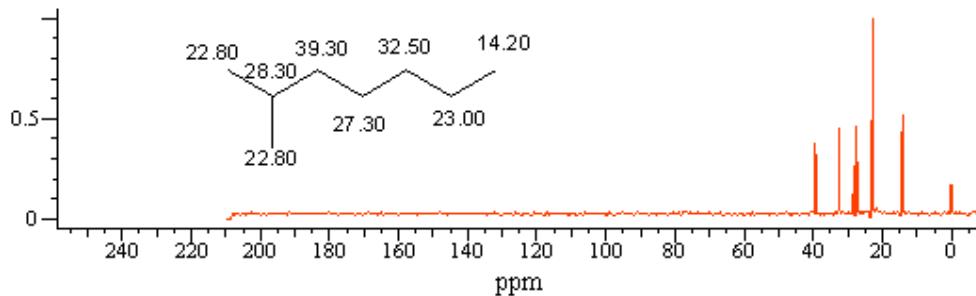


C-7	C-6	C-5	C-4	C-3	C-2	C-1	Compound	Solvent
-----	-----	-----	-----	-----	-----	-----	----------	---------

		14.2	22.8	34.8	22.8	14.2		CDCl <sub>3</sub>
	14.2	23.0	32.1	32.1	23.0	14.2		CDCl <sub>3</sub>
14.1	23.1	32.4	29.5	32.4	23.1	14.1		CDCl <sub>3</sub>
R2-	32.3	29.8	29.8	32.3	23.1	14.1		CDCl <sub>3</sub>
R5-	30.1	30.1	29.7	32.3	23.0	14.2		CDCl <sub>3</sub>
R12-	29.9	29.9	29.6	32.2	22.9	14.2		CDCl <sub>3</sub>

## 2□Branched Alkanes

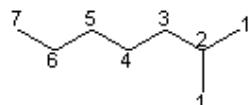
### Branched Alkanes



This section contains the carbon-13 NMR chemical shifts of the branched alkanes.

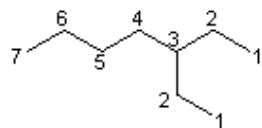
The aliphatic additivity constants presented in many of the section heading discussions are usually very useful when utilized with these parent alkane chemical shifts in the calculation of theoretical chemical shifts for branched aliphatic compounds.

### 2-Methyl Alkanes



C-7	C-6	C-5	C-4	C-3	C-2	C-1	Solvent
			11.8	32.0	30.1	22.3	CDCl <sub>3</sub>
	14.1	23.2	29.9	39.0	28.2	22.7	CDCl <sub>3</sub>
14.2	23.0	32.5	27.3	39.3	28.3	22.8	CDCl <sub>3</sub>
R2-	32.3	29.9	27.7	39.4	28.3	22.8	CDCl <sub>3</sub>

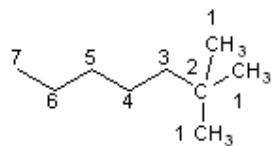
### 3-Ethyl Alkanes



C-7	C-6	C-5	C-4	C-3	C-2	C-1	Solvent
			18.9	36.6	29.5	11.6	CDCl <sub>3</sub>
		11.1	25.5	42.5	25.5	11.1	CDCl <sub>3</sub>
14.2	23.4	29.3	32.8	40.7	25.7	11.0	CDCl <sub>3</sub>

---

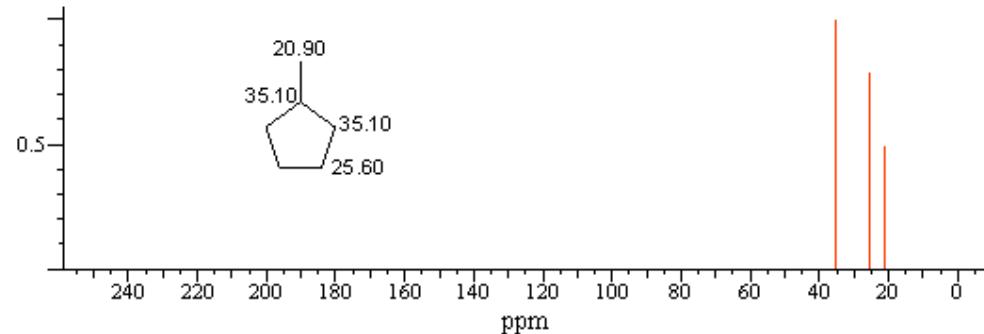
### 2,2-Dimethyl Alkanes



C-7	C-6	C-5	C-4	C-3	C-2	C-1	Solvent
			8.9	36.7	30.5	29.0	CDCl <sub>3</sub>
14.1	22.9	33.1	24.4	44.5	30.4	29.5	CDCl <sub>3</sub>
R2-	32.3	30.6	24.8	44.6	30.4	29.6	CDCl <sub>3</sub>

### 3 □ Cyclic Alkanes

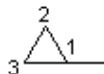
#### Cyclic Alkanes



This section contains the carbon-13 NMR chemical shifts of cyclic hydrocarbons.

The chemical shift tables presented below illustrate the carbon resonances of both the ring carbons of substituted forms and the shifts of the side chain carbons of alkyl cycloalkanes.

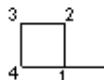
### Cyclopropanes



C-2,3	C-1	-X	Solvent
7.1	-3.5	-C≡N	CDCl <sub>3</sub>
4.7	11.9		CDCl <sub>3</sub>
9.1	15.5		CDCl <sub>3</sub>

---

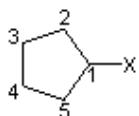
### Cyclobutanes



C-3	C-2,4	C-1	-X	Solvent
18.7	25.5	38.5		CDCl <sub>3</sub>
15.6	27.8	46.2	-NH <sub>2</sub> HCl	D <sub>2</sub> O
12.1	33.41	67.0	-OH	CDCl <sub>3</sub>

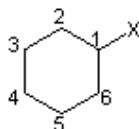
---

### Cyclopentanes

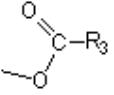


C-3,4	C-2,5	C-1	-X	Solvent
23.9	39.8	28.1	-I	CDCl <sub>3</sub>
25.6	35.1	35.1	-CH <sub>3</sub>	CDCl <sub>3</sub>
25.5	33.1	40.6	-R5	CDCl <sub>3</sub>
23.4	38.0	53.0	-Br	CDCl <sub>3</sub>
23.2	37.3	61.8	-Cl	CDCl <sub>3</sub>

## Cyclohexanes

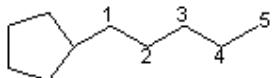


C-4	C-3,5	C-2,6	C-1	-X	Solvent
25.4	24.2	29.7	28.1	-C≡N	CDCl <sub>3</sub>
26.0	24.9	32.6	28.9	-C≡C-H	CDCl <sub>3</sub>
25.2	27.1	39.5	32.0	-I	CDCl <sub>3</sub>
26.7	26.7	35.8	33.1	-CH <sub>3</sub>	CDCl <sub>3</sub>
27.0	26.7	34.0	35.6		CDCl <sub>3</sub>
27.1	26.7	33.7	37.9	-R7	CDCl <sub>3</sub>
25.5	26.3	38.0	38.3	-SH	CDCl <sub>3</sub>
27.1	26.8	33.3	39.9	-CH <sub>2</sub> CH <sub>3</sub>	CDCl <sub>3</sub>
24.8	24.2	30.4	50.1	-NH <sub>2</sub> HCl	Polysol
26.0	25.3	37.1	50.5	-NH <sub>2</sub>	CDCl <sub>3</sub>
26.0	25.1	33.4	51.5		CDCl <sub>3</sub>
25.3	25.9	37.6	52.9	-Br	CDCl <sub>3</sub>

26.6	29.2	34.0	56.9	-NH-CH <sub>2</sub> CH <sub>3</sub>	CDCl <sub>3</sub>
25.1	24.0	27.6	59.5	-NH-NH <sub>2</sub> HCl	Polysol
25.8	24.0	32.0	72.2		CDCl <sub>3</sub>
25.2	24.4	31.3	84.8		CDCl <sub>3</sub>

---

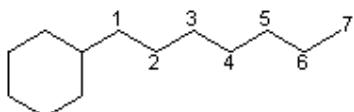
### Alkyl Cyclopentanes; Alkyl Shifts



C-5	C-4	C-3	C-2	C-1	-X	Solvent
				20.9	-C5	CDCl <sub>3</sub>
	14.2	23.3	31.5	36.4	-C5	CDCl <sub>3</sub>
14.2	23.0	32.6	28.9	36.6	-C5	CDCl <sub>3</sub>

---

### Alkyl Cyclohexanes; Alkyl Shifts



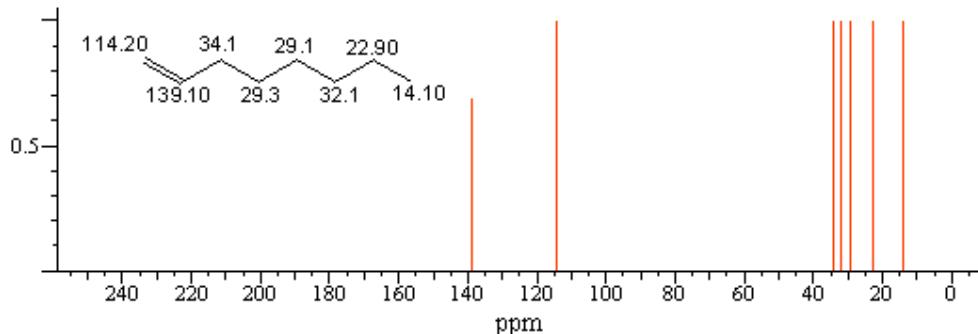
C-7	C-6	C-5	C-4	C-3	C-2	C-1	-X	Solvent
						22.9	-C6	CDCl <sub>3</sub>
					11.4	30.4	-C6	CDCl <sub>3</sub>
				14.4	20.1	40.2	-C6	CDCl <sub>3</sub>
			14.2	23.3	29.4	37.6	-C6	CDCl <sub>3</sub>
		14.2	23.0	32.6	26.8	37.8	-C6	CDCl <sub>3</sub>

	14.1	22.9	32.3	30.0	27.1	38.0	-C6	CDCl <sub>3</sub>
14.1	22.9	32.2	29.6	30.2	27.1	37.9	-C6	CDCl <sub>3</sub>

## B □ Unsaturated Hydrocarbons

### 1. Acyclic Alkenes

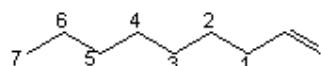
#### Acyclic Alkenes



The carbon-13 NMR chemical shifts of alkenes that are contained in this section illustrate the low field chemical shifts of the alkenyl carbon atoms (100-150ppm) and the weakly deshielding effect of alkene linkages on the chemical shifts of adjacent aliphatic groups. The aliphatic additivity constants for two forms are given below.

C-4	C-3	C-2	C-1	-X
0.4	-2.5	6.5	19.9	CH <sub>2</sub> =CH-
0.4	-2.4	5.1	24.0	

#### The Alkenes; Alkyl Chemical Shifts

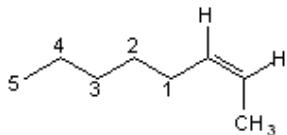


C-6	C-5	C-4	C-3	C-2	C-1	-X	Solvent
		14.0	22.5	31.6	33.8	-CH=CH <sub>2</sub>	CDCl <sub>3</sub>
	14.1	22.8	31.7	29.0	34.1	-CH=CH <sub>2</sub>	CDCl <sub>3</sub>
14.1	22.9	32.1	29.1	29.3	34.1	-CH=CH <sub>2</sub>	CDCl <sub>3</sub>

R2-	32.2	29.4	29.4	29.4	34.1	-CH=CH <sub>2</sub>	CDCl <sub>3</sub>
R7-	29.9	29.9	29.6	29.3	34.0	-CH=CH <sub>2</sub>	CDCl <sub>3</sub>

---

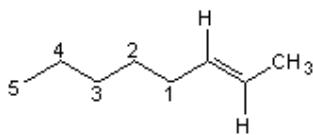
### The CIS Alkenes; Alkyl Chemical Shifts



C-5	C-4	C-3	C-2	C-1	-X	Solvent
				12.7	-CH=CH-R5	CDCl <sub>3</sub>
				12.7	-CH=CH-R3	CDCl <sub>3</sub>
		13.7	23.1	29.2	-CH=CH-CH <sub>3</sub>	CDCl <sub>3</sub>
14.2	22.9	31.9	29.7	27.1	-CH=CH-CH <sub>3</sub>	CDCl <sub>3</sub>

---

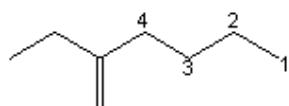
### The TRANS Alkenes; Alkyl Chemical Shifts

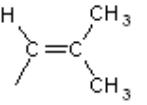
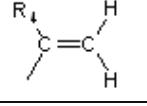
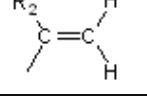
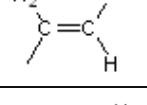
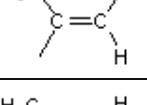
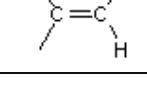


C-5	C-4	C-3	C-2	C-1	-X	Solvent
				17.8	-CH=CH-R3	CDCl <sub>3</sub>
			14.0	17.9	-CH=CH-R5	CDCl <sub>3</sub>
		13.7	23.1	35.0	-CH=CH-CH <sub>3</sub>	CDCl <sub>3</sub>
	14.1	22.5	32.2	32.6	-CH=CH-R4	CDCl <sub>3</sub>
14.2	22.9	31.9	29.7	33.0	-CH=CH-CH <sub>3</sub>	CDCl <sub>3</sub>

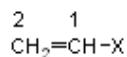
---

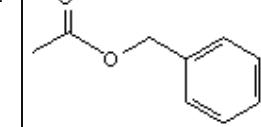
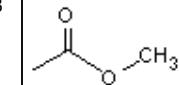
## 2,2-Disubstituted Ethenes; Alkyl Chemical Shifts

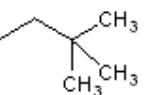
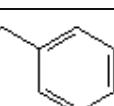
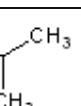
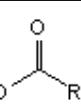
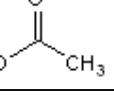
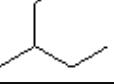
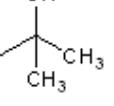
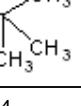


C-5	C-4	C-3	C-2	C-1	-X	Solvent
			17.5	21.6		CDCl <sub>3</sub>
			12.5	29.0		CDCl <sub>3</sub>
			12.6	29.3		CDCl <sub>3</sub>
	14.1	22.8	30.5	36.3		CDCl <sub>3</sub>
14.1	22.8	31.9	27.7	38.1		CDCl <sub>3</sub>
R4-	22.9	31.9	29.7	33.0		CDCl <sub>3</sub>

## Alkenyl Chemical Shifts

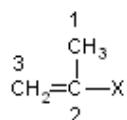


C-2	C-1	-X	Solvent
130.7	128.2		CDCl <sub>3</sub>
130.4	128.8		CDCl <sub>3</sub>

116.5	136.0		CDCl <sub>3</sub>
113.5	137.0		CDCl <sub>3</sub>
115.6	137.4		CDCl <sub>3</sub>
115.0	137.7	-CH <sub>2</sub> OH	CDCl <sub>3</sub>
115.5	137.8		CDCl <sub>3</sub>
137.8	138.6		CDCl <sub>3</sub>
114.3	139.2	-R4	CDCl <sub>3</sub>
97.0	141.5		CDCl <sub>3</sub>
97.2	141.6		CDCl <sub>3</sub>
114.4	143.1		CDCl <sub>3</sub>
110.7	146.5		CDCl <sub>3</sub>
109.0	149.8		CDCl <sub>3</sub>
86.1	152.3	-O-R4	CDCl <sub>3</sub>

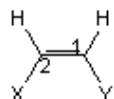
---

### Alkenyl Chemical Shifts



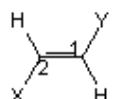
C-3	C-2	C-1	-X	Solvent
112.3	143.2	21.8		CDCl <sub>3</sub>
112.0	144.9	22.0		CDCl <sub>3</sub>
109.7	146.0	22.4	-R9	CDCl <sub>3</sub>
109.9	146.0	22.4	-R5	CDCl <sub>3</sub>
108.8	147.5	22.3	-R2	CDCl <sub>3</sub>

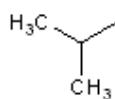
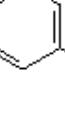
### E (CIS) Isomers



X-	C-2	C-1	-Y	Solvent
Br-	107.1	107.1	-Br	CDCl <sub>3</sub>
CH <sub>3</sub> -	123.9	130.7	-CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	CDCl <sub>3</sub>
CH <sub>3</sub> -	123.7	131.0	-R5	CDCl <sub>3</sub>
	135.2	135.2		CDCl <sub>3</sub>

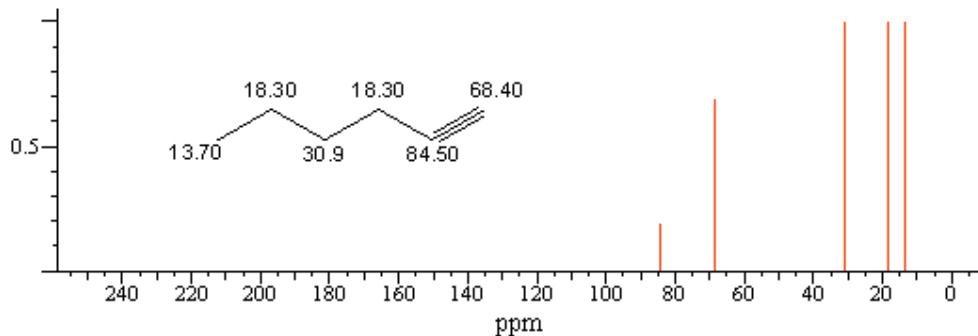
### Z (TRANS) Isomers



X-	C-2	C-1	-Y	Solvent
Br-	113.3	113.3	-Br	CDCl <sub>3</sub>
CH <sub>3</sub> -	124.9	131.6	-CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	CDCl <sub>3</sub>
CH <sub>3</sub> -	124.6	131.8	-R5	CDCl <sub>3</sub>
R4-	130.6	130.6	-R4	CDCl <sub>3</sub>
	134.7	134.7		CDCl <sub>3</sub>
	126.0	137.6		CDCl <sub>3</sub>
HO-N=CH-	116.3	137.7		Polysol
	122.6	147.5	-CH <sub>3</sub>	CDCl <sub>3</sub>
	131.8	148.8		CDCl <sub>3</sub>
N≡C-	96.4	150.3		CDCl <sub>3</sub>
	121.2	152.0	-R3	CDCl <sub>3</sub>
	131.1	152.3		CDCl <sub>3</sub>
	133.3	158.2	-R3	CDCl <sub>3</sub>

2 □ [Alkynes](#)

## Alkynes



The alkynyl ( $\text{C}=\text{C}$ ) carbons resonate in the chemical shift range from 68–92 ppm. Because of their relatively long relaxation times, they tend to be "weak" peaks overlapping in many cases with the  $\text{CDCl}_3$  solvent bands.

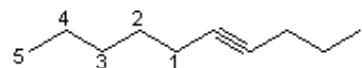
The alkynyl functional group has only a very weak deshielding effect on the C—1 and C—2 carbons ( $\delta\text{C}1=+4.4\text{ ppm}$ ,  $\delta\text{C}2=+6.0\text{ ppm}$ ). It displays a similar shielding effect on the alpha carbon of the alkynyl benzenes.

The aromatic additivity constants are given below.

C-4	C-3	C-2	C-1	$-\text{X}$
0.3	-0.1	3.8	-6.0	$\text{H}-\text{C}\equiv\text{C}-$
-0.3	-0.2	3.2	-5.1	

The chemical shifts of selected alkynyl compounds are presented in the following tables.

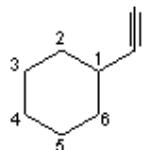
### Alkyl Acetylenes: Alkyl Chemical Shifts



C-5	C-4	C-3	C-2	C-1	$-\text{C}\equiv\text{C-X}$	Solvent
				3.4		$\text{CDCl}_3$
				3.4		$\text{CDCl}_3$
				4.1		$\text{CDCl}_3$

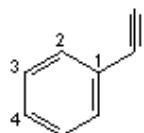
		13.5	22.9	21.0	-C≡C-R5	CDCl <sub>3</sub>
	13.7	22.1	30.9	18.3	-C≡C-H	CDCl <sub>3</sub>
14.0	22.4	31.3	29.1	18.6	-C≡C-R4	CDCl <sub>3</sub>
14.1	22.5	31.4	29.2	18.9	-C≡C-R3	CDCl <sub>3</sub>
R2-	31.4	28.6	27.7	18.7		CDCl <sub>3</sub>
R3-	29.1	29.4	29.1	18.9	-C≡C-CH <sub>3</sub>	CDCl <sub>3</sub>
R12-	29.3	29.0	28.8	18.5	-C≡C-H	CDCl <sub>3</sub>

### Ethyneylcyclohexane: Cyclohexyl Chemical Shifts



C-4	C-3,5	C-2,6	C-1	-X	Solvent
26.0	24.9	32.6	28.9	-C≡C-H	CDCl <sub>3</sub>

### Alkynyl Benzenes; Phenyl Chemical Shifts

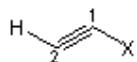


C-4	C-3	C-2	C-1	-X	Solvent
128.7	128.3	132.2	122.4	-C≡C-H	CDCl <sub>3</sub>
129.1	128.4	132.4	121.8		CDCl <sub>3</sub>
127.6	128.3	131.7	124.4	-C≡C-CH <sub>3</sub>	CDCl <sub>3</sub>

128.1	128.2	131.6	123.3		CDCl <sub>3</sub>
-------	-------	-------	-------	--	-------------------

---

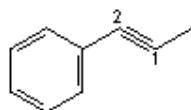
### Alkynyl Carbons Chemical Shifts



H-	C-2	C-1	-X	Solvent
H-	68.4	84.5	-R4	CDCl <sub>3</sub>
H-	68.2	84.4	-R12	CDCl <sub>3</sub>
H-	68.1	88.5		CDCl <sub>3</sub>
H-	77.4	83.8		CDCl <sub>3</sub>
CH <sub>3</sub> -	75.2	79.4	-R7	CDCl <sub>3</sub>
CH <sub>3</sub> -	75.6	78.9		CDCl <sub>3</sub>
CH <sub>3</sub> -	80.1	85.9		CDCl <sub>3</sub>
CH <sub>3</sub> -CH <sub>2</sub> -	81.9	79.2		CDCl <sub>3</sub>
R3-	80.0	80.4	-R5	CDCl <sub>3</sub>
R4-	80.0	80.0	-R4	CDCl <sub>3</sub>

---

### Alkynyl Benzenes; Alkynyl Chemical Shifts

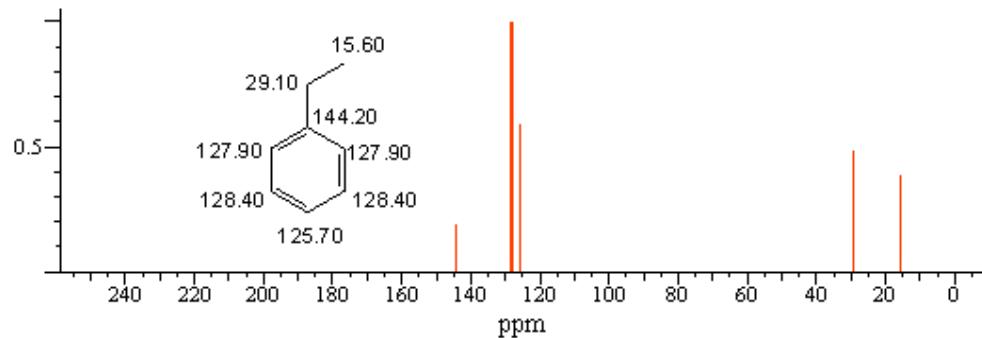


X-	C-2	C-1	-X	Solvent
	81.5	74.1		CDCl3
	85.9	80.1	-CH3	CDCl3
	85.2	84.7		CDCl3
	91.8	87.3		CDCl3
	90.0	88.4		CDCl3
	89.6	89.6		CDCl3

C□Aromatic Hydrocarbons

### 1. [Monocyclic \(Benzenes\) and Polycyclic](#)

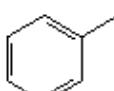
## Monocyclics and Polycyclics



This section contains the carbon-13 NMR chemical shifts of a selection of aromatic hydrocarbons. The chemical shifts of benzenes substituted by other than hydrocarbon groups are included in the section.

As a substituent, the phenyl group exerts an intermediate deshielding effect on adjacent aliphatic carbon nuclei.

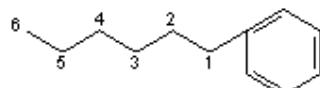
Aliphatic additivity constants for the phenyl group are given below.

	C-4	C-3	C-2	C-1
	0.3	-2.5	8.8	22.0

The following tables provide aliphatic and aromatic chemical shifts for a selected variety of aromatic hydrocarbon compounds.

---

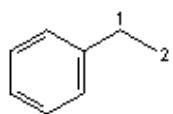
### Alkyl Benzenes; Alkyl Carbon Chemical Shifts



C-6	C-5	C-4	C-3	C-2	C-1	-X	Solvent
					21.43		CDCl <sub>3</sub>
				15.6	29.1		CDCl <sub>3</sub>
		14.4	22.6	33.8	35.9		CDCl <sub>3</sub>
R7-	298	29.8	29.6	31.6	36.1		CDCl <sub>3</sub>

---

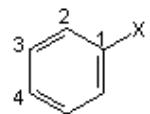
### Substituted Ethyl Benzenes; Ethyl Carbon Chemical Shifts



C-2	C-1	-X	Solvent
15.6	29.1		CDCl3
15.3	25.6		CDCl3
15.7	29.1		CDCl3
15.7	28.7		CDCl3

### Phenyl Carbon Chemical Shifts

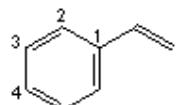
Alkyl Benzenes



C-4	C-3	C-2	C-1	-X	Solvent
125.6	129.2	130.0	137.7	-CH <sub>3</sub>	CDCl <sub>3</sub>
125.7	128.4	127.9	144.2	-R2	CDCl <sub>3</sub>
125.7	128.5	128.3	142.6	-R3	CDCl <sub>3</sub>
125.6	128.4	128.4	142.9	-R17	CDCl <sub>3</sub>
126.0	128.4	128.4	140.0		CDCl <sub>3</sub>
125.9	129.3	128.8	141.0		CDCl <sub>3</sub>

125.9	128.5	128.5	141.5		CDCl <sub>3</sub>
125.9	128.4	128.4	141.9		CDCl <sub>3</sub>
125.7	128.3	128.3	142.1		CDCl <sub>3</sub>
125.8	128.3	127.0	147.5		CDCl <sub>3</sub>
125.8	128.4	126.4	148.8		CDCl <sub>3</sub>
126.2	129.4	128.2	143.8		CDCl <sub>3</sub>
125.9	131.2	127.5	146.8		CDCl <sub>3</sub>

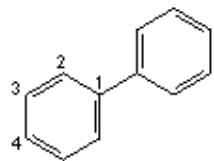
### Alkenyl Benzenes



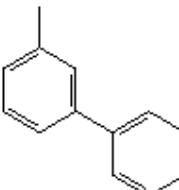
C-4	C-3	C-2	C-1	-X	Solvent
127.8	128.5	126.2	137.7		CDCl <sub>3</sub>
128.7	128.7	126.5	137.3		CDCl <sub>3</sub>

125.5	128.8	128.0	138.8		CDCl <sub>3</sub>
127.4	128.2	125.6	141.4		CDCl <sub>3</sub>
128.2	128.2	127.7	141.6		CDCl <sub>3</sub>
125.5	128.5	128.0	138.8		CDCl <sub>3</sub>

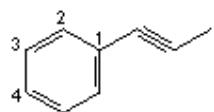
### Biphenyls

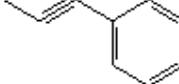
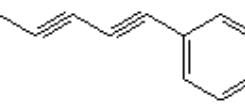


C-4	C-3	C-2	C-1	-X	Solvent
127.1	128.7	127.1	141.2		CDCl <sub>3</sub>
126.9	128.6	126.9	141.1		CDCl <sub>3</sub>
127.0	128.6	127.0	140.9		CDCl <sub>3</sub>
127.3	129.8	127.8	140.6		CDCl <sub>3</sub>

127.2	128.7	127.2	141.2		CDCl <sub>3</sub>
-------	-------	-------	-------	---	-------------------

### Alkynyl Benzenes



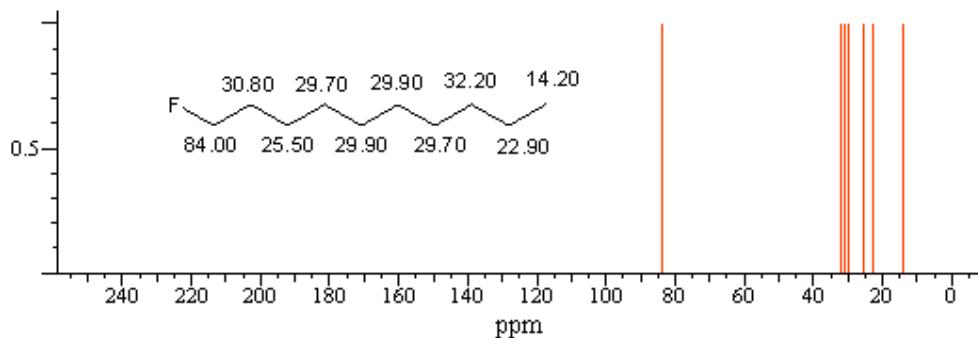
C-4	C-3	C-2	C-1	-X	Solvent
128.7	128.3	132.2	122.4	-C≡C-H	CDCl <sub>3</sub>
127.6	128.3	131.7	124.4		CDCl <sub>3</sub>
128.1	128.2	131.6	123.3		CDCl <sub>3</sub>
129.1	128.4	132.4	121.8		CDCl <sub>3</sub>

## II. Halogenated Hydrocarbons

### A. Fluorinated Hydrocarbons

#### 1. Aliphatic

#### Aliphatics

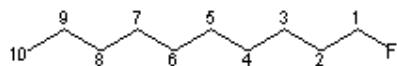


This section contains the carbon-13 NMR chemical shifts of fluorinated hydrocarbons. The chemical shifts of these compounds illustrate not only that fluorine is one of the most strongly deshielding substituents in its effect on the alpha carbon (alkanes: F- $\alpha$ C = +69.9 ppm, benzenes: F- $\alpha$ C = +34.9 ppm) but that fluorine with  $I = 1/2$ , couples with nearby carbons through as many as four bonds. As the coupling constant tables indicate, the magnitude of J decreases with the increase in intervening bonds, i.e. F- $\alpha$ C > F- $\beta$ C > F- $\delta$ C > F- $\sigma$ C.

In addition, the spectra of fluorobenzenes illustrate that coupling across substituted carbons or to substituted carbons tends to be smaller in magnitude than the corresponding coupling constant to or across carbons that possess bonded hydrogens.

The following tables present the observed chemical shifts and coupling constant information for this group of compounds.

### Fluorodecane



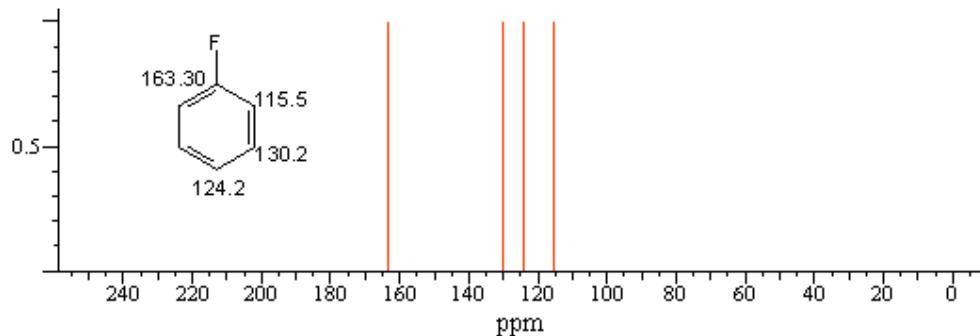
C-5	C-4	C-3	C-2	C-1	-F	Solvent
29.9	29.7	25.5	30.8	84.0	-F	CDCl <sub>3</sub>

### Aliphatic Additivity Constants

sigma	gamma	beta	alpha	-F	Solvent
0.2	-6.6	8.0	69.9	-F	CDCl <sub>3</sub>

2□[Aromatic](#)

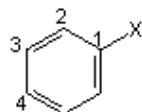
### Aromatics



This section contains the carbon-13 NMR chemical shifts of fluorinated hydrocarbons. The chemical shifts of these compounds illustrate not only that fluorine is one of the most strongly deshielding substituents in its effect on the alpha carbon (alkanes: F- $\alpha$ C = +69.9 ppm, benzenes: F- $\alpha$ C = +34.9 ppm) but that fluorine with  $I = 1/2$ , couples with nearby carbons through as many as four bonds. As the coupling constant tables indicate, the magnitude of J decreases with the increase in intervening bonds, i.e. F- $\alpha$ C > F- $\beta$ C > F- $\delta$ C > F- $\sigma$ C.

In addition, the spectra of fluorobenzenes illustrate that coupling across substituted carbons or to substituted carbons tends to be smaller in magnitude than the corresponding coupling constant to or across carbons that possess bonded hydrogens.

### Fluorinated Aromatic Hydrocarbons

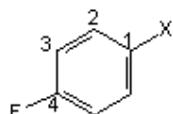


C-4	C-3	C-2	C-1	-X	Solvent
124.2	130.2	115.5	163.3	-F	CDCl <sub>3</sub>
132.1	129.0	125.5	131.5	-CF <sub>3</sub>	CDCl <sub>3</sub>

### Aromatic Additivity Constants for Fluorine

sigma	gamma	beta	alpha	-F	Solvent
-4.2	1.8	-12.9	34.9	-F	CDCl <sub>3</sub>
3.7	0.5	-3.0	2.7	-CF <sub>3</sub>	CDCl <sub>3</sub>

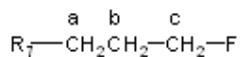
### Selected Para-Substituted Fluorobenzenes



F-	C-4	C-3	C-2	C-1	-X	Solvent

F-	156.4	115.7	116.1	143.1	-NH <sub>2</sub>	CDCl <sub>3</sub>
F-	157.7	116.3	116.6	151.1	-OH	Polysol
F-	159.4	116.7	116.7	159.4	-F	CDCl <sub>3</sub>
F-	161.4	115.0	130.5	133.5	-CH <sub>3</sub>	CDCl <sub>3</sub>
F-	161.5	116.1	131.9	125.2	-SH	CDCl <sub>3</sub>
F-	161.7	116.8	130.2	129.5	-Cl	CDCl <sub>3</sub>
F-	161.9	117.2	132.5	116.7	-Br	CDCl <sub>3</sub>
F-	162.0	115.4	130.5	134.0	-CH <sub>2</sub> -CH <sub>2</sub> -Cl	CDCl <sub>3</sub>
F-	162.5	115.6	128.6	137.4		CDCl <sub>3</sub>
F-	165.2	116.9	134.8	108.8	-C≡N	Polysol
F-	165.5	115.4	132.3	127.6		CDCl <sub>3</sub>
F-	165.8	115.7	131.1	133.9		CDCl <sub>3</sub>
F-	166.0	115.6	132.3	126.8		CDCl <sub>3</sub>
F-	166.7	116.6	126.6	144.9		CDCl <sub>3</sub>

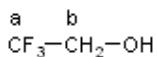
### Fluorine-Carbon Coupling Constants



$$J^{19}\text{F-a} = 4.9 \text{ Hz CDCl}_3$$

$$J^{19}\text{F-b} = 19.8 \text{ Hz CDCl}_3$$

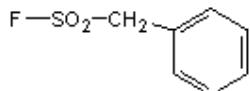
$$J^{19}\text{F-c} = 125.5 \text{ Hz CDCl}_3$$



$J^{19}\text{F-a} = 125.5$  Hz  $\text{H}_2\text{O}$

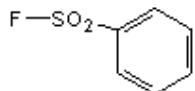
$J^{19}\text{F-b} = 60.7$  Hz  $\text{H}_2\text{O}$

---



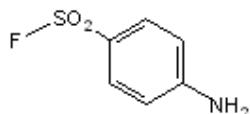
$J^{19}\text{F-CH}_2 = 16.9$  Hz  $\text{CDCl}_3$

---



$J^{19}\text{F-SO}_2\text{-C} = 22$  Hz  $\text{CDCl}_3$

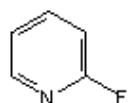
---



$J^{19}\text{F-SO}_2\text{-C} = 21.2$  Hz  $\text{CDCl}_3$

---

## 2-Fluoropyridine



$J^{19}\text{F-C}2 = 239.2$  Hz  $\text{CDCl}_3$

$J^{19}F\text{-C}3 = 36.7$  Hz  $\text{CDCl}_3$

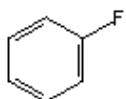
$J^{19}F\text{-C}4 = 7.3$  Hz  $\text{CDCl}_3$

$J^{19}F\text{-C}5 = 4.8$  Hz  $\text{CDCl}_3$

$J^{19}F\text{-C}6 = 14.5$  Hz  $\text{CDCl}_3$

---

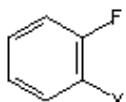
### Fluorobenzene



$J^{19}F$	C-1	C-2	C-3	C-4	C5	C-6	-H	Solvent
	245.7	21.7	7.3		7.3	21.7	-H	$\text{CDCl}_3$

---

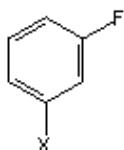
### Ortho-Substituted Fluorobenzenes



$J^{19}F$	C-1	C-2	C-3	C-4	C5	C-6	-X	Solvent
	238.3	14.7			6.4	17.0	-OH	$\text{CDCl}_3$
	244.1	17.5			6.3	23.3	-CH <sub>3</sub>	$\text{CDCl}_3$
	248.7	16.8	7.0		4.0	21.1	-Cl	$\text{CDCl}_3$
	249.1	16.7			7.4	22.0	-CH <sub>2</sub> -C≡N	$\text{CDCl}_3$
	254.1	12.6			8.8	24.2		$\text{CDCl}_3$

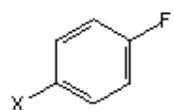
---

### Meta-Substituted Fluorobenzenes



$J^{19}\text{F}$	C-1	C-2	C-3	C-4	C5	C-6	-X	Solvent
	241.7	24.4	12.2		9.7	22.0	-NH <sub>2</sub>	CDCl <sub>3</sub>
	244.2	23.6	11.7		10.0	21.1	-OH	CDCl <sub>3</sub>
	246.2	22.3	7.3		7.9	21.7		CDCl <sub>3</sub>
	246.6	22.0	7.3		7.3	26.8	-CH <sub>2</sub> C≡N	CDCl <sub>3</sub>
	249.1	24.4	7.4		7.3	19.5		CDCl <sub>3</sub>
	249.1	24.4			7.3	22.0		CDCl <sub>3</sub>

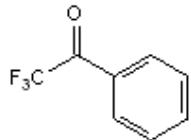
### Para-Substituted Fluorobenzenes



$J^{19}\text{F}$	C-1	C-2	C-3	C-4	C5	C-6	-X	Solvent
	239.2	22.0	7.3		7.3	22.0	-OH	Polysol
	242.3	21.1	7.3		7.3	21.2	-CH <sub>3</sub>	CDCl <sub>3</sub>
	244.4	23.1	7.0		7.0	23.1	-SH	CDCl <sub>3</sub>
	248.3	23.2	9.3		9.3	23.2	-Br	CDCl <sub>3</sub>
	252.9	23.3	8.9	3.5	8.9	23.3		Polysol

	255.1	21.4	9.4		9.4	21.4		CDCl <sub>3</sub>
	256.1	23.6	11.1		11.1	23.6		CDCl <sub>3</sub>
	256.3	23.3	9.1	3.5	9.1	23.3	-C≡N	CDCl <sub>3</sub>

---

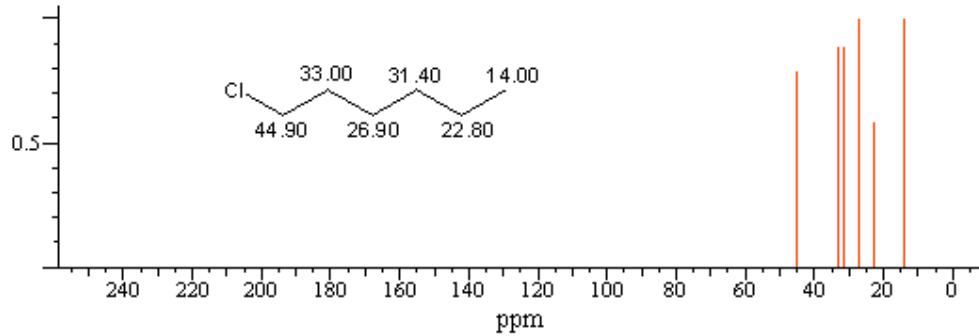


J <sup>19</sup> F	C-1	C-2	C-3	Solvent
	291.1 Hz	35.1 Hz		CDCl <sub>3</sub>

## B □ Chlorinated Hydrocarbons

### 1. [Aliphatic](#)

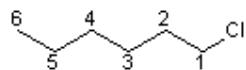
#### Aliphatics



This section contains selected chlorinated hydrocarbons. As a substituent in alkyl structures the chlorine atom possesses a moderately strong deshielding effect, i.e. Cl- $\alpha$ C = +30.6ppm.

As a substituent on aromatic rings, chlorine has a weakly deshielding effect, i.e. Cl- $\alpha$ C=+6.0ppm.

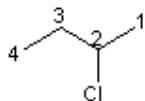
#### 1-Chloroalkanes



C-6	C-5	C-4	C-3	C-2	C-1	-Cl	Solvent
		13.4	20.3	35.0	44.6	-Cl	CDCl <sub>3</sub>
14.0	22.8	31.4	26.9	33.0	44.9	-Cl	CDCl <sub>3</sub>
R2-	32.0	28.8	27.2	33.0	44.8	-Cl	CDCl <sub>3</sub>

---

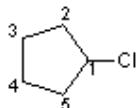
### 2-Chlorobutane



C-4	C-3	C-2	C-1	-Cl	Solvent
11.1	33.6	25.0	60.1	-Cl	CDCl <sub>3</sub>

---

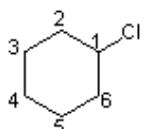
### Chlorocyclopentane



C-3,5	C-2,4	C-1	-Cl	Solvent
23.2	37.3	61.8	-Cl	CDCl <sub>3</sub>

---

### Chlorocyclohexane

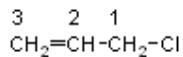


C-4	C-3,5	C-2,6	C-1	-Cl	Solvent

25.4	25.0	36.9	59.9	-Cl	CDCl <sub>3</sub>
------	------	------	------	-----	-------------------

---

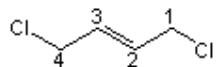
### 3-Chloropropene



C-3	C-2	C-1	-Cl	Solvent
118.3	134.3	45.1	-Cl	CDCl <sub>3</sub>

---

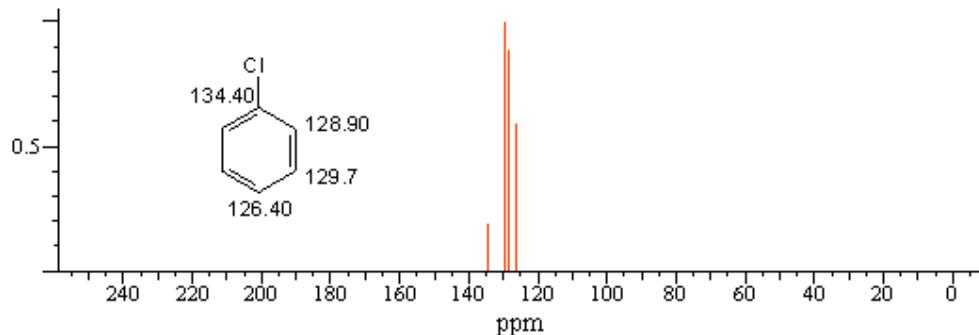
### 1,4-Dichloro-2-butene



Cl-	C-4	C-3	C-2	C-1	-Cl	Solvent
Cl-	43.7	130.2	130.3	43.7	-Cl	CDCl <sub>3</sub>

2□[Aromatic](#)

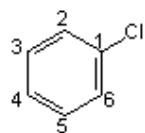
### Aromatics



This section contains selected chlorinated hydrocarbons. As a substituent in alkyl structures the chlorine atom possesses a moderately strong deshielding effect, i.e. Cl- $\alpha$ C = +30.6ppm.

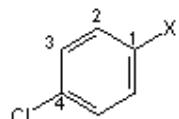
As a substituent on aromatic rings, chlorine has a weakly deshielding effect, i.e. Cl- $\alpha$ C = +6.0ppm.

## Chlorinated Aromatic Hydrocarbons



C-4	C-3,5	C-2,6	C-1	-X	Solvent
126.8	129.7	128.63	134.4	-Cl	CDCl <sub>3</sub>
128.2	128.6	128.6	137.5	-CH <sub>2</sub> -Cl	CDCl <sub>3</sub>
129.8	128.6	126.0	140.2	-CH-Cl <sub>2</sub>	CDCl <sub>3</sub>
130.1	128.1	125.3	144.1	-CCl <sub>3</sub>	CDCl <sub>3</sub>
127.5	129.5	127.5	145.2		CDCl <sub>3</sub>

## 4-Substituted Chlorobenzenes



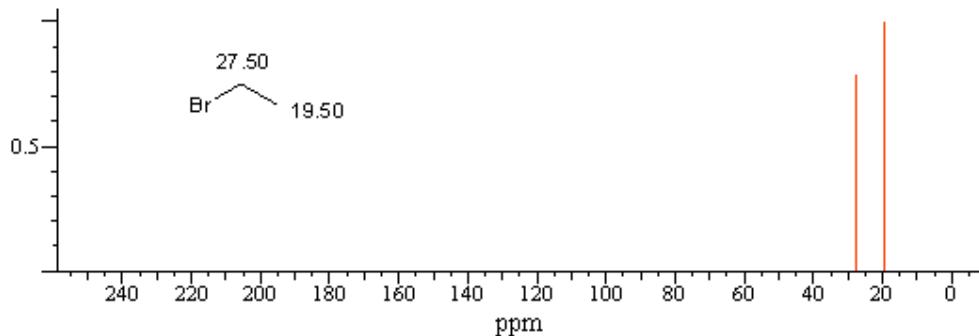
Cl-	C-4	C-3	C-2	C-1	-X	Solvent
Cl-	122.8	129.0	116.3	145.2	-NH <sub>2</sub>	CDCl <sub>3</sub>
Cl-	126.2	129.7	116.9	153.6	-OH	CDCl <sub>3</sub>
Cl-	129.5	130.2	116.8	161.7	-F	CDCl <sub>3</sub>
Cl-	132.6	129.8	129.8	132.6	-Cl	CDCl <sub>3</sub>
Cl-	133.2	130.1	132.6	120.2	-Br	CDCl <sub>3</sub>
Cl-	134.1	130.3	138.6	91.1	-I	CDCl <sub>3</sub>
Cl-	138.1	128.5	131.5	135.7		Polysol
Cl-	138.3	128.5	131.1	129.8		Polysol

Cl-	139.3	129.6	133.4	111.0	-C≡N	CDCl <sub>3</sub>
Cl-	141.4	129.6	125.0	147.0		CDCl <sub>3</sub>

## C□Brominated Hydrocarbons

### 1. Aliphatic

## Aliphatics



This section contains bromine containing hydrocarbons. As a substituent, bromine exerts a weakly deshielding effect on the adjacent carbon atom. The aliphatic additivity constants for bromine are:

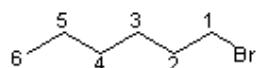
Br- C1=+19.4, C2 = +10.2, C3 = -3.8, C4 = -0.6 ppm

In aromatic molecules, bromine has the effect of actually shielding the C1 carbon atom. The aromatic additivity constants for bromine are:

Br- C1=-5.9, C2, 6 = + 3.0, C3, 5 = + 1.4, C4 = -1.7 ppm

The tables shown below illustrate the chemical shifts of a selected variety of bromine containing organic compounds.

### N-Alkyl Bromides



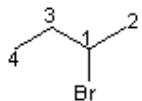
C-6	C-5	C-4	C-3	C-2	C-1	-Br	Solvent
				19.5	27.5	-Br	CDCl <sub>3</sub>
			13.0	26.5	35.5	-Br	CDCl <sub>3</sub>
		13.2	21.5	35.0	33.1	-Br	CDCl <sub>3</sub>
	13.9	22.0	30.5	32.8	33.4	-Br	CDCl <sub>3</sub>
14.0	22.7	31.2	28.1	33.1	33.4	-Br	CDCl <sub>3</sub>

R2-	31.7	28.5	28.2	33.0	33.7	-Br	CDCl <sub>3</sub>
R13-	29.9	29.0	28.4	33.2	33.2	-Br	CDCl <sub>3</sub>

---

### Branched Alkyl Bromides

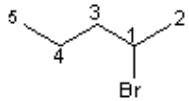
#### 2-Bromobutane



C-4	C-3	C-2	C-1	-Br	Solvent
12.1	34.3	26.1	52.8	-Br	CDCl <sub>3</sub>

---

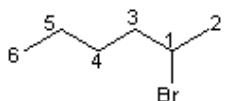
#### 2-Bromopentane



C-5	C-4	C-3	C-2	C-1	-Br	Solvent
13.4	21.0	43.3	26.5	50.9	-Br	CDCl <sub>3</sub>

---

#### 2-Bromohexane

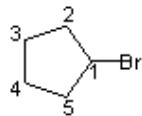


C-6	C-5	C-4	C-3	C-2	C-1	-Br	Solvent
13.9	22.1	29.9	41.0	26.5	51.0	-Br	CDCl <sub>3</sub>

---

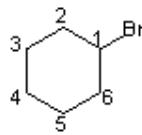
## Alicyclic Bromides

Bromocyclopentane



C-3,4	C-2,5	C-1	-Br	Solvent
23.4	38.0	53.0	-Br	CDCl <sub>3</sub>

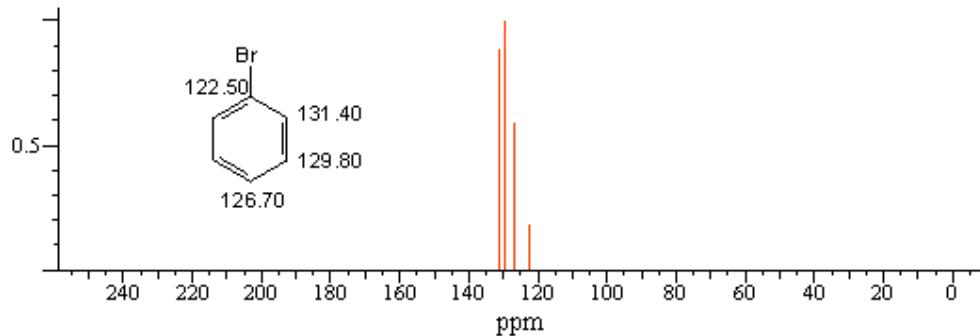
Cyclohexanes



C-4	C-3,5	C-2,6	C-1	-X	Solvent
26.6	26.2	32.9	36.5	-CH <sub>2</sub> CH <sub>2</sub> Br	CDCl <sub>3</sub>
25.3.1	25.9	37.6	52.9	-Br	CDCl <sub>3</sub>

2□[Aromatic](#)

Aromatics



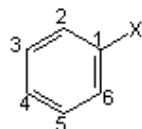
This section contains bromine containing hydrocarbons. As a substituent, bromine exerts a weakly deshielding effect on the adjacent carbon atom. The aliphatic additivity constants for bromine are:

Br- C1=+19.4, C2 = +10.2, C3 = -3.8, C4 = -0.6 ppm

In aromatic molecules, bromine has the effect of actually shielding the C1 carbon atom. The aromatic additivity constants for bromine are:

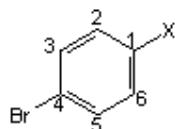
Br- C1=-5.9, C2, 6 = + 3.0, C3, 5 = + 1.4, C4 = -1.7ppm

### Aromatic Bromides

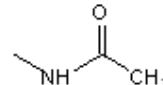
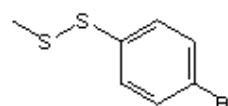
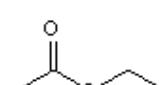


C-4	C-3,5	C-2,6	C-1	-X	Solvent
126.7	129.8	131.4	122.5	-Br	CDCl <sub>3</sub>
128.1	128.5	128.8	137.6	-CH <sub>2</sub> -Br	CDCl <sub>3</sub>
128.9	128.6	127.5	138.5		CDCl <sub>3</sub>
127.3	128.3	127.3	142.3		CDCl <sub>3</sub>

### 4-Substituted Bromobenzenes



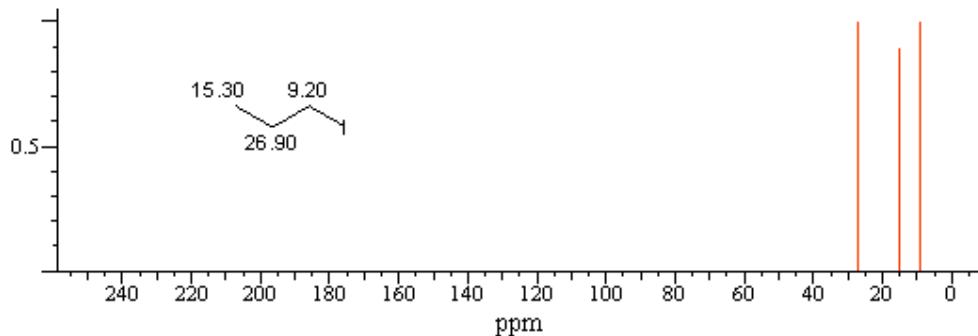
Br-	C-1	C-2,6	C-3,5	C-4	-X	Solvent
Br-	106.9	131.8	113.4	146.7		CDCl <sub>3</sub>

Br-	109.8	131.9	116.7	145.6	-NH <sub>2</sub>	CDCl <sub>3</sub>
Br-	113.2	132.5	117.2	153.9	-OH	CDCl <sub>3</sub>
Br-	114.8	131.2	121.0	138.5		Polysol
Br-	116.7	132.6	117.2	161.9	-F	CDCl <sub>3</sub>
Br-	119.1	131.2	130.7	136.5	-CH <sub>3</sub>	CDCl <sub>3</sub>
Br-	120.2	132.6	130.1	133.2	-Cl	CDCl <sub>3</sub>
Br-	121.0	133.0	133.0	121.0	-Br	CDCl <sub>3</sub>
Br-	121.4	132.2	129.3	135.7		CDCl <sub>3</sub>
Br-	122.1	133.3	139.0	91.9	-I	CDCl <sub>3</sub>
Br-	127.1	131.5	131.2	130.2		Polysol
Br-	127.8	132.5	133.3	111.2	-C≡N	CDCl <sub>3</sub>
Br-	127.8	131.6	131.1	129.5		CDCl <sub>3</sub>
Br-	127.8	131.8	129.5	136.0		CDCl <sub>3</sub>
Br-	129.4	132.3	130.8	135.2		CDCl <sub>3</sub>

## DQIodinated Hydrocarbons

### 1. [Aliphatic](#)

## Aliphatics



The carbon-13 NMR chemical shifts of the iodinated hydrocarbons are distinguished by the unusually high field chemical shifts observed for carbon atoms bonded to the iodine substituent. These shifts appear as negative shifts resonating above TMS.

$\text{CHI}_3$  -146.5 ppm

$\text{CH}_2\text{I}_2$  ~ 61.6 ppm

$\text{CH}_3\text{I}$  - 22.5 ppm

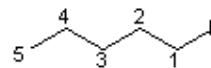
The aliphatic additivity constants for iodine are:

I- C1 = -7.6, C2 = +10.9, C3 = -1.5, C4 = -0.9 ppm

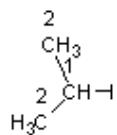
A similar shielding effect is noted in the spectra of the iodinated benzenes. The aromatic additivity constants for iodobenzenes are:

I- C1 = -34.1, C2 = +8.6, C3 = +1.4, C4 = -1.4 ppm

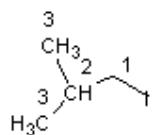
### Alkyl Iodides



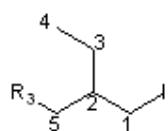
	C-5	C-4	C-3	C-2	C-1	-I	Solvent
					-22.5	-I	$\text{CDCl}_3$
				20.6	-1.3	-I	$\text{CDCl}_3$
			15.3	26.9	9.2	-I	$\text{CDCl}_3$
		12.9	23.6	35.6	6.2	-I	$\text{CDCl}_3$
	13.8	21.6	32.7	33.2	6.5	-I	$\text{CDCl}_3$
R2-	31.6	28.2	30.4	33.7	6.4	-I	$\text{CDCl}_3$
R5-	29.5	28.6	30.5	33.7	6.5	-I	$\text{CDCl}_3$



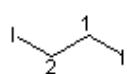
C-2	C-1	-I	Solvent
31.2	20.9	-I	CDCl <sub>3</sub>



C-3	C-2	C-1	-I	Solvent
22.5	30.3	18.1	-I	CDCl <sub>3</sub>

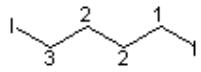


C-5	C-4	C-3	C-2	C-1	-I	Solvent
33.7	15.4	28.8	40.4	10.9	-I	CDCl <sub>3</sub>



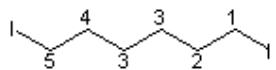
I-	C-2	C-1	-I	Solvent
I-	3.0	3.0	-I	CDCl <sub>3</sub>

---



I-	C-3	C-2	C-1	-I	Solvent
I-	5.2	33.6	5.2	-I	CDCl <sub>3</sub>

---

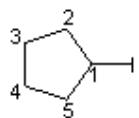


I-	C-5	C-4	C-3	C-2	C-1	-I	Solvent
I-	6.7	32.9	29.0	32.9	6.7	-I	CDCl <sub>3</sub>

---

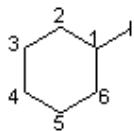
## Alicyclic Iodides

Cyclopentyl Iodide



C-3,4	C-2,5	C-1	-I	Solvent
23.9	39.8	28.1	-I	CDCl <sub>3</sub>

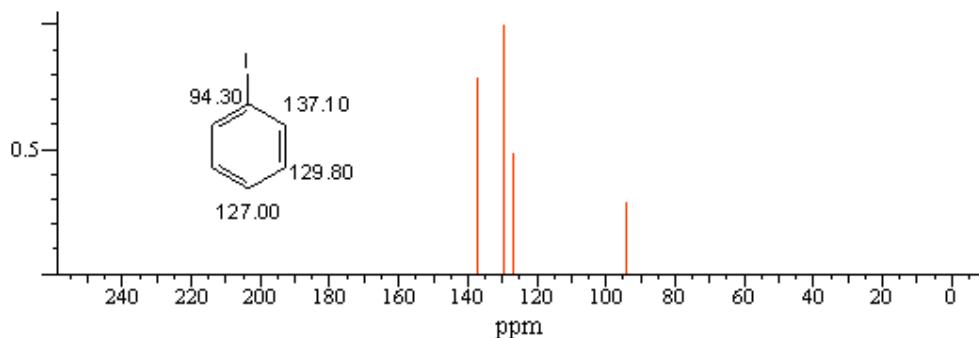
Cyclohexyl Iodide



C-4	C-3,5	C-2,6	C-1	-I	Solvent
25.2	27.1	39.5	32.0	-I	CDCl <sub>3</sub>

## 2□Aromatic

### Aromatics



The carbon-13 NMR chemical shifts of the iodinated hydrocarbons are distinguished by the unusually high field chemical shifts observed for carbon atoms bonded to the iodine substituent. These shifts appear as negative shifts resonating above TMS.

CHI<sub>3</sub> -146.5 ppm

CH<sub>2</sub>I<sub>2</sub> ~ 61.6 ppm

CH<sub>3</sub>I - 22.5 ppm

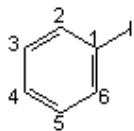
The aliphatic additivity constants for iodine are:

I- C1 = -7.6, C2 = +10.9, C3 = -1.5, C4 = -0.9 ppm

A similar shielding effect is noted in the spectra of the iodinated benzenes. The aromatic additivity constants for iodobenzenes are:

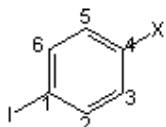
I- C1 = -34.1, C2 = +8.6, C3 = +1.4, C4 = -1.4 ppm

### Iodinated Aromatic Hydrocarbons



C-4	C-3,5	C-2,6	C-1	-X	Solvent
127.0	129.8	137.1	94.3	-I	CDCl <sub>3</sub>
126.0	128.3	128.3	140.1	-(CH <sub>2</sub> ) <sub>3</sub> I	CDCl <sub>3</sub>
126.5	128.3	128.0	140.2	-CH <sub>2</sub> CH <sub>2</sub> I	CDCl <sub>3</sub>

#### 4-Substituted Iodobenzenes



I-	C-1	C-2	C-3	C-4	-X	Solvent
I-	76.8	137.1	116.7	147.4	-NH <sub>2</sub>	Polysol
I-	80.4	137.7	118.1	157.1	-OH	Polysol
I-	90.1	137.1	131.0	137.1	-CH <sub>3</sub>	CDCl <sub>3</sub>
I-	91.1	138.6	130.3	134.1	-Cl	CDCl <sub>3</sub>
I-	91.9	139.0	133.3	122.1	-Br	CDCl <sub>3</sub>
I-	93.0	137.7	128.8	139.8		CDCl <sub>3</sub>
I-	96.5	137.0	127.5	144.7	-SO <sub>2</sub> -OH	Polysol

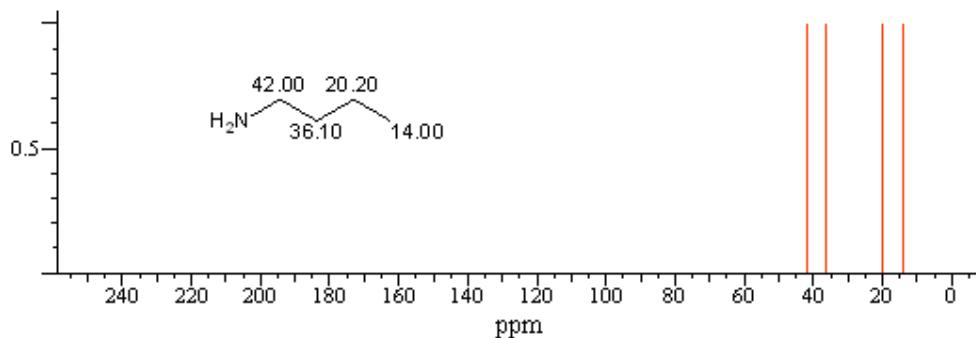
### III. Nitrogen Containing Compounds

#### A. Amines

##### 1. Primary

###### a. Aliphatic

#### Aliphatics



This section contains the carbon-13 NMR chemical shifts of the primary amines. Other functional groups containing an -NH<sub>2</sub> group include the hydrazines, amine salts and primary amides. The additivity effect of the primary amine group on adjacent aliphatic carbon atoms is that of a moderately strong deshielding group, i.e.

H<sub>2</sub>N- C1 = + 28.3, C2 = + 11.3, C3 = -5.0, C4 = + 0.3ppm

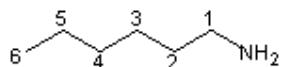
The aromatic additivity values of the aniline -NH<sub>2</sub> are:

H<sub>2</sub>N- C1 = + 18.3, C2 = - 13.3, C3 = + 0.8, C4 = - 10.2ppm

Frequently the carbon-13 NMR spectra of primary amines display a singlet near 79 ppm which represents the resonance of chloroform that is formed by reaction with the solvent:



#### Aliphatic Amines

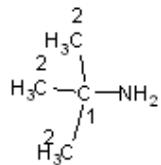


	C-5	C-4	C-3	C-2	C-1	-NH <sub>2</sub>	Solvent
			11.3	27.1	44.3	-NH <sub>2</sub>	CDCl <sub>3</sub>
		14.0	20.2	36.1	42.0	-NH <sub>2</sub>	CDCl <sub>3</sub>
	14.1	22.8	29.5	33.9	42.5	-NH <sub>2</sub>	CDCl <sub>3</sub>

14.0	22.7	31.9	26.7	33.7	42.1	-NH <sub>2</sub>	CDCl <sub>3</sub>
R3-	29.5	29.7	27.2	34.0	42.3	-NH <sub>2</sub>	CDCl <sub>3</sub>
R5-	29.8	29.8	27.2	34.1	42.4	-NH <sub>2</sub>	CDCl <sub>3</sub>

---

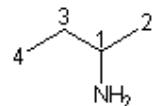
### tert-Butylamine



C-2	C-1	-NH <sub>2</sub>	Solvent
32.7	47.3	-NH <sub>2</sub>	CDCl <sub>3</sub>

---

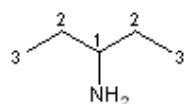
### 2-Aminobutane



C-4	C-3	C-2	C-1	-NH <sub>2</sub>	Solvent
10.7	33.3	23.8	48.7	-NH <sub>2</sub>	CDCl <sub>3</sub>

---

### 3-Aminopentane

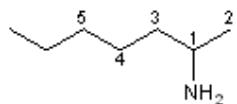


C-3	C-2	C-1	-NH <sub>2</sub>	Solvent

10.4	30.4	54.4	-NH <sub>2</sub>	CDCl <sub>3</sub>
------	------	------	------------------	-------------------

---

### 2-Aminoheptane

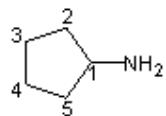


C-5	C-4	C-3	C-2	C-1	-NH <sub>2</sub>	Solvent
32.2	26.3	40.6	24.2	47.2	-NH <sub>2</sub>	CDCl <sub>3</sub>

---

### Alicyclic Amines

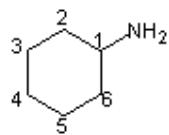
#### Cyclopentylamine



C-3,4	C-2,5	C-1	-NH <sub>2</sub>	Solvent
24.0	36.3	53.4	-NH <sub>2</sub>	CDCl <sub>3</sub>

---

#### Cyclohexylamine

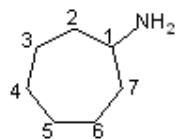


C-4	C-3,5	C-2,6	C-1	-NH <sub>2</sub>	Solvent

26.0	25.3	37.1	50.5	-NH <sub>2</sub>	CDCl <sub>3</sub>
------	------	------	------	------------------	-------------------

---

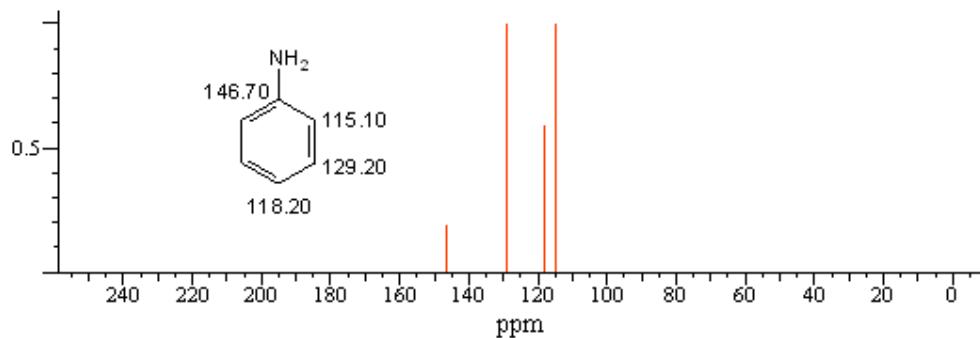
### Cycloheptylamine



C-4,5	C-3,6	C-2,7	C-1	-NH <sub>2</sub>	Solvent
28.4	24.3	38.8	52.8	-NH <sub>2</sub>	CDCl <sub>3</sub>

b□[Aromatic](#)

### Aromatics



This section contains the carbon-13 NMR chemical shifts of the primary amines. Other functional groups containing an -NH<sub>2</sub> group include the hydrazines, amine salts and primary amides. The additivity effect of the primary amine group on adjacent aliphatic carbon atoms is that of a moderately strong deshielding group, i.e.

H<sub>2</sub>N- C1 = + 28.3, C 2 = + 11.3, C3 = -5.0, C4 = + 0.3ppm

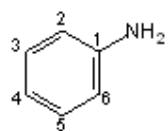
The aromatic additivity values of the aniline -NH<sub>2</sub> are:

H<sub>2</sub>N- C1 = + 18.3, C2 = - 13.3, C3 = + 0.8, C 4 = - 10.2ppm

Frequently the carbon-13 NMR spectra of primary amines display a singlet near 79 ppm which represents the resonance of chloroform that is formed by reaction with the solvent:

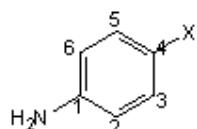


## Primary Aromatic Amines



C-4	C-3,5	C-2,6	C-1	-X	Solvent
126.9	128.9	128.2	139.0		CDCl <sub>3</sub>
126.1	128.2	126.3	139.0		CDCl <sub>3</sub>
126.0	128.7	128.3	140.0		CDCl <sub>3</sub>
126.6	128.3	127.0	143.4	-CH <sub>2</sub> -NH <sub>2</sub>	CDCl <sub>3</sub>
118.2	129.2	115.1	146.7	-NH <sub>2</sub>	CDCl <sub>3</sub>
126.6	128.3	125.7	148.0		CDCl <sub>3</sub>

## 4-Substituted Anilines



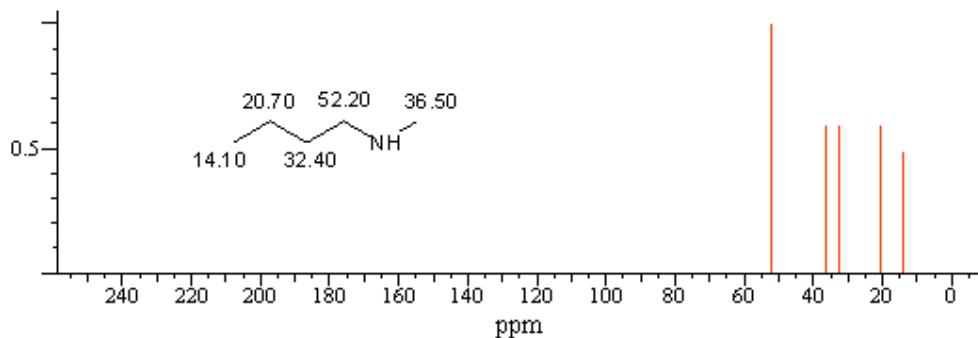
H <sub>2</sub> N-	C-1	C-2,6	C-3,5	C-4	Compound	Solvent
H <sub>2</sub> N-	138.8	116.1	116.1	138.8	-NH <sub>2</sub>	Polysol
H <sub>2</sub> N-	139.6	115.7	115.9	149.1	-OH	Polysol
H <sub>2</sub> N-	140.5	116.3	114.9	152.6	-O-CH <sub>3</sub>	CDCl <sub>3</sub>

H <sub>2</sub> N-	142.0	115.0	123.1	133.6		CDCl <sub>3</sub>
H <sub>2</sub> N-	142.7	116.1	121.0	148.5		CDCl <sub>3</sub>
H <sub>2</sub> N-	143.1	116.1	115.7	156.4	-F	CDCl <sub>3</sub>
H <sub>2</sub> N-	143.9	114.9	125.8	140.9		CDCl <sub>3</sub>
H <sub>2</sub> N-	144.3	115.2	129.7	127.2	-CH <sub>3</sub>	CDCl <sub>3</sub>
H <sub>2</sub> N-	144.4	115.3	129.1	132.7	-R4	CDCl <sub>3</sub>
H <sub>2</sub> N-	144.6	115.3	127.0	138.7		CDCl <sub>3</sub>
H <sub>2</sub> N-	145.2	116.3	129.0	122.8	-Cl	CDCl <sub>3</sub>
H <sub>2</sub> N-	145.6	116.7	131.9	109.8	-Br	CDCl <sub>3</sub>
H <sub>2</sub> N-	147.4	116.7	137.1	76.8	-I	Polysol
H <sub>2</sub> N-	151.1	114.5	133.8	99.5	-C≡N	CDCl <sub>3</sub>
H <sub>2</sub> N-	153.1	113.2	131.4	117.2		Polysol

2□Secondary

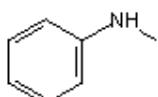
a. [Aliphatic](#)

## Aliphatics



This section contains the carbon-13 NMR chemical shifts of several types of secondary amine compounds (R'- NH— R''). The secondary amine groups exert a moderately strong deshielding effect on adjacent aliphatic carbons. Aliphatic additivity constants for the secondary amine groups are:

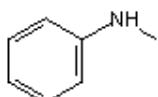
R4-NH- C1= + 36.3, C2 = + 7.7, C3 = - 4.4, C4 = + 0.4 ppm



C1= + 29.9, C2 = + 7.0, C3 = - 4.7, C4 = + 0.3 ppm

The additivity constants for the N-substituted anilines vary significantly in magnitude depending on the type of substituent bonded to the — NH— group:

NH<sub>2</sub>- C1= + 18.3, C2 = -13.3, C3 = + 0.8, C4 = -10.2 ppm

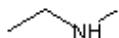


C1= +14.7, C2 = -10.6, C3 = + 0.8, C4 = - 7.6 ppm

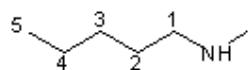
R5-NH- C1= + 20.2, C2 = -15.7, C3 = + 0.7, C4 = - 11.4 ppm

CH<sub>3</sub>-NH- C1= + 21.2, C2 = -16.0, C3 = + 0.8, C4 = - 11.4 ppm

### Aliphatic Secondary Amines



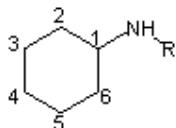
CH <sub>3</sub>	-NH-R	Solvent
29.4	-NH-R	Polysol
30.4		CDCl <sub>3</sub>
31.5		CDCl <sub>3</sub>
33.4		CDCl <sub>3</sub>
35.9	-NH-C6	CDCl <sub>3</sub>
36.3	-NH-R18	CDCl <sub>3</sub>
36.5	-NH-R4	CDCl <sub>3</sub>



C-6	C-5	C-4	C-3	C-2	C-1	-NH-R	Solvent
				14.8	38.3		CDCl <sub>3</sub>
				14.8	38.7		CDCl <sub>3</sub>
				15.9	41.2	-NH-C <sub>6</sub>	CDCl <sub>3</sub>
				15.3	43.6		CDCl <sub>3</sub>
			11.8	23.3	51.4		CDCl <sub>3</sub>
			11.9	23.6	52.3	-NH-R <sub>3</sub>	CDCl <sub>3</sub>
		13.9	20.3	31.7	43.6		CDCl <sub>3</sub>
		14.0	20.5	32.4	49.2		CDCl <sub>3</sub>
		14.1	20.8	32.7	49.8	-NH-CH <sub>2</sub> CH <sub>3</sub>	CDCl <sub>3</sub>
		14.1	20.7	32.6	50.0	-NH-R <sub>12</sub>	CDCl <sub>3</sub>
		14.1	20.7	32.4	52.2	-NH-CH <sub>3</sub>	CDCl <sub>3</sub>
	14.0	22.5	29.3	29.3	43.9		CDCl <sub>3</sub>
14.0	22.8	32.1	27.3	30.5	50.4	-NH-R <sub>6</sub>	CDCl <sub>3</sub>
R8-	29.9	29.9	27.7	30.5	50.4	-NH-R <sub>4</sub>	CDCl <sub>3</sub>

---

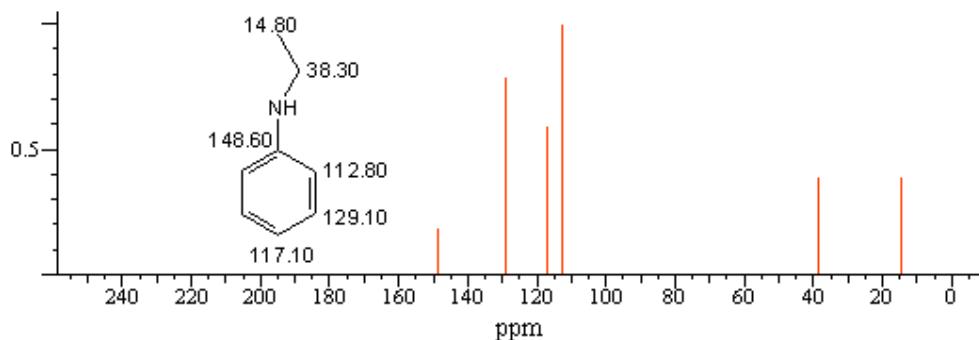
### Secondary Cyclohexylamines



C-4	C-3,5	C-2,6	C-1	-NH-R	Solvent
26.0	25.1	33.4	51.5		CDCl <sub>3</sub>
26.5	25.4	34.6	53.2	-NH-C6	CDCl <sub>3</sub>
26.6	25.2	34.0	56.9	-NH-R2	CDCl <sub>3</sub>
26.5	25.2	33.3	58.7	-NH-CH <sub>3</sub>	CDCl <sub>3</sub>

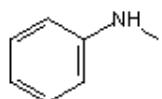
b□[Aromatic](#)

## Aromatics



This section contains the carbon-13 NMR chemical shifts of several types of secondary amine compounds (R'— NH— R"). The secondary amine groups exert a moderately strong deshielding effect on adjacent aliphatic carbons. Aliphatic additivity constants for the secondary amine groups are:

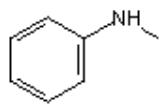
$$\text{R}_4\text{-NH-} \quad \text{C1} = +36.3, \quad \text{C2} = +7.7, \quad \text{C3} = -4.4, \quad \text{C4} = +0.4 \text{ ppm}$$



$$\text{C1} = +29.9, \quad \text{C2} = +7.0, \quad \text{C3} = -4.7, \quad \text{C4} = +0.3 \text{ ppm}$$

The additivity constants for the N-substituted anilines vary significantly in magnitude depending on the type of substituent bonded to the — NH— group:

$$\text{NH}_2- \quad \text{C1} = +18.3, \quad \text{C2} = -13.3, \quad \text{C3} = +0.8, \quad \text{C4} = -10.2 \text{ ppm}$$

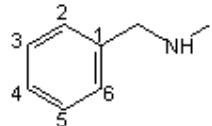


C1 = +14.7, C2 = -10.6, C3 = + 0.8, C4 = - 7.6 ppm

R5-NH- C1 = + 20.2, C2 = -15.7, C3 = + 0.7, C4 = - 11.4 ppm

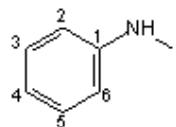
CH<sub>3</sub>-NH- C1 = + 21.2, C2 = -16.0, C3 = + 0.8, C4 = - 11.4 ppm

### Secondary Benzylamines



C-4	C-3,5	C-2,6	C-1	-X	Solvent
126.9	128.4	127.2	139.5		CDCl <sub>3</sub>
126.8	128.3	128.0	140.5	-CH <sub>2</sub> -NH-CH <sub>3</sub>	CDCl <sub>3</sub>
126.7	128.4	128.0	140.8	-CH <sub>2</sub> -NH-R2	CDCl <sub>3</sub>

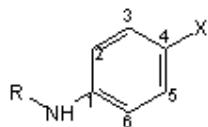
### N-Substituted Anilines



C-4	C-3,5	C-2,6	C-1	-NH-R	Solvent
128.1	128.1	119.0	141.4		Polysol
120.8	129.2	117.8	143.1		CDCl <sub>3</sub>

118.6	129.0	115.5	145.0		Polysol
118.0	128.9	115.8	145.8		Polysol
118.8	129.1	116.0	145.9		CDCl3
116.7	129.2	113.2	147.5	-NH-C6	CDCl3
116.9	129.3	113.4	147.7		CDCl3
117.3	129.1	112.7	148.1		CDCl3
117.0	129.1	112.7	148.6	-NH-R5	CDCl3
117.1	129.1	112.8	148.6	-NH-CH2CH3	CDCl3
117.0	129.2	112.4	149.6	-NH-CH3	CDCl3

#### 4-Substituted Secondary Anilines



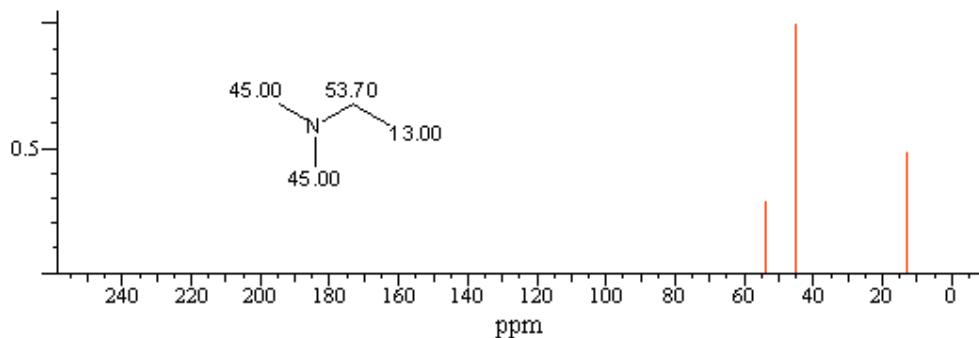
R-NH-	C-1	C-2,4	C-3,5	C-4	-X	Solvent
	133.6	123.1	115.0	142.0	-NH2	CDCl3
	134.5	121.8	114.6	152.3	-OH	Polysol

	136.8	120.1	120.1	136.8		Polysol
CH <sub>3</sub> -NH-	143.9	113.6	115.0	152.1	-O-CH <sub>3</sub>	CDCl <sub>3</sub>
R2-NH-	146.3	113.0	129.6	126.0	-CH <sub>3</sub>	CDCl <sub>3</sub>
CH <sub>3</sub> -NH-	147.4	112.5	129.7	125.9	-CH <sub>3</sub>	CDCl <sub>3</sub>
CH <sub>3</sub> -NH-	147.5	112.5	126.9	137.5		CDCl <sub>3</sub>
CH <sub>3</sub> -NH-	155.3	110.4	126.1	136.3		Polysol

### 3□Tertiary

#### a. Aliphatic

## Aliphatics



This section contains the carbon-13 NMR chemical shifts of selected tertiary amine and nitroso amine compounds. The tertiary amine groups exert a stronger deshielding effect on adjacent aliphatic carbons than the primary or secondary amine groups. A comparison of the aliphatic additivity constants follows:

H<sub>2</sub>N- C1= + 28.3, C2 = +11.3 C3 = -5.0, C4 = + 0.3 ppm

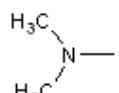
CH<sub>3</sub>-NH- C1= + 37.9, C2 = + 6.7, C3 = - 4.8, C4 = 0.0 ppm

C1= + 46.0, C2 = + 4.9, C3 = -4.1, C4 = + 0.3 ppm

A similar comparison is provided below to illustrate the deshielding/shielding properties of the primary, secondary and tertiary amine groups on the carbon resonances of benzene. The aromatic additivity constants are:

$\text{H}_2\text{N}-$  C1 = + 18.3, C2 = -13.2, C3 = + 0.8, C4 = -10.2 ppm

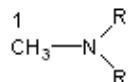
$\text{CH}_3\text{-HN-}$  C1 = + 21.2, C2 = -16.0, C3 = + 0.8, C4 = -11.4 ppm



C1 = + 22.3, C2 = -15.7, C3 = + 0.6, C4 = -11.8 ppm

The chemical shift data for a variety of tertiary amine compounds is presented in the following tables.

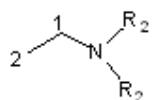
### Alkyl Tertiary Amines



C-1	-N(R) <sub>2</sub>	Solvent
38.1		$\text{CDCl}_3$
40.3		$\text{CDCl}_3$
41.6		$\text{CDCl}_3$
42.4		$\text{CDCl}_3$
45.0		$\text{CDCl}_3$
45.7		$\text{CDCl}_3$

46.6		CDCl <sub>3</sub>
------	--	-------------------

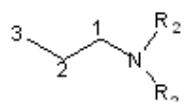
---



C-2	C-1	-N(R) <sub>2</sub>	Solvent
17.4	40.2		CDCl <sub>3</sub>
14.4	43.9		CDCl <sub>3</sub>
12.5	44.3		CDCl <sub>3</sub>
12.7	44.4		CDCl <sub>3</sub>
12.0	46.7		CDCl <sub>3</sub>
11.8	46.8		CDCl <sub>3</sub>
11.9	46.9		CDCl <sub>3</sub>
11.9	47.1		CDCl <sub>3</sub>

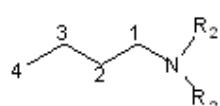
11.9	47.5		CDCl <sub>3</sub>
12.7	48.0		CDCl <sub>3</sub>
13.0	53.7		CDCl <sub>3</sub>

---

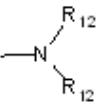


C-3	C-2	C-1	-N(R) <sub>2</sub>	Solvent
11.1	19.8	45.3		CDCl <sub>3</sub>
11.1	20.1	46.0		CDCl <sub>3</sub>
11.9	20.8	56.8		CDCl <sub>3</sub>
12.0	20.8	57.2		CDCl <sub>3</sub>

---

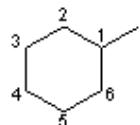


C-4	C-3	C-2	C-1	-N(R) <sub>2</sub>	Solvent
-----	-----	-----	-----	--------------------	---------

14.1	20.9	29.8	54.1		CDCl <sub>3</sub>
14.1	20.9	29.8	54.3		CDCl <sub>3</sub>
14.1	20.9	29.8	57.9		CDCl <sub>3</sub>

---

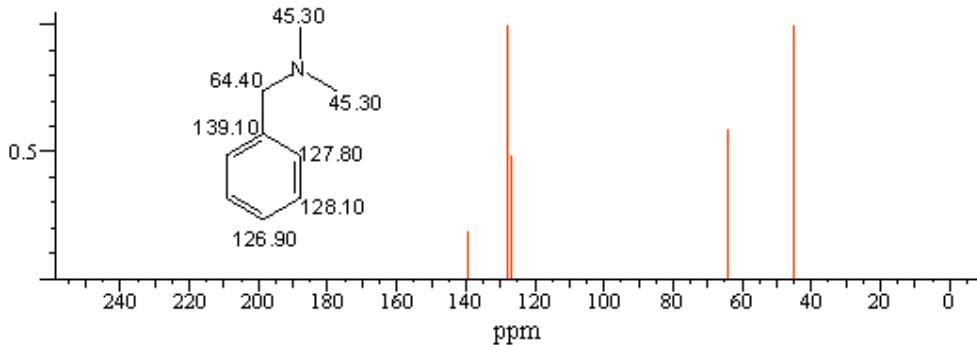
### Cyclohexylamines



C-4	C-3,5	C-2,6	C-1		Solvent
26.6	26.6	32.0	58.2		CDCl <sub>3</sub>
26.7	26.5	29.7	60.0		CDCl <sub>3</sub>
26.6	25.9	29.2	63.9		CDCl <sub>3</sub>

b□[Aromatic](#)

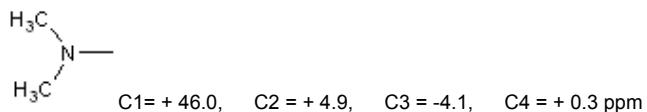
### Aromatics



This section contains the carbon-13 NMR chemical shifts of selected tertiary amine and nitroso amine compounds. The tertiary amine groups exert a stronger deshielding effect on adjacent aliphatic carbons than the primary or secondary amine groups. A comparison of the aliphatic additivity constants follows:

$\text{H}_2\text{N}-$     C1 = + 28.3,    C2 = + 11.3    C3 = - 5.0,    C4 = + 0.3 ppm

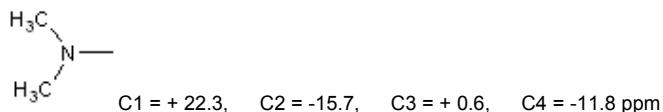
$\text{CH}_3\text{-NH}-$     C1 = + 37.9,    C2 = + 6.7,    C3 = - 4.8,    C4 = 0.0 ppm



A similar comparison is provided below to illustrate the deshielding/shielding properties of the primary, secondary and tertiary amine groups on the carbon resonances of benzene. The aromatic additivity constants are:

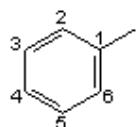
$\text{H}_2\text{N}-$     C1 = + 18.3,    C2 = - 13.2,    C3 = + 0.8,    C4 = - 10.2 ppm

$\text{CH}_3\text{-HN}-$     C1 = + 21.2,    C2 = - 16.0,    C3 = + 0.8,    C4 = - 11.4 ppm

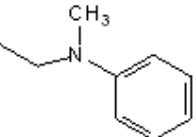
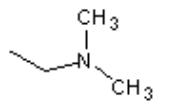
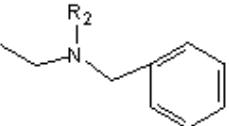


The chemical shift data for a variety of tertiary amine compounds is presented in the following tables.

### Benzylamines

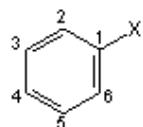


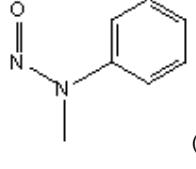
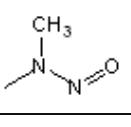
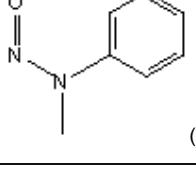
C-4	C-3,5	C-2,6	C-1	-X	Solvent
-----	-------	-------	-----	----	---------

126.7	128.4	126.7	138.9		CDCl <sub>3</sub>
126.9	128.1	127.8	139.1		CDCl <sub>3</sub>
126.7	128.6	128.1	139.9		CDCl <sub>3</sub>

---

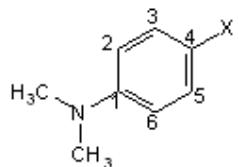
### Tertiary Anilines



C-4	C-3,5	C-2,6	C-1	-X	Solvent
119.6	129.2	126.8	136.7		CDCl <sub>3</sub>
125.4	129.4	120.2	140.7		CDCl <sub>3</sub>
127.1	129.3	119.0	142.3		CDCl <sub>3</sub>
119.6	129.6	127.3	142.5		CDCl <sub>3</sub>

122.6	129.1	124.1	147.8		CDCl <sub>3</sub>
115.8	129.2	112.4	148.0		CDCl <sub>3</sub>
116.5	129.1	112.4	149.6		CDCl <sub>3</sub>
116.6	129.0	112.7	150.7		CDCl <sub>3</sub>

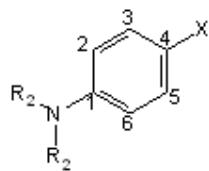
#### 4-Substituted Tertiary Amines



C-1	C-2,6	C-3,5	C-4	-X	Solvent
144.0	115.3	115.3	144.0		CDCl <sub>3</sub>
149.0	113.2	129.6	125.8	-CH <sub>3</sub>	CDCl <sub>3</sub>
149.3	113.1	126.9	129.8		CDCl <sub>3</sub>
149.5	114.1	131.7	108.5	-Br	CDCl <sub>3</sub>
150.1	112.4	125.9	125.9		CDCl <sub>3</sub>

153.1	110.6	131.1	117.4		Polysol
153.3	110.7	131.2	117.3		CDCl3

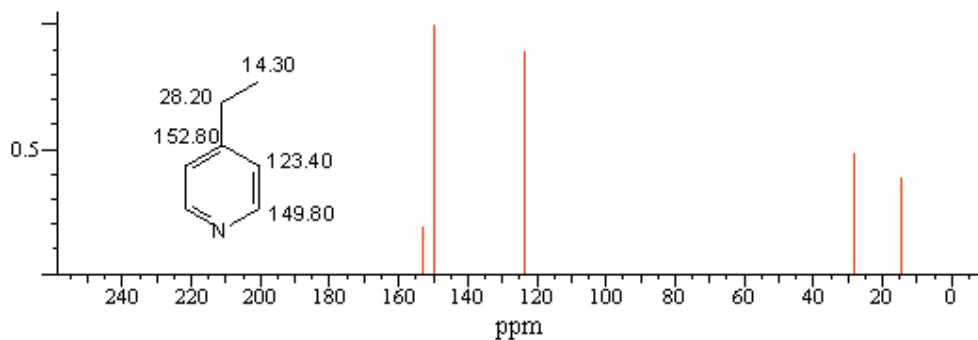
---



C-1	C-2,6	C-3,5	C-4	-X	Solvent
146.0	112.8	129.8	124.7	-CH <sub>3</sub>	CDCl <sub>3</sub>
146.7	113.4	131.8	106.9	-Br	CDCl <sub>3</sub>
151.0	110.3	131.5	116.7		CDCl <sub>3</sub>
152.2	110.7	132.0	124.9		CDCl <sub>3</sub>

## B □ Pyridines

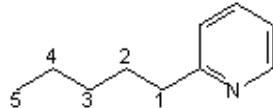
### Pyridines



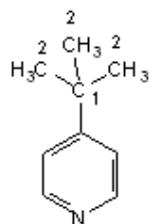
This section contains the carbon-13 NMR chemical shifts of monosubstituted pyridines. The spectra display characteristically very low chemical shifts for positions 2 and 6 carbon nuclei.

The chemical shift tables presented below contain a selected listing of carbon-13 resonances for a variety of pyridine compounds.

### Alkyl Chemical Shifts



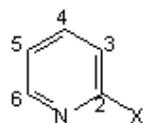
C-5	C-4	C-3	C-2	C-1	-Pyridine-R-	Solvent
				17.9		CDCl <sub>3</sub>
				23.7		CDCl <sub>3</sub>
				24.3		CDCl <sub>3</sub>
			14.3	23.6		CDCl <sub>3</sub>
			15.3	26.1		CDCl <sub>3</sub>
			14.3	28.2		CDCl <sub>3</sub>
14.0	22.6	31.8	29.5	14.2		CDCl <sub>3</sub>



C-2	C-1	-4-Pyridine	Solvent
30.3	34.4		CDCl3

### Pyridine Ring Carbon Chemical Shifts

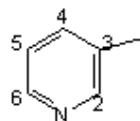
#### 2-Substituted Pyridines



C-6	C-5	C-4	C-3	C-2	-X	Solvent
151.2	128.8	137.4	127.3	133.8	-C≡N	CDCl3
150.1	122.7	138.5	128.2	142.1	-Br	CDCl3
149.2	127.0	137.6	124.8	148.4		Polysol
149.8	122.4	138.9	124.5	151.5	-Cl	CDCl3
149.1	127.1	136.8	121.4	153.8		CDCl3
147.5	114.3	137.1	109.9	156.2		Polysol
149.5	122.1	136.9	123.5	156.9		CDCl3

149.6	122.0	136.6	120.3	157.3		CDCl <sub>3</sub>
147.7	111.4	136.9	105.7	159.3		CDCl <sub>3</sub>
147.6	112.6	137.3	108.5	159.7	-NH <sub>2</sub>	Polysol
141.1	120.2	135.0	105.7	163.8	-OH	Polysol
147.8	121.3	141.2	109.7	163.8	-F	CDCl <sub>3</sub>
147.1	116.6	138.3	111.1	164.4	-O-CH <sub>3</sub>	CDCl <sub>3</sub>

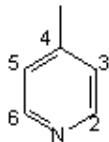
### 3-Substituted Pyridines



C-6	C-5	C-4	C-3	C-2	-X	Solvent
147.8	125.0	143.9	93.6	155.6	-I	CDCl <sub>3</sub>
153.4	123.6	135.4	132.5	149.9		CDCl <sub>3</sub>
138.9	123.9	121.3	143.7	137.2	-NH <sub>2</sub>	CDCl <sub>3</sub>
152.7	123.2	137.0	132.9	150.9		CDCl <sub>3</sub>
147.8	124.7	138.5	120.8	151.0	-Br	CDCl <sub>3</sub>
149.6	123.3	135.2	139.2	147.3	-CH <sub>2</sub> -CH <sub>3</sub>	CDCl <sub>3</sub>
147.6	124.3	135.6	132.1	148.9	-Cl	CDCl <sub>3</sub>
139.9	122.7	124.1	154.3	138.1	-OH	Polysol
147.8	123.6	133.1	129.1	145.5	-CH=N-OH	Polysol
150.4	123.5	133.2	128.7	145.1	-CH=N-O-R3	CDCl <sub>3</sub>
147.3	123.3	134.0	133.2	150.1		CDCl <sub>3</sub>

---

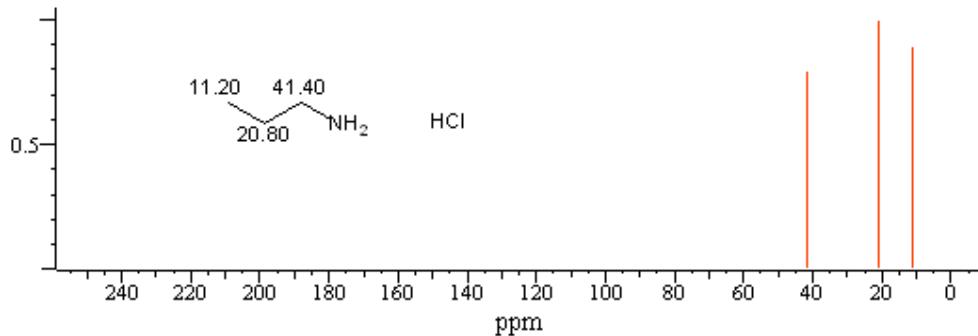
### 4-Substituted Pyridines



C-4	C-3,5	C-2,6	-X	Solvent
150.8	121.3	142.9		CDCl <sub>3</sub>
150.3	122.8	144.3		CDCl <sub>3</sub>
149.5	123.9	149.5		CDCl <sub>3</sub>
149.8	124.0	149.8		CDCl <sub>3</sub>
149.6	120.6	159.5		CDCl <sub>3</sub>
149.8	123.4	152.8		CDCl <sub>3</sub>
149.7	121.9	157.4		CDCl <sub>3</sub>
149.3	109.2	154.4		Polysol
140.7	120.7	149.9		Polysol
139.5	120.8	150.1		CDCl <sub>3</sub>

C□[Amine Salts](#)

## Amine Salts

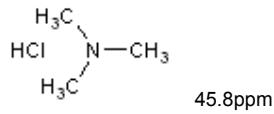
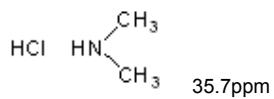
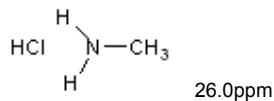


The amine salts formed with inorganic acids display intermediate aliphatic chemical shifts similar in magnitude to those of the free amine forms. The aliphatic additivity constants are:

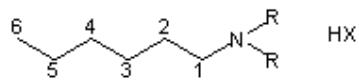
Free amine    C1 = + 28.3,    C2 = + 11.3,    C3 = - 5.0ppm

Amine salt    C1 = + 26.1,    C2 = + 4.6,    C3 = - 5.6ppm

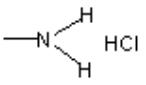
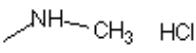
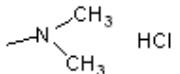
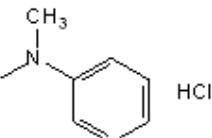
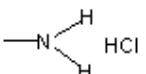
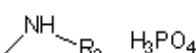
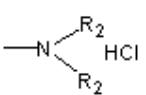
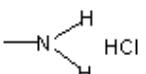
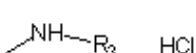
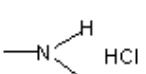
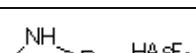
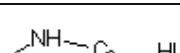
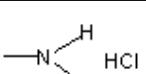
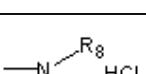
As with the free amine forms, the aliphatic primary amine salts resonate at higher fields than corresponding secondary amines and the secondary amine salts resonate at higher fields than the corresponding tertiary amine salts.



## Alkyl Amine Salts

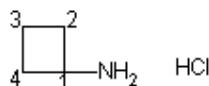


C-6	C-5	C-4	C-3	C-2	C-1	-X	Solvent
-----	-----	-----	-----	-----	-----	----	---------

					26.0		D <sub>2</sub> O
					35.7		D <sub>2</sub> O
					45.8		D <sub>2</sub> O
					47.4		D <sub>2</sub> O
				13.3	36.3		H <sub>2</sub> O
				11.5	42.8		D <sub>2</sub> O
				9.5	47.6		H <sub>2</sub> O
			11.2	20.8	41.4		Polysol
			11.3	19.5	49.7		CDCl <sub>3</sub>
		13.6	19.7	29.2	39.3		CDCl <sub>3</sub>
		13.4	19.5	27.8	47.2		Polysol
		13.5	20.3	27.8	44.6		CDCl <sub>3</sub>
14.0	22.5	31.3	26.5	27.6	40.3		CDCl <sub>3</sub>
R3-	29.1	29.1	23.5	27.0	52.7		CDCl <sub>3</sub>

---

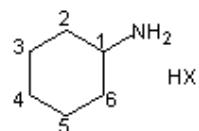
### Cyclobutylamine, Hydrochloride



C-3	C-2,4	C-1	Compound	Solvent
15.6	27.6	46.2		D <sub>2</sub> O

---

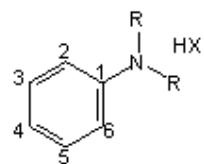
### Cyclohexylamine Salts



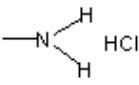
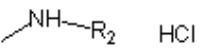
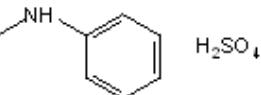
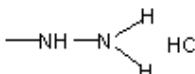
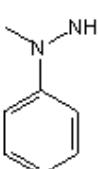
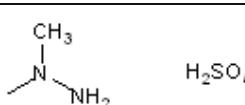
C-4	C-3	C-2	C-1	-NH <sub>2</sub> (HX)	Solvent
24.8	24.2	30.4	50.1		Polysol
24.6	24.6	29.0	58.1		CDCl <sub>3</sub>
25.1	24.0	27.6	59.5		Polysol

---

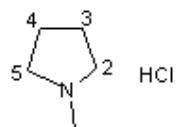
### Aniline Salts

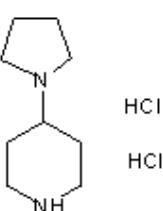
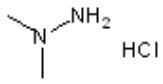


C-4	C-3,5	C-2,6	C-1	-N(R) <sub>2</sub> (HX)	Solvent
-----	-------	-------	-----	-------------------------	---------

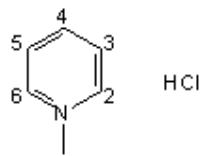
130.1	131.0	123.8	131.0		D <sub>2</sub> O
128.9	129.7	123.2	135.9		Polysol
122.8	129.3	119.0	141.6		Polysol
124.8	130.6	116.5	144.3		D <sub>2</sub> O
125.6	129.2	122.2	145.8		Polysol
120.5	128.8	115.4	150.5		Polysol

### N-Substituted Pyrrolidine Hydrochlorides



C-3,4	C-2,5	-NH <sub>2</sub> (HX)	Solvent
23.3	52.8		D <sub>2</sub> O
22.1	56.8		Polysol

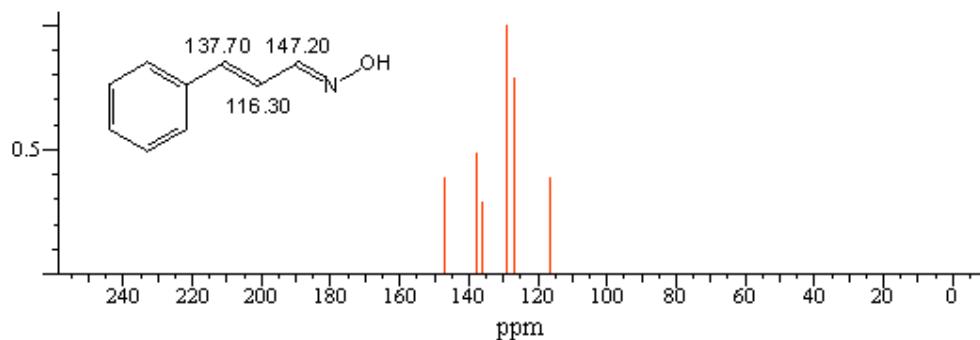
## Substituted Pyridine Salts



C-6	C-5	C-4	C-3	C-2	Compound	Solvent
149.5	131.7	143.6	128.8	141.3		D <sub>2</sub> O
149.0	128.6	143.0	128.3	151.1		D <sub>2</sub> O

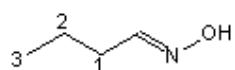
D [Oximes](#) (-CH=N-OH)

## Oximes



This section contains the chemical shifts of the oximes and derivatives which contain the -CH=N- group. The carbon-13 spectra usually display resonance bands for both the syn- and anti- forms. The oxime -CH=N- resonance is found in the chemical shift range from 137 to 158 ppm depending upon its environment.

## Alkyl Chemical Shifts

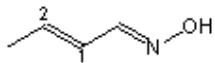


C-3	C-2	C-1	-CH=N-OH	Solvent

		11.1	147.9 (syn)	CDCl <sub>3</sub>
		15.0	148.2 (anti)	CDCl <sub>3</sub>
13.9	19.5	27.1	152.5 (syn)	CDCl <sub>3</sub>
13.5	20.1	31.5	152.1 (anti)	CDCl <sub>3</sub>

---

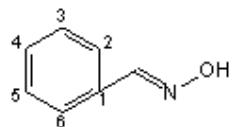
### Alkenyl Chemical Shifts



CH=	CH	-CH=N-OH	Solvent
137.7	116.3	147.2	Polysol

---

### Aromatic Chemical Shifts



C-4	C-3,5	C-2,6	C-1	-CH=N-OH	Solvent
130.0	128.7	127.2	131.9	150.6	CDCl <sub>3</sub>

---

### Chemical Shifts of the -CH=N-OH Group

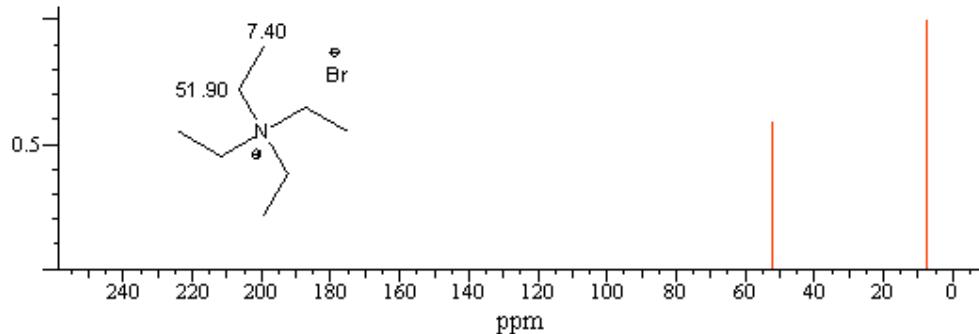
HO-N=CH	-R	Solvent
137.1	 (syn)	CDCl <sub>3</sub>

140.3		CDCl <sub>3</sub>
144.0		Polysol
146.4		Polysol
146.8		CDCl <sub>3</sub>
147.2		Polysol
147.7		CDCl <sub>3</sub>
147.9	-CH <sub>3</sub> (syn)	CDCl <sub>3</sub>
148.2	-CH <sub>3</sub> (anti)	CDCl <sub>3</sub>
149.3		Polysol
149.8		Polysol
150.3		CDCl <sub>3</sub>
150.6		CDCl <sub>3</sub>
152.0		CDCl <sub>3</sub>
152.5		CDCl <sub>3</sub>

	(anti)	
152.6		CDCl <sub>3</sub>
156.7		CDCl <sub>3</sub>
157.6		CDCl <sub>3</sub>

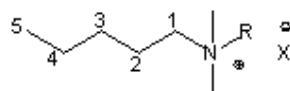
## E □ Quaternary Ammonium Salts

### Quaternary Ammonium Salts

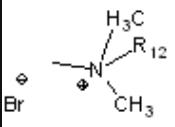
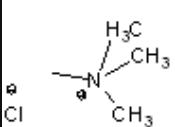
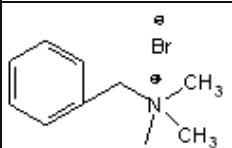
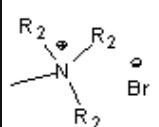
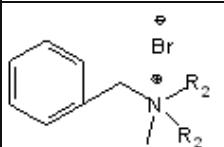
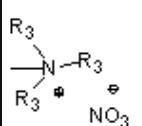
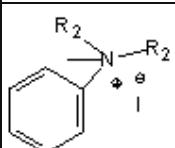
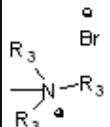
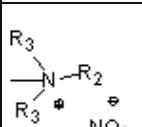
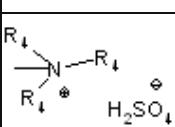
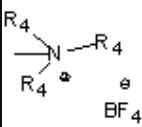


The carbon-13 NMR chemical shifts of the quaternary ammonium compounds contained in this section display the strongly deshielding effect of the N(+) group. Additionally, they illustrate the spin-spin coupling that exists between Nitrogen-14 and adjacent carbon atoms. With methyl groups (N(+) - CH<sub>3</sub>), the coupling may result in the formation of a narrow triplet ( $J = 3.5\text{Hz}$ ) for the -CH<sub>3</sub> resonance. In other cases, the coupling is too narrow to be resolved resulting in only a distinctly broadened resonance for the adjacent carbon nuclei.

### Alkyl Chemical Shifts



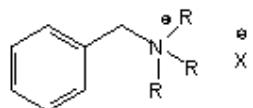
C-5	C-4	C-3	C-2	C-1	-X	Solvent
				52.4		CDCl <sub>3</sub>

			53.4		CDCl <sub>3</sub>
			56.2		H <sub>2</sub> O
			57.0		Polysol
			7.451.9		Polysol
			8.653.0		CDCl <sub>3</sub>
			10.754.2		CDCl <sub>3</sub>
			8.756.9		CDCl <sub>3</sub>
		11.0	16.160.9		CDCl <sub>3</sub>
		10.7	15.459.8		CDCl <sub>3</sub>
	13.6	19.4	23.658.0		Polysol
	13.5	19.6	23.858.5		CDCl <sub>3</sub>

R10-	28.7	25.6		31.5 60.8		Polysol
R12-	29.8	26.2		32.0 62.1		CDCl3
R8-	29.3	26.2		23.2 66.8		CDCl3

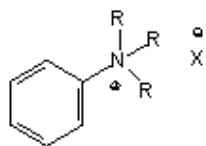
### Aromatic Chemical Shifts

#### Benzyl Ammonium Salts



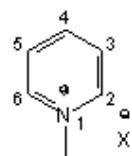
C-4	C-3	C-2	C-1	CH <sub>2</sub>	-X	Solvent
130.4	129.1	132.6	127.4	CH <sub>2</sub>		CDCl <sub>3</sub>
130.5	129.0	133.1	127.9	CH <sub>2</sub>		CDCl <sub>3</sub>

#### Phenyl Ammonium Salts



C-4	C-3,5	C-2,6	C-1	-X	Solvent
130.3	130.7	122.7	141.0		CDCl3
130.2	130.2	119.6	146.2		Polysol
131.5	131.5	120.8	147.6		D2O

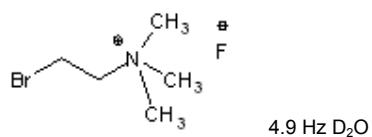
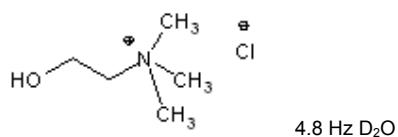
### Pyridinium Salts



C-4	C-3,5	C-2,6	-X	Solvent
145.6	128.3	145.1		Polysol
146.9	129.1	145.5		D2O
145.3	128.7	145.6		CDCl3

147.6	128.9	146.7		D <sub>2</sub> O
-------	-------	-------	--	------------------

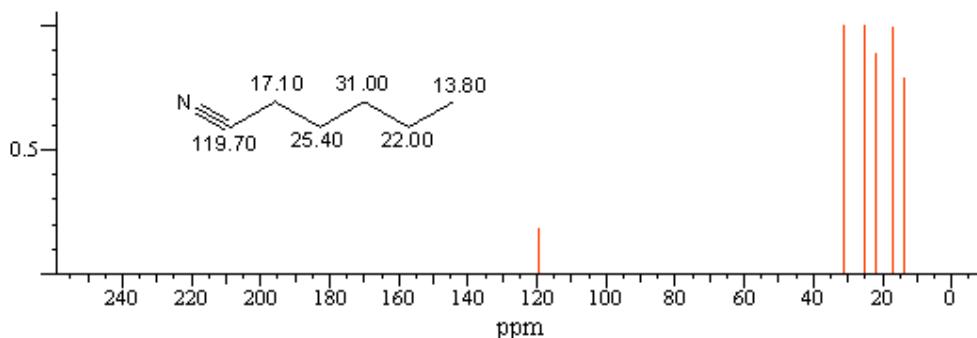
### Coupling Constants (<sup>14</sup>N-CH<sub>3</sub>)



### F□Nitriles (-C≡N)

#### 1. Aliphatic

#### Aliphatics



The carbon-13 NMR chemical shifts of the carbonitrile compounds contained in this section display the characteristically weak resonance of the C≡N carbon over the chemical shift range from 111 to 126 ppm. The long

relaxation time exhibited by the nitrile carbon often requires the utilization of relatively small pulse widths and/or the addition of a relaxation agent to the sample solution.

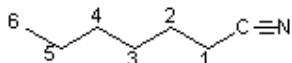
The C≡N group exerts a very weakly deshielding effect on the adjacent aliphatic carbon and a strongly shielding effect on C-1 of aromatic ring systems.

The aliphatic additivity constants for the nitrile groups are:

N≡C-    C1 = + 3.0,    C2 = + 2.8,    C3 = -3.3,    C4 = 0.0 ppm

The tables presented below illustrate the chemical shifts of a variety of selected nitrile compounds.

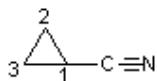
### Alkyl Chemical Shifts



C-6	C-5	C-4	C-3	C-2	C-1	-C≡N	Solvent
					1.7	117.4	CDCl <sub>3</sub>
				10.9	10.6	121.0	CDCl <sub>3</sub>
			13.2	19.0	19.4	119.8	CDCl <sub>3</sub>
		13.2	22.0	27.6	16.7	119.9	CDCl <sub>3</sub>
	13.8	22.0	31.0	25.4	17.1	119.7	CDCl <sub>3</sub>
R4-	29.7	29.5	28.9	25.6	17.1	119.6	CDCl <sub>3</sub>
R9-	29.8	29.5	28.8	25.6	17.1	119.5	CDCl <sub>3</sub>

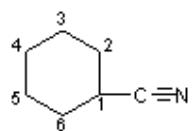
### Alicyclic Carbonitriles

Cyclopropanecarbonitrile



C-2,3	C-1	-C≡N	Solvent
7.1	-3.5	122.3	CDCl <sub>3</sub>

### Cyclohexanecarbonitrile



C-4	C-3,5	C-2,6	C-1	$-\text{C}\equiv\text{N}$	Solvent
25.4	24.2	29.7	28.1	122.4	$\text{CDCl}_3$

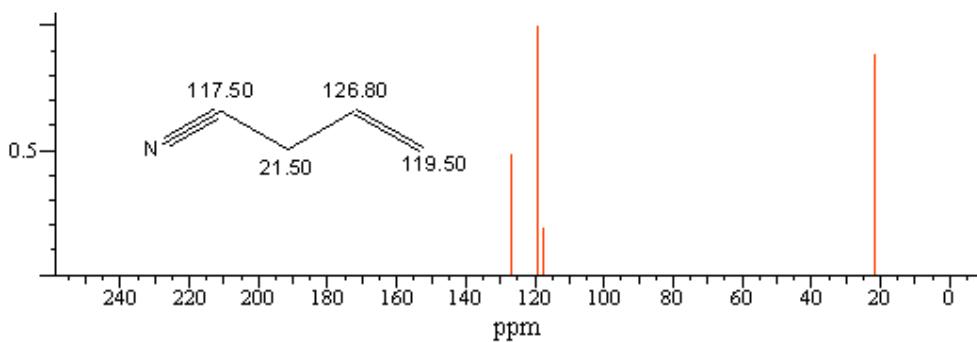
### Chemical Shifts of the $-\text{C}\equiv\text{N}$ Group

$\text{N}\equiv\text{C}-$	-X	Solvent
111.7		Polysol
112.9		$\text{CDCl}_3$
113.7		$\text{CDCl}_3$
114.5		$\text{CDCl}_3$
114.8		Polysol
115.9		$\text{CDCl}_3$
117.1		$\text{CDCl}_3$
117.4	$-\text{CH}_3$	$\text{CDCl}_3$

118.3		CDCl <sub>3</sub>
118.8		CDCl <sub>3</sub>
119.7		CDCl <sub>3</sub>
119.9	-R4	CDCl <sub>3</sub>
121.0		CDCl <sub>3</sub>
122.3		CDCl <sub>3</sub>
122.4		CDCl <sub>3</sub>
123.9		CDCl <sub>3</sub>
125.6		CDCl <sub>3</sub>

## 2□[Olefinic](#)

### Olefins



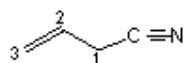
The carbon-13 NMR chemical shifts of the carbonitrile compounds contained in this section display the characteristically weak resonance of the C≡N carbon over the chemical shift range from 111 to 126 ppm. The long relaxation time exhibited by the nitrile carbon often requires the utilization of relatively small pulse widths and/or the addition of a relaxation agent to the sample solution.

The C≡N group exerts a very weakly deshielding effect on the adjacent aliphatic carbon and a strongly shielding effect on C-1 of aromatic ring systems.

The aliphatic additivity constants for the nitrile groups are:

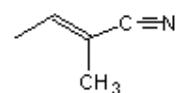
N≡C- C1 = + 3.0, C2 = + 2.8, C3 = -3.3, C4 = 0.0 ppm

### Alkenyl Nitriles



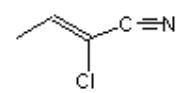
C-3	C-2	C-1	-C≡N	Solvent
24.2	29.7	28.1	122.4	CDCl <sub>3</sub>

---



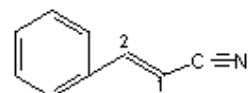
CH <sub>2</sub> =	C(CH <sub>3</sub> )	-C≡N	Solvent
131.2	118.5(20.6)	119.3	CDCl <sub>3</sub>

---



CH <sub>2</sub> =	C(Cl)	-C≡N	Solvent
131.8	110.8	114.5	CDCl <sub>3</sub>

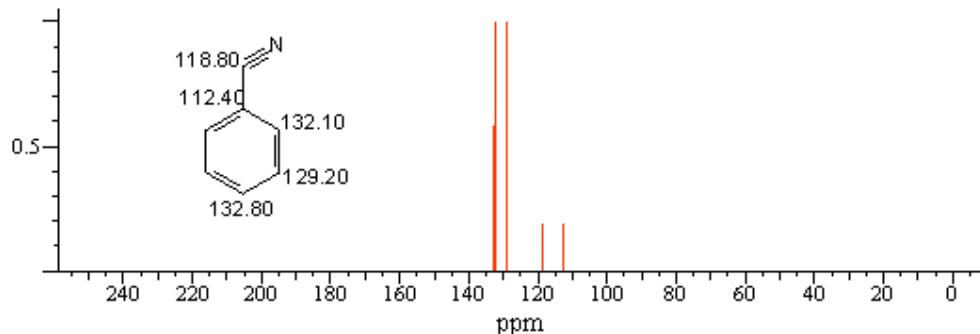
---



C-2	C-1	-C≡N	Solvent
150.3	96.4	118.3	CDCl <sub>3</sub>

### 3□Aromatic

## Aromatics



The carbon-13 NMR chemical shifts of the carbonitrile compounds contained in this section display the characteristically weak resonance of the C≡N carbon over the chemical shift range from 111 to 126 ppm. The long relaxation time exhibited by the nitrile carbon often requires the utilization of relatively small pulse widths and/or the addition of a relaxation agent to the sample solution.

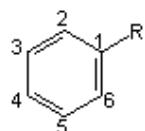
The C≡N group exerts a very weakly deshielding effect on the adjacent aliphatic carbon and a strongly shielding effect on C-1 of aromatic ring systems.

The aromatic additivity constants for this group are:

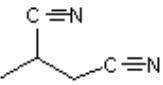
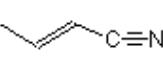
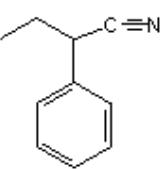
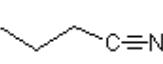
N≡C- C1=-16.0, C2,6 = + 3.7, C3,5 = + 0.8, C4 = + 4.4 ppm

The tables presented below illustrate the chemical shifts of a variety of selected nitrile compounds.

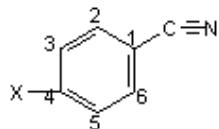
## Aromatic Nitriles



C-4	C-3,5	C-6	C-1	-R	Solvent
132.8	129.2	132.1	112.4	-C≡N	CDCl <sub>3</sub>
127.9	127.9	129.0	130.5		CDCl <sub>3</sub>

127.2	129.4	127.2	132.5		CDCl <sub>3</sub>
131.1	127.4	129.0	133.5		CDCl <sub>3</sub>
128.1	129.1	127.6	136.1		CDCl <sub>3</sub>
128.8	128.4	127.1	138.5		CDCl <sub>3</sub>

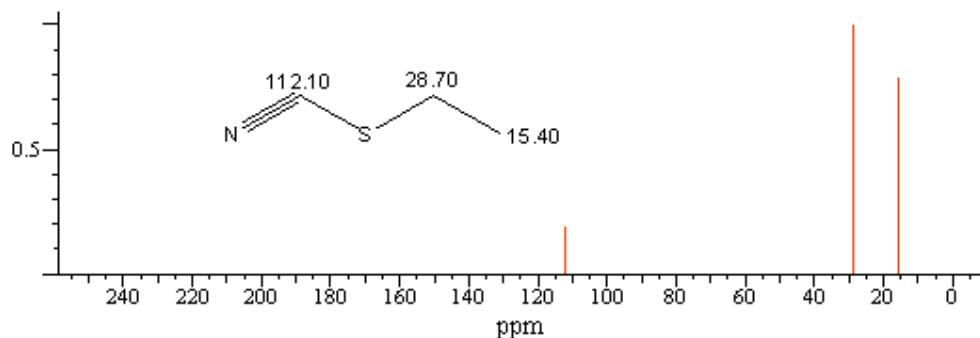
#### 4-Substituted Benzonitriles



N≡C-	C-1	C-2,6	C-3,5	C-4	-x	Solvent
117.0	116.2	132.9	132.9	116.2	-C≡N	Polysol
117.9	111.2	133.3	132.5	127.8	-Br	CDCl <sub>3</sub>
117.8	116.4	133.3	126.5	134.2	-CF <sub>3</sub>	Polysol
118.1	115.5	132.2	130.0	135.1		Polysol
117.8	111.0	133.4	129.6	139.3	-Cl	CDCl <sub>3</sub>
119.0	109.5	131.9	130.0	143.7	-CH <sub>3</sub>	CDCl <sub>3</sub>
118.8	111.0	132.5	129.1	145.6		CDCl <sub>3</sub>
120.5	99.5	133.8	114.5	151.1	-NH <sub>2</sub>	CDCl <sub>3</sub>
119.6	101.9	134.0	116.5	161.4	-OH	Polysol
118.0	108.8	134.8	116.9	165.2	-F	CDCl <sub>3</sub>

G □ [Thiocyanates](#) (-S-C≡N)

## Thiocyanates



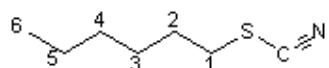
The thiocyanate group (S-C≡N) exerts a relatively weak chemical effect on adjacent aliphatic carbon atoms. The aliphatic additivity constants for the thiocyanate group are shown below.

N≡C-S-    C1=+20.0,    C2=+6.7,    C3=-4.1,    C4=-0.5 ppm.

The carbon resonance of the S-C≡N group of thiocyanate esters absorbs over a narrow chemical shift range from 110 - 114 ppm compared to 111 - 126 ppm for the nitrile (R-C≡N) group. The thiocyanate salts show a C≡N resonance near 133 ppm in D<sub>2</sub>O solution.

A selection of thiocyanate chemical shifts are show in the tables presented below.

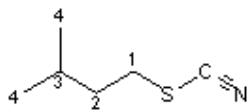
### Alkyl Thiocyanates



	C-5	C-4	C-3	C-2	C-1	-S-C≡N	Solvent
					16.5	113.4	CDCl <sub>3</sub>
				15.4	28.7	112.1	CDCl <sub>3</sub>
	13.8	22.1	30.1	29.7	34.1	112.1	CDCl <sub>3</sub>
R7-	29.5	29.0	28.0	29.5	34.1	111.7	CDCl <sub>3</sub>

---

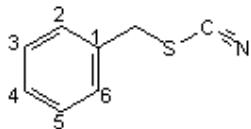
### Isopentyl Thiocyanate



C-4	C-3	C-2	C-1	-S-C≡N	Solvent
22.0	26.9	38.8	32.2	112.0	CDCl <sub>3</sub>

---

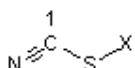
### Benzyl Thiocyanate



C-4	C-3,5	C-2,6	C-1	CH <sub>2</sub> -	-S-C≡N	Solvent
128.7	128.9	128.9	134.6	37.9	112.0	CDCl <sub>3</sub>

---

### Chemical Shifts of the (S-C≡N) Group

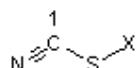


C-1	-X	Solvent
110.9		CDCl <sub>3</sub>
111.7		CDCl <sub>3</sub>
112.0		CDCl <sub>3</sub>
112.0		CDCl <sub>3</sub>

112.1	-R5	CDCl <sub>3</sub>
112.8		CDCl <sub>3</sub>
113.4	-CH <sub>3</sub>	CDCl <sub>3</sub>

---

### Thiocyanate Salts

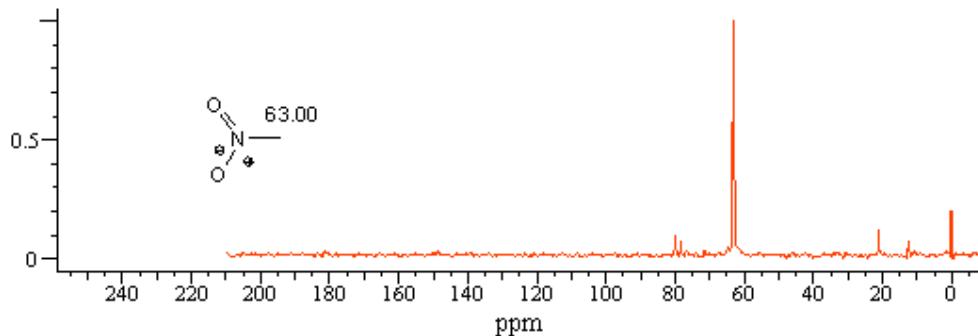


C-1	-X	Solvent
132.9	-K	D <sub>2</sub> O
133.4	-NH <sub>4</sub>	D <sub>2</sub> O

H □ Nitro Compounds (-NO<sub>2</sub>)

#### 1. Aliphatic

### Aliphatics



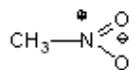
As the carbon-13 NMR chemical shifts in this section illustrate, the -NO<sub>2</sub> group has a strongly deshielding effect on the adjacent carbon (C-1) of both aliphatic and aromatic compounds. The additivity constants for nitrobenzenes are:

$$\text{NO}_2^- \quad \text{C}1 = +19.9, \quad \text{C}2 = -4.9, \quad \text{C}3 = +1.1, \quad \text{C}4 = +6.4 \text{ ppm}$$

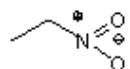
The C-1 carbons of the nitrobenzenes tend to have an abnormally long relaxation time requiring short pulse widths and/or the addition of relaxation agents.

---

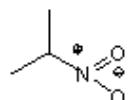
### Nitro Alkanes



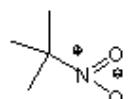
C-1	-NO <sub>2</sub>	Solvent
63.0	-NO <sub>2</sub>	CDCl <sub>3</sub>



C-2	C-1	-NO <sub>2</sub>	Solvent
12.4	70.9	-NO <sub>2</sub>	CDCl <sub>3</sub>



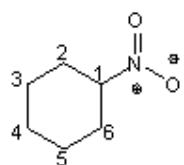
C-2	C-1	-NO <sub>2</sub>	Solvent
20.8	79.2	-NO <sub>2</sub>	CDCl <sub>3</sub>



C-2	C-1	-NO <sub>2</sub>	Solvent
27.8	85.2	-NO <sub>2</sub>	CDCl <sub>3</sub>

---

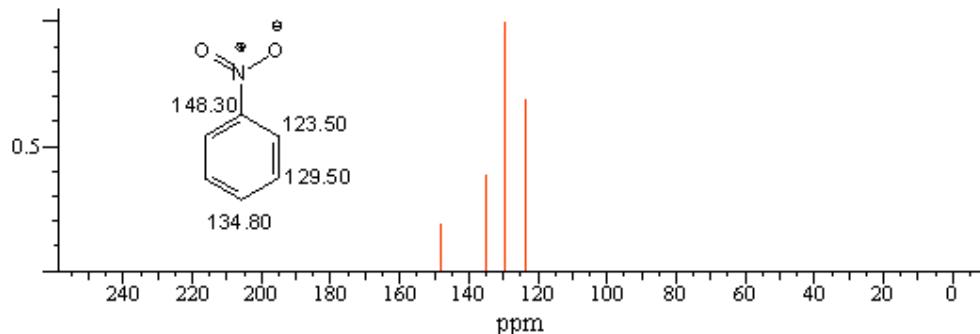
### Nitrocyclohexane



C-4	C-3,5	C-2,6	C-1	-NO <sub>2</sub>	Solvent
25.2	24.4	31.3	84.8	-NO <sub>2</sub>	CDCl <sub>3</sub>

2□[Aromatic](#)

## Aromatics

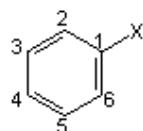


As the carbon-13 NMR chemical shifts in this section illustrate, the -NO<sub>2</sub> group has a strongly deshielding effect on the adjacent carbon (C-1) of both aliphatic and aromatic compounds. The additivity constants for nitrobenzenes are:

$$\text{NO}_2^- \quad \text{C}1 = +19.9, \quad \text{C}2 = -4.9, \quad \text{C}3 = +1.1, \quad \text{C}4 = +6.4 \text{ ppm}$$

The C-1 carbons of the nitrobenzenes tend to have an abnormally long relaxation time requiring short pulse widths and/or the addition of relaxation agents.

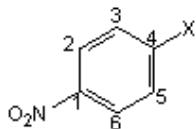
## Aromatic Nitro Compounds



C-4	C-3,5	C-2,6	C-1	-X	Solvent
128.3	128.7	128.3	131.1		CDCl <sub>3</sub>
134.8	129.5	123.5	148.5		CDCl <sub>3</sub>

---

#### 4-Substituted Nitrobenzenes

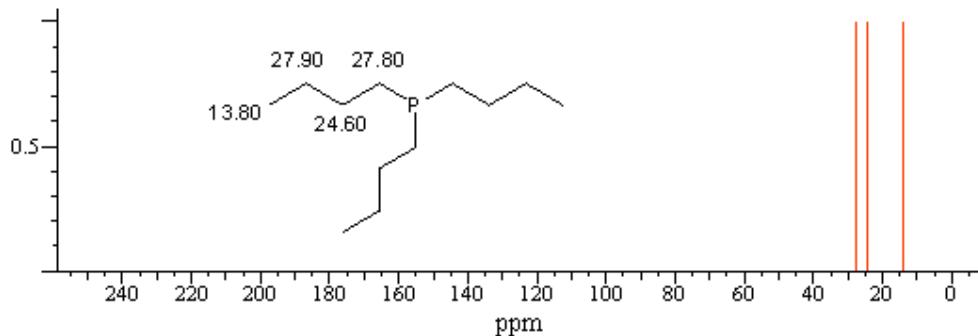


	C-1	C-2,6	C-3,5	C-4	-X	Solvent
NO <sub>2</sub> <sup>-</sup>	150.6	123.5	130.7	136.1		CDCl <sub>3</sub>
NO <sub>2</sub> <sup>-</sup>	147.0	125.0	129.6	141.4	-Cl	CDCl <sub>3</sub>
NO <sub>2</sub> <sup>-</sup>	150.4	123.7	129.4	141.7		CDCl <sub>3</sub>
NO <sub>2</sub> <sup>-</sup>	147.5	123.8	129.8	144.9	-CH <sub>2</sub> -Cl	CDCl <sub>3</sub>
NO <sub>2</sub> <sup>-</sup>	146.4	123.5	129.9	146.1	-CH <sub>3</sub>	CDCl <sub>3</sub>
NO <sub>2</sub> <sup>-</sup>	136.9	126.3	112.8	155.1	-NH <sub>2</sub>	CDCl <sub>3</sub>
NO <sub>2</sub> <sup>-</sup>	136.3	126.1	110.4	155.3	-NH-CH <sub>3</sub>	CDCl <sub>3</sub>
NO <sub>2</sub> <sup>-</sup>	141.4	125.8	114.5	164.3	-O-CH <sub>2</sub> CH <sub>3</sub>	CDCl <sub>3</sub>
NO <sub>2</sub> <sup>-</sup>	140.9	126.6	116.3	164.5	-OH	CDCl <sub>3</sub>
NO <sub>2</sub> <sup>-</sup>	144.9	126.6	116.6	166.7	-F	CDCl <sub>3</sub>

#### □ □ Silicon Containing Compounds (Except Si-O) □ □ □

#### □ □ Phosphorus Containing Compounds (Except P-O and P(=O)-O)

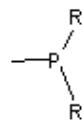
#### Phosphorus Compounds



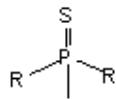
The carbon-13 NMR chemical shifts of organic compounds containing phosphorus characteristically display <sup>31</sup>P - <sup>13</sup>C coupling across as many as 4 intervening bonds.

The chemical shift effect exerted by all of the different valence states in which phosphorus can exist varies from that of a weakly deshielding substituent on adjacent aliphatic carbons to either a weakly shielding or weakly deshielding substituent on aromatic phenyl C-1 carbons.

The aliphatic additivity constants for compounds in this group are:

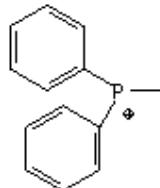


$$\text{C1} = +13.5, \quad \text{C2} = +3.0, \quad \text{C3} = +0.6, \quad \text{C4} = -0.4 \text{ ppm}$$

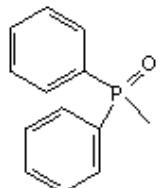


$$\text{C1} = +17.0, \quad \text{C2} = -0.7, \quad \text{C3} = -1.4, \quad \text{C4} = -0.6 \text{ ppm}$$

The aromatic additivity constants are:



$$\text{C1} = -10.9, \quad \text{C2, 6} = +6.0, \quad \text{C3, 5} = +2.1, \quad \text{C4} = +7.1 \text{ ppm}$$

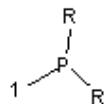


$$\text{C1} = +5.3, \quad \text{C2, 6} = +3.5, \quad \text{C3, 5} = 0.0, \quad \text{C4} = +3.2 \text{ ppm}$$

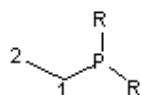
The tables that are presented below illustrate the chemical shifts and coupling constants for a variety of phosphorus containing organic molecules.

---

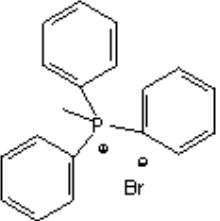
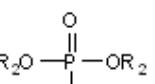
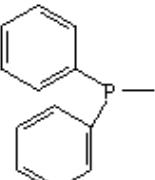
### Alkyl Chemical Shifts



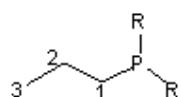
C-1	-P(R) <sub>n</sub>	Solvent
5.8		CDCl <sub>3</sub>
12.4		CDCl <sub>3</sub>

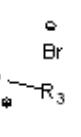


C-2	C-1	-P(R) <sub>n</sub>	Solvent
7.6	10.0		CDCl <sub>3</sub>
5.6	11.0		Polysol

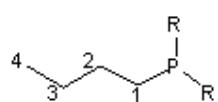
6.9	17.0		CDCl <sub>3</sub>
6.6	19.1		CDCl <sub>3</sub>
9.9	20.5		CDCl <sub>3</sub>

---

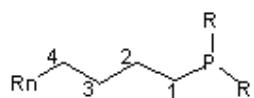


C-3	C-2	C-1	-P(R) <sub>n</sub>	Solvent
15.5	15.7	21.3		CDCl <sub>3</sub>
15.2	15.6	22.7		CDCl <sub>3</sub>

---

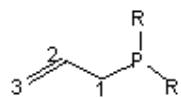


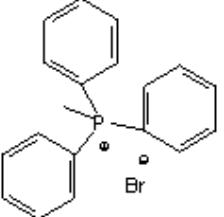
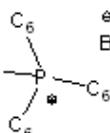
C-4	C-3	C-2	C-1	$-P(R)_n$	Solvent
13.7	23.6	24.5	22.7		CDCl <sub>3</sub>
13.6	24.8	23.1	26.2		CDCl <sub>3</sub>
13.8	27.9	24.6	27.8		CDCl <sub>3</sub>



R <sub>n</sub> -	C-4	C-3	C-2	C-1	$-P(R)_n$	Solvent
R4-	29.4	31.7	26.1	27.6		CDCl <sub>3</sub>
R8-	29.3	29.1	22.3	30.5		CDCl <sub>3</sub>
R4-	29.2	30.9	22.5	31.1		CDCl <sub>3</sub>

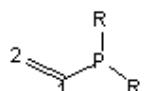
### Allyl Phosphorus Compounds

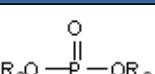


C-3	C-2	C-1	$-\text{P}(\text{R})_n$	Solvent
123.2	126.2	28.9		$\text{CDCl}_3$
125.3	124.1	21.7		$\text{CDCl}_3$

---

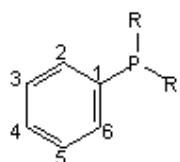
### Vinyl Chemical Shifts



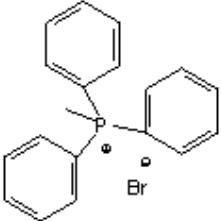
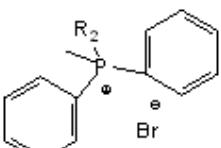
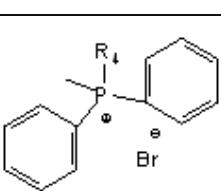
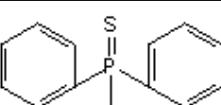
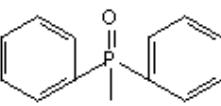
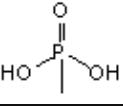
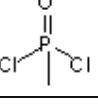
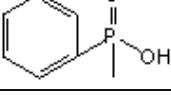
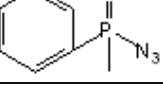
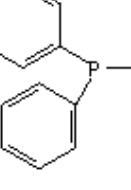
C-2	C-1	$-\text{P}(\text{R})_n$	Solvent
135.1	126.8		$\text{CDCl}_3$

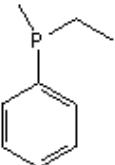
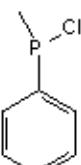
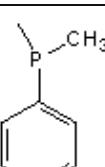
---

### Phenyl Group Chemical Shifts

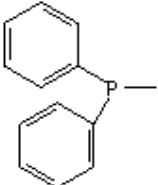
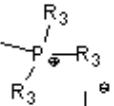


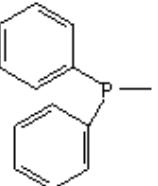
C-4	C-3	C-2	C-1	$-\text{P}(\text{R})_n$	Solvent
-----	-----	-----	-----	-------------------------	---------

135.5	130.5	134.4	117.5		Polysol
135.1	130.6	133.6	117.9		CDCl3
135.1	130.6	133.5	118.2		CDCl3
131.6	128.5	131.9	132.8		Polysol
131.6	128.4	131.9	133.7		CDCl3
131.2	128.0	130.5	134.1		Polysol
134.7	129.3	130.1	134.3		CDCl3
131.5	129.2	131.7	138.6		NaOD
133.2	128.9	131.2	142.9		CDCl3
128.6	128.4	133.6	137.2		CDCl3

128.4	128.3	132.6	138.5		CDCl <sub>3</sub>
130.1	128.4	131.6	138.6		CDCl <sub>3</sub>
128.4	128.2	132.0	140.1		CDCl <sub>3</sub>

### Aliphatic Coupling Constants (<sup>31</sup>P-<sup>13</sup>C)

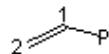
C-1	- <sup>31</sup> P(R) <sub>n</sub>	Solvent
14.0 Hz		CDCl <sub>3</sub>
50.7 Hz		CDCl <sub>3</sub>

C-2	C-1	- <sup>31</sup> P(R) <sub>n</sub>	Solvent
16.4 Hz	10.0 Hz		CDCl <sub>3</sub>

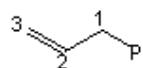
5.9 Hz	47.6 Hz		Polysol
4.8 Hz	51.3 Hz		CDCl3
6.6 Hz	144.1 Hz		CDCl3

C-3	C-2	C-1	${}^{-31}\text{P}(\text{R})_n$	Solvent
13.4 Hz	14.4 Hz	11.9 Hz		CDCl3
7.7 Hz	11.5 Hz	33.5 Hz		CDCl3
14.6 Hz	4.9 Hz	46.8 Hz		CDCl3
12.0 Hz	4.2 Hz	48.5 Hz		CDCl3
14.6 Hz	3.9 Hz	50.4 Hz		CDCl3
16.2 Hz	4.5 Hz	53.0 Hz		CDCl3

### Alkenyl Coupling Constants ( $^{31}\text{P}$ - $^{13}\text{C}$ )



C-2	C-1	-X	Solvent
	183.1 Hz	$\text{R}_2\text{O}-\overset{\text{O}}{\underset{ }{\text{P}}}(\text{OR}_2)_2$	$\text{CDCl}_3$

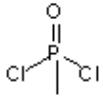


C-3	C-2	C-1	-X	Solvent
9.7 Hz	13.0 Hz	49.6 Hz		$\text{CDCl}_3$

### Phenyl Coupling Constants ( $^{31}\text{P}$ - $^{13}\text{C}$ )

C-3 Hz	C-2 Hz	C-1 Hz	-P(R) <sub>n</sub>	Solvent
6.8	19.5	11.9		$\text{CDCl}_3$
6.5	15.9	12.0		$\text{CDCl}_3$

5.0	18.7	12.8		CDCl <sub>3</sub>
5.5	24.2	33.3		CDCl <sub>3</sub>
12.3	9.8	85.5		CDCl <sub>3</sub>
12.2	9.9	86.4		CDCl <sub>3</sub>
13.7	9.7	89.4		Polysol
14.7	12.2	85.4		Polysol
18.3	14.5	117.4		CDCl <sub>3</sub>
12.1	8.9	63.2		CDCl <sub>3</sub>
14.4	9.8	118.4		Polysol
11.8	8.9	131.3		NaOD
14.1	12.2	141.6		CDCl <sub>3</sub>

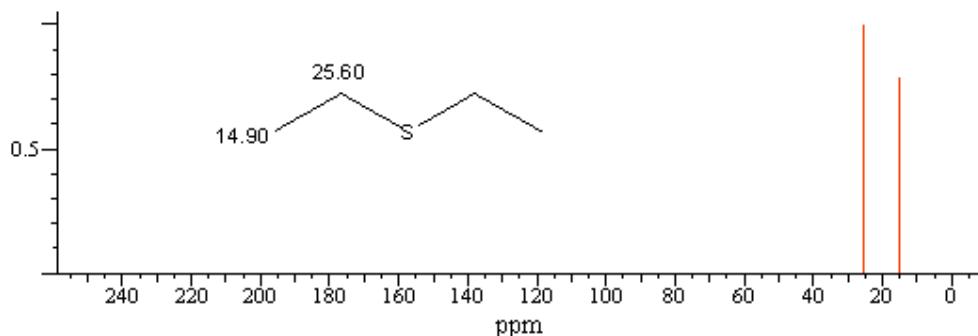
21.5	16.9	155.1		CDCl <sub>3</sub>
------	------	-------	---	-------------------

# Sulfur Containing Compounds

#### A. Sulfides (R-S-R)

## 1. Aliphatic

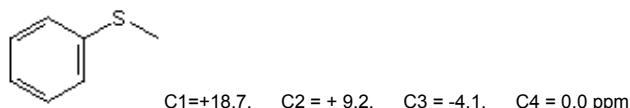
## Aliphatics



This section contains the carbon-13 NMR chemical shifts of the alkyl and aromatic sulfides and the thiophenes. As expected, the deshielding effect of the various sulfide groups on the adjacent carbon is significantly stronger than that of the thiols. A comparison of their additivity constants is shown below.

The aliphatic additivity constants are:

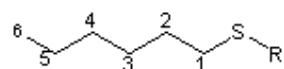
HS- C1=+10.5, C2- + 11.4, C3 = -3.6, C4 = - 0.2 ppm



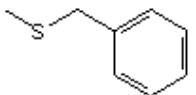
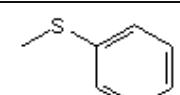
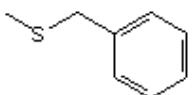
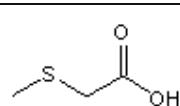
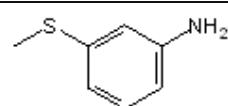
$\text{CH}_3\text{-S-}$  C1 = +20.4, C2 = +6.2, C3 = -2.7, C4 = +0.3 ppm

The assignment of thiophene resonances based on chemical shifts is complicated by the fact that the chemical shift of C-2 and C-5 is very similar to that of C-3 and C-4 (125.0 vs. 126.7 ppm). In general, it is found that there is a rough correlation between a substituent's shielding effect on benzene carbon atoms and its effect on the corresponding thiophene ring positions.

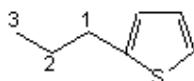
## Alkyl Sulfides

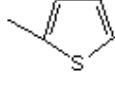
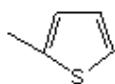


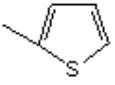
C-6	C-5	C-4	C-3	C-2	C-1	-S-R	Solvent
-----	-----	-----	-----	-----	-----	------	---------

					14.7		CDCl <sub>3</sub>
					15.5	-S-R12	CDCl <sub>3</sub>
					15.6		CDCl <sub>3</sub>
				14.3	25.1		CDCl <sub>3</sub>
				14.9	25.6	-S-R2	CDCl <sub>3</sub>
				14.1	26.1	-S-R4	CDCl <sub>3</sub>
				14.2	26.7		CDCl <sub>3</sub>
		13.7	22.2	32.2	32.2	-S-R4	CDCl <sub>3</sub>
14.1	22.7	31.7	28.8	29.9	32.4	-S-R6	CDCl <sub>3</sub>
R2-	31.9	29.1	29.1	29.9	32.4	-S-R7	CDCl <sub>3</sub>
R11-	29.4	29.1	28.7	31.6	32.8		Polysol
R7-	29.8	29.8	29.4	29.0	34.5	-S-CH <sub>3</sub>	CDCl <sub>3</sub>

### Alkyl Group Chemical Shifts

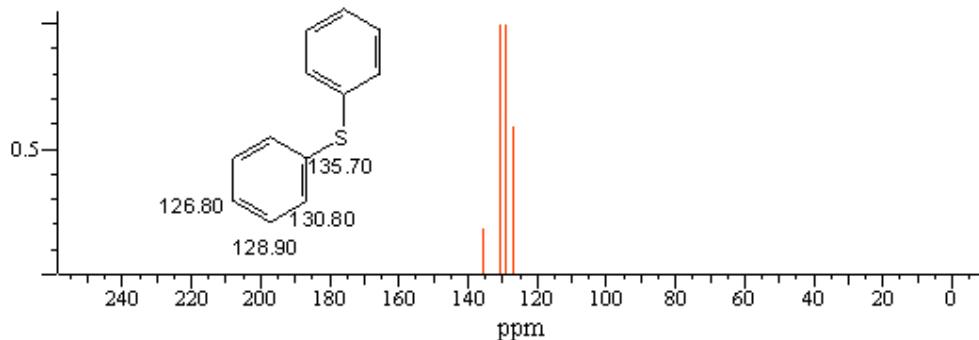


C-3	C-2	C-1	-2-Thiophene	Solvent
		14.9		CDCl <sub>3</sub>
	16.1	23.7		CDCl <sub>3</sub>

13.7	25.1	32.0		CDCl <sub>3</sub>
------	------	------	---	-------------------

2□[Aromatic](#)

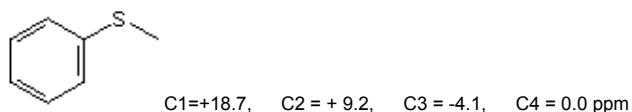
## Aromatics



This section contains the carbon-13 NMR chemical shifts of the alkyl and aromatic sulfides and the thiophenes. As expected, the deshielding effect of the various sulfide groups on the adjacent carbon is significantly stronger than that of the thiois. A comparison of their additivity constants is shown below.

The aliphatic additivity constants are:

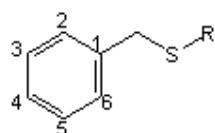
HS-      C1=+10.5,    C2= + 11.4,    C3 = -3.6,    C4 = - 0.2 ppm

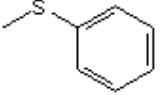
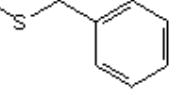


CH<sub>3</sub>-S-    C1= + 20.4,    C2 = + 6.2,    C3 = -2.7,    C4 = + 0.3 ppm

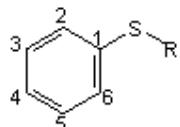
The assignment of thiophene resonances based on chemical shifts is complicated by the fact that the chemical shift of C-2 and C-5 is very similar to that of C-3 and C-4 (125.0 vs. 126.7 ppm). In general, it is found that there is a rough correlation between a substituent's shielding effect on benzene carbon atoms and its effect on the corresponding thiophene ring positions.

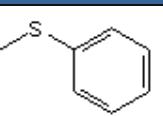
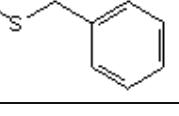
## Benzyl Sulfides



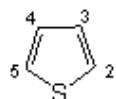
C-4	C-3,5	C-2,6	C-1	-CH <sub>2</sub> -	-S-R	Solvent
126.9	129.5	128.3	137.3	38.7		CDCl <sub>3</sub>
127.3	129.3	128.4	137.3	43.2		CDCl <sub>3</sub>
126.9	128.8	128.4	138.4	38.3	-S-CH <sub>3</sub>	CDCl <sub>3</sub>
126.7	128.8	128.3	138.6	35.8	-S-R2	CDCl <sub>3</sub>

### Phenyl Sulfides



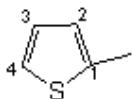
C-4	C-3,5	C-2,6	C-1	-S-R	Solvent
126.8	128.9	130.8	135.7		CDCl <sub>3</sub>
126.0	128.7	128.3	136.5		CDCl <sub>3</sub>
124.9	128.7	126.7	138.6	-S-CH <sub>3</sub>	CDCl <sub>3</sub>

### Thiophene



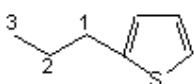
C-5	C-4	C-3	C-2	Solvent
125.0	126.7	126.7	125.0	CDCl <sub>3</sub>

## 2-Substituted Thiophenes

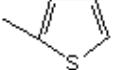


C-4	C-3	C-2	C-1	-X	Solvent
131.0	128.4	136.4	73.2	-I	CDCl <sub>3</sub>
133.1	127.9	137.6	109.6	-C≡N	CDCl <sub>3</sub>
124.0	126.0	126.5	130.1	-Cl	CDCl <sub>3</sub>
132.3	127.8	133.3	134.9		Polysol
129.9	127.7	127.7	138.0		Polysol
125.1	126.6	123.9	142.9		CDCl <sub>3</sub>
131.7	128.2	133.2	144.3		CDCl <sub>3</sub>
122.8	126.6	124.1	145.3	-R3	CDCl <sub>3</sub>

## Alkyl Group Chemical Shifts

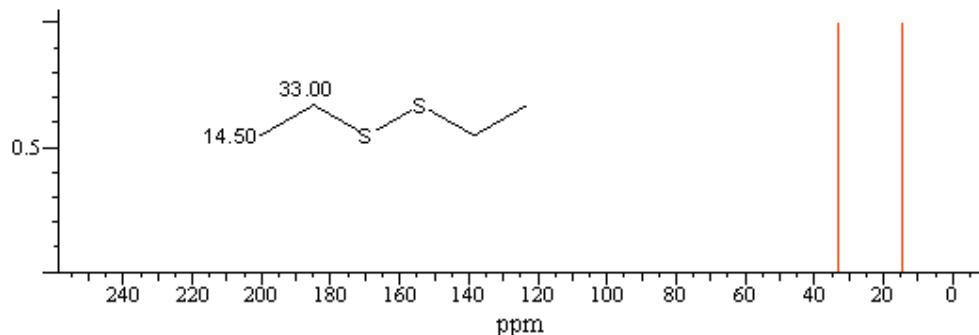


C-3	C-2	C-1	-2-Thiophene	Solvent
		14.9		CDCl <sub>3</sub>
	16.1	23.7		CDCl <sub>3</sub>

13.7	25.1	32.0		CDCl <sub>3</sub>
------	------	------	---	-------------------

### B □ Disulfides (R-S-S-R)

## Disulfides



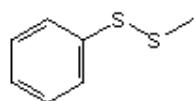
The chemical shift effect of the disulfide functional group displayed by the carbon-13 NMR chemical shifts in this section is that of a moderately strong deshielding substituent in relation to adjacent aliphatic carbons. A comparison of the aliphatic additivity constants for the sulfide and disulfide groups is given below.

The aliphatic additivity constants are:

R-S-S- C1= + 25.2, C2 = + 6.6, C3 = - 3.4, C4 = -0.1 ppm

R-S- C1=+17.9, C2 = + 7.1, C3 = -3.0, C4 = -0.1 ppm

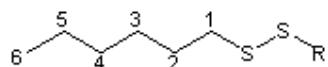
A similar moderately strong deshielding effect is noted in the chemical shift of aromatic C-1's. The aromatic additivity constants are:



C1= + 7.5, C2,6 = -1.0, C3,5 = + 0.4, C4 = -1.5 ppm

The following tables contain representative chemical shifts for a variety of disulfide compounds.

## Alkyl Disulfides

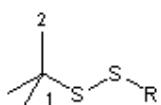


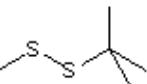
C-6	C-5	C-4	C-3	C-2	C-1	-S-S-R	Solvent
					22.2	-S-S-CH <sub>3</sub>	CDCl <sub>3</sub>

				14.5	33.0	-S-S-R2	CDCl <sub>3</sub>
			13.1	22.6	41.2	-S-S-R3	CDCl <sub>3</sub>
		13.7	21.7	31.4	38.9	-S-S-R4	CDCl <sub>3</sub>
	13.9	22.4	30.8	29.1	39.4	-S-S-R5	CDCl <sub>3</sub>
R5-	29.7	29.4	28.7	29.4	39.3	-S-S-R10	CDCl <sub>3</sub>

---

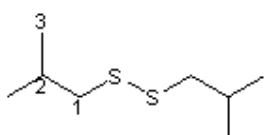
### tert-Butyl Disulfide

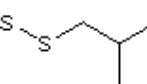


C-2	C-1	-S-S-R	Solvent
30.5	45.8		CDCl <sub>3</sub>

---

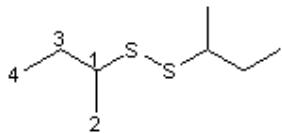
### Isobutyl Disulfide



C-3	C-2	C-1	-S-S-R	Solvent
21.8	28.3	48.7		CDCl <sub>3</sub>

---

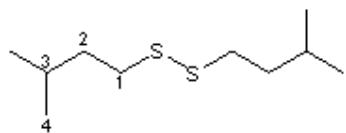
### sec-Butyl Disulfide



C-4	C-3	C-2	C-1	-S-S-R	Solvent
11.5	29.1	20.2	48.2		CDCl3

---

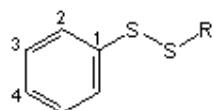
### Isopentyl Disulfide



C-4	C-3	C-2	C-1	-S-S-R	Solvent
22.3	27.2	37.2	38.4		CDCl3

---

### Aromatic Disulfides



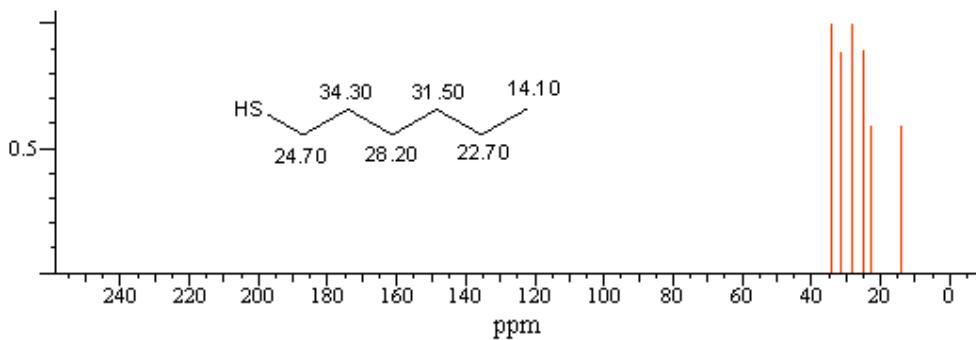
	C-4	C-3	C-2	C-1	-R	Solvent
	127.2	129.3	128.3	137.3		CDCl3
	126.9	128.8	127.4	136.9		CDCl3

<chem>CH3-</chem>	127.1	129.6	128.5	133.9		<chem>CDCl3</chem>
<chem>Br-</chem>	121.4	132.2	129.3	135.7		Polysol

## C $\square$ Thiols

### 1. Aliphatic

## Aliphatics



The spectra of the thiol containing compounds in this section indicate that the -SH group exerts a very weak deshielding effect on both aliphatic and aromatic position 1 carbons.

The aliphatic additivity constants are:

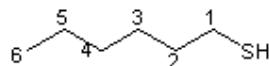
HS- C1=+10.5, C2 = + 11.4, C3 = -3.6, C4 = - 0.2 ppm

The aromatic additivity constants are:

HS- C1= + 2.3, C2, 6 = + 0.9, C3, 5 = + 0.5, C4 = -3.0 ppm

A selection of thiol chemical shifts is presented in the tables below.

## N-Alkyl Thiols

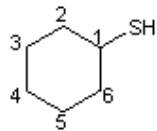


C-6	C-5	C-4	C-3	C-2	C-1	-SH	Solvent
				19.7	19.1	-SH	<chem>CDCl3</chem>

		13.5	21.6	36.3	24.3	-SH	$\text{CDCl}_3$
14.1	22.7	31.5	28.2	34.3	24.7	-SH	$\text{CDCl}_3$
R4-	29.7	29.4	28.6	34.3	24.6	-SH	$\text{CDCl}_3$
R13-	29.8	29.2	28.5	34.2	24.6	-SH	$\text{CDCl}_3$

---

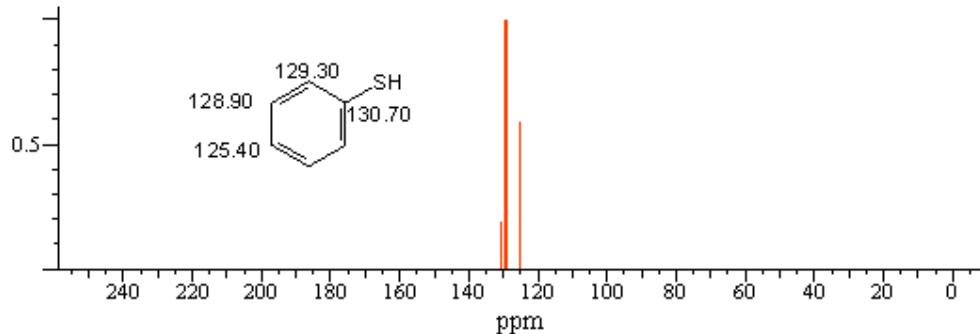
### Cyclohexanethiol



C-4	C-3,5	C-2,6	C-1	-SH	Solvent
25.5	26.3	38.0	38.3	-SH	$\text{CDCl}_3$

2□[Aromatic](#)

### Aromatics



The spectra of the thiol containing compounds in this section indicate that the -SH group exerts a very weak deshielding effect on both aliphatic and aromatic position 1 carbons.

The aliphatic additivity constants are:

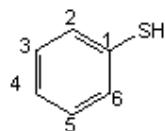
HS- C1=+10.5, C2 = + 11.4, C3 = -3.6, C4 = - 0.2 ppm

The aromatic additivity constants are:

HS- C1= + 2.3, C2, 6 = + 0.9, C3, 5 = + 0.5, C4 = -3.0 ppm

---

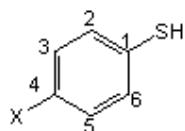
### Aromatic Thiols



C-4	C-3,5	C-2,6	C-1	-X	Solvent
125.4	128.9	129.3	130.7	-SH	CDCl <sub>3</sub>
126.8	128.5	127.9	141.0	-CH <sub>2</sub> -SH	CDCl <sub>3</sub>
126.9	128.4	126.3	145.7		CDCl <sub>3</sub>
126.8	129.3	127.7	147.2		CDCl <sub>3</sub>

---

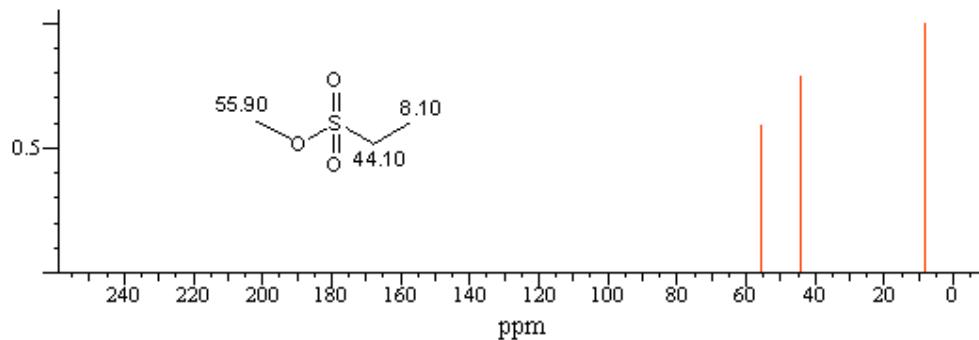
### 4-Substituted Benzenethiols



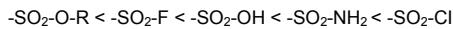
HS-	C-1	C-2,6	C-3,5	C-4	-X	Solvent
HS-	119.9	132.3	114.7	158.4	-O-CH <sub>3</sub>	CDCl <sub>3</sub>
HS-	125.2	131.9	116.1	161.5	-F	CDCl <sub>3</sub>
HS-	126.7	129.8	129.8	135.3	-CH <sub>3</sub>	CDCl <sub>3</sub>
HS-	126.8	129.6	126.0	148.7		CDCl <sub>3</sub>
HS-	129.0	130.7	129.0	131.6	-Cl	CDCl <sub>3</sub>

D □ **Sulfones** ( $\text{R-SO}_2\text{-R}$ )

## Sulfones

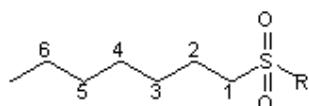


The wide variety of functional groups containing the  $-\text{SO}_2-$  group displays differing deshielding effects ranging from moderately to strongly deshielding depending upon the type of substituent involved. The aliphatic deshielding observed follows the general sequence shown below for increasing chemical shift effect.

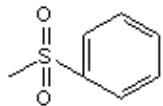
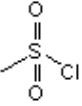
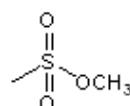
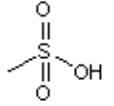
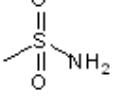
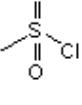
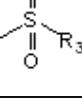
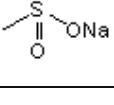
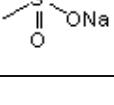
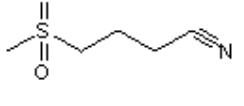


A similar range of values is noted for the ipso carbon chemical shifts of aromatic  $-\text{SO}_2-$  compounds as shown in the following tables.

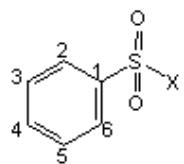
## Alkyl Chemical Shifts



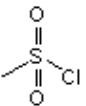
C-6	C-5	C-4	C-3	C-2	C-1	Compound	Solvent
					37.0	$\begin{array}{c} \text{O} \\ \parallel \\ \text{S} \\ \parallel \\ \text{O} \\ \text{OR}'_4 \end{array}$	$\text{CDCl}_3$
					37.5	$\begin{array}{c} \text{O} \\ \parallel \\ \text{S} \\ \parallel \\ \text{O} \\ \text{F} \end{array}$	$\text{CDCl}_3$
					43.1	$\begin{array}{c} \text{O} \\ \parallel \\ \text{S} \\ \parallel \\ \text{O} \\ \text{NH}_2 \end{array}$	Polysol

					44.3		CDCl <sub>3</sub>
					52.6		CDCl <sub>3</sub>
				0.81	44.1		CDCl <sub>3</sub>
				0.81	46.7		CDCl <sub>3</sub>
				0.84	49.1		Polysol
				0.92	60.3		CDCl <sub>3</sub>
			13.2	15.9	54.4		CDCl <sub>3</sub>
	14.2	22.6	31.1	24.6	51.9		D <sub>2</sub> O
R6-	30.5	29.5	25.2	30.1	52.1		D <sub>2</sub> O
R7-	29.5	29.2	28.4	22.0	53.6		CDCl <sub>3</sub>

## Phenyl Group Chemical Shifts



C-4	C-3,5	C-2,6	C-1	$-\text{SO}_2\text{-X}$	Solvent
135.9	130.0	128.5	133.3		$\text{CDCl}_3$
134.1	128.0	129.5	135.2		$\text{CDCl}_3$
133.0	128.3	128.7	137.3		Polysol
133.6	129.3	127.2	140.6		$\text{CDCl}_3$
133.2	129.3	127.6	141.6		$\text{CDCl}_3$
131.9	128.7	125.7	143.5		Polysol
132.2	129.8	126.3	143.7		$\text{H}_2\text{O}$
130.6	128.5	125.7	144.1		Polysol

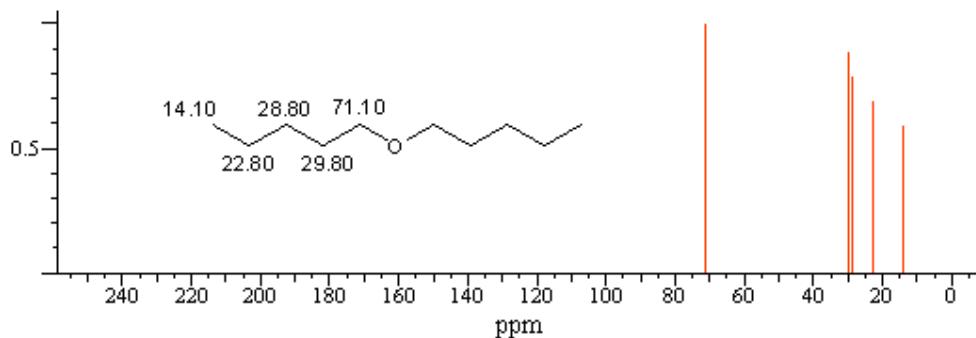
135.5	129.8	126.8	144.2		CDCl <sub>3</sub>
-------	-------	-------	-------	---	-------------------

## VII. Oxygen Containing Compounds (Except -C(=O)-)

### A. Ethers

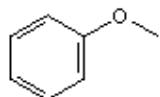
#### 1. Aliphatic Ethers (R-O-R)

#### Aliphatics



This section deals with the carbon-13 NMR chemical shifts of aliphatic ethers.

The very strong deshielding effect of the oxygen linkage of the ethers is second only to that of fluorine in the chemical shifts observed for adjacent carbon nuclei. The aliphatic additivity constants for several ether groups are:



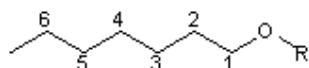
C1 = + 53.8, C2 = + 6.3, C3 = - 6.1, C4 = 0.0 ppm

R10-O

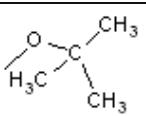
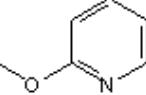
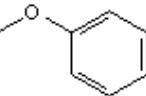
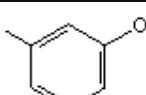
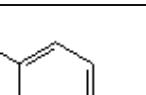
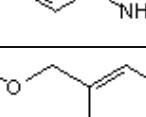
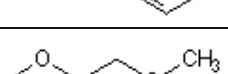
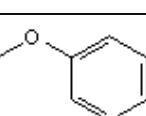
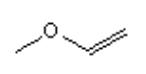
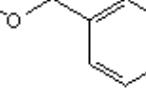
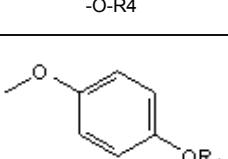
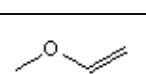
C1 = + 57.0, C2 = + 7.3, C3 = - 5.6, C4 = - 0.3 ppm

The tables presented below illustrate representative chemical shifts for a variety of selected spectra of ethers.

#### Alkyl Chemical Shifts

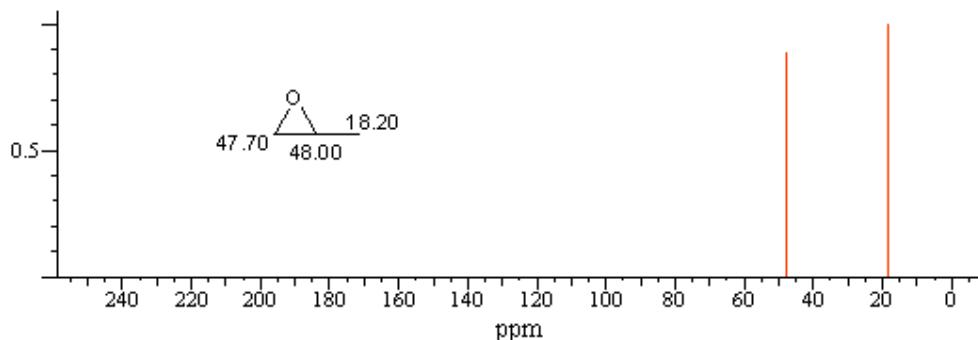


C-6	C-5	C-4	C-3	C-2	C-1	Compound	Solvent
-----	-----	-----	-----	-----	-----	----------	---------

					49.4		CDCl <sub>3</sub>
					53.1		CDCl <sub>3</sub>
					54.8		CDCl <sub>3</sub>
					55.1		CDCl <sub>3</sub>
					55.8		CDCl <sub>3</sub>
					57.8		CDCl <sub>3</sub>
					58.8		CDCl <sub>3</sub>
				14.9	63.2		CDCl <sub>3</sub>
				14.6	63.6		CDCl <sub>3</sub>
				15.2	65.7		CDCl <sub>3</sub>
				15.3	66.2	-O-R4	CDCl <sub>3</sub>
		13.9	19.4	31.8	68.3		CDCl <sub>3</sub>
		13.9	19.5	31.5	67.9		CDCl <sub>3</sub>
		14.0	19.7	32.3	70.6	-O-R2	CDCl <sub>3</sub>
		14.0	19.7	32.2	72.9	-O-CH <sub>3</sub>	CDCl <sub>3</sub>
	14.1	22.8	28.8	29.8	71.1	-O-R5	CDCl <sub>3</sub>
14.1	22.9	32.0	26.1	30.0	71.1	-O-R6	CDCl <sub>3</sub>
R5	29.8	29.8	26.5	30.1	71.1	-O-R10	CDCl <sub>3</sub>

## 2 □ [Alicyclic Ethers](#)

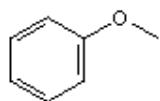
### Alicyclics



This section deals with the carbon-13 NMR chemical shifts of alicyclic ethers.

The very strong deshielding effect of the oxygen linkage of the ethers is second only to that of fluorine in the chemical shifts observed for adjacent carbon nuclei.

The aliphatic additivity constants for several ether groups are:



C1 = + 53.8, C2 = + 6.3, C3 = - 6.1, C4 = 0.0 ppm

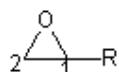
R10-O

C1 = + 57.0, C2 = + 7.3, C3 = - 5.6, C4 = - 0.3 ppm

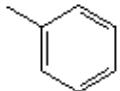
---

### Alicyclic Ethers

#### 1,2-Epoxides

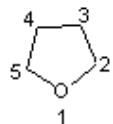


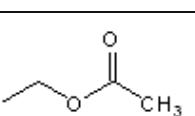
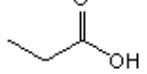
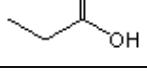
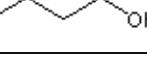
C-2	C-1	-R	Solvent
47.7	48.0	-CH <sub>3</sub>	CDCl <sub>3</sub>
44.4	50.1		CDCl <sub>3</sub>
44.1	50.8		CDCl <sub>3</sub>

50.8	52.0		CDCl <sub>3</sub>
46.5	53.2		CDCl <sub>3</sub>

---

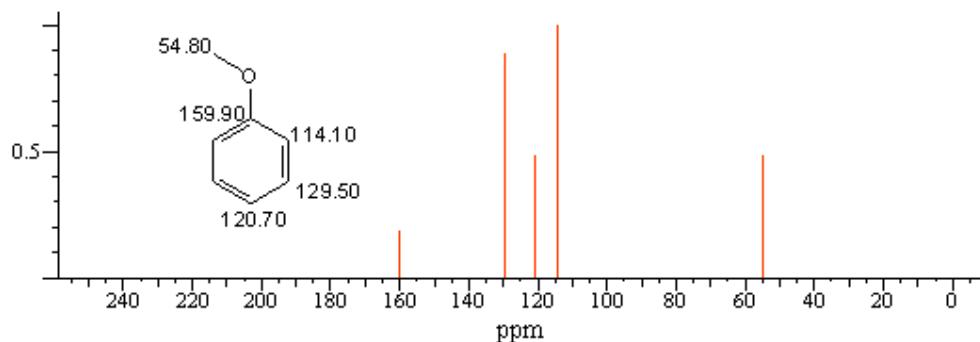
### Tetrahydrofurans



C-5	C-4	C-3	C-2	-R	Solvent
68.0	26.0	26.0	68.0		CDCl <sub>3</sub>
68.2	25.8	28.3	66.5		CDCl <sub>3</sub>
67.7	26.2	33.5	75.3		CDCl <sub>3</sub>
67.8	25.2	31.2	75.4		CDCl <sub>3</sub>
67.6	25.8	32.2	79.4		CDCl <sub>3</sub>

### 3 □ [Aromatic Ethers](#)

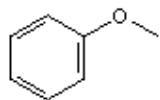
### Aromatics



This section deals with the carbon-13 NMR chemical shifts of aromatic ethers.

The very strong deshielding effect of the oxygen linkage of the ethers is second only to that of fluorine in the chemical shifts observed for adjacent carbon nuclei.

The aromatic additivity constants for certain ethers are:



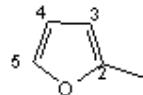
C1 = + 29.0, C2, 6 = - 9.5, C3, 5 = + 1.3, C4 = - 5.3ppm

R2-O- C1= + 30.9, C2, 6 =-13.8, C3, 5=+1.1, C4 = - 7.8ppm

---

## Aromatic Chemical Shifts

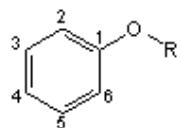
### Furan and 2-Substituted Derivatives



C-5	C-4	C-3	C-2	-R	Solvent
142.8	109.7	109.7	142.8		CDCl <sub>3</sub>
148.0	111.9	122.5	126.5	-C≡N	CDCl <sub>3</sub>
146.7	112.0	118.1	145.0		CDCl <sub>3</sub>
146.5	112.1	118.0	145.3		Polysol
145.7	112.2	116.3	149.5		CDCl <sub>3</sub>
145.9	112.9	116.7	150.6		CDCl <sub>3</sub>
140.9	110.4	105.6	152.2	-CH <sub>3</sub>	CDCl <sub>3</sub>
142.3	110.3	107.7	154.4		CDCl <sub>3</sub>

141.5	110.2	104.8	157.4		CDCl <sub>3</sub>
-------	-------	-------	-------	--	-------------------

### Phenyl Ethers



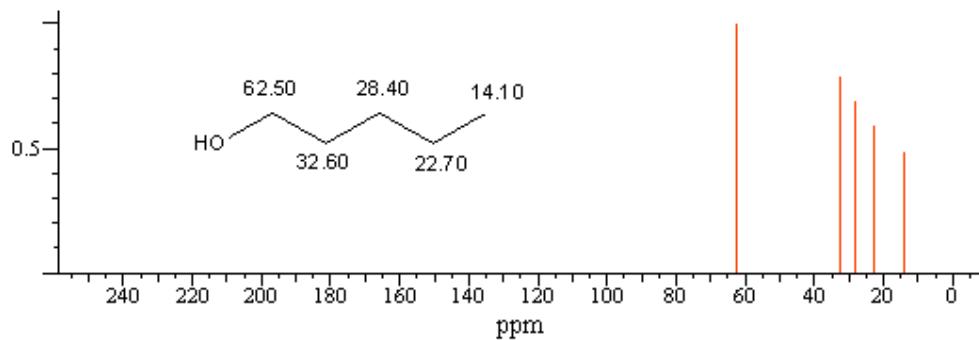
C-4	C-3	C-2	C-1	Compound	Solvent
122.1	129.4	116.2	157.1		CDCl <sub>3</sub>
123.1	129.7	118.9	157.4		CDCl <sub>3</sub>
122.0	129.5	117.2	158.9		CDCl <sub>3</sub>
120.6	129.5	114.6	159.3	-O-R2	CDCl <sub>3</sub>
120.7	129.5	114.1	159.9	-O-CH <sub>3</sub>	CDCl <sub>3</sub>

### B □ Alcohols (R-OH)

#### 1. Primary

##### a. Aliphatic and Alicyclic

### Aliphatics and Alicyclics



This section contains the carbon-13 NMR chemical shifts of the primary alcohols. The -OH group produces a strongly deshielded chemical shift for the adjacent carbon of both aliphatic and aromatic compounds.

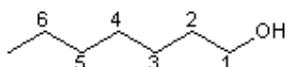
The aliphatic additivity constants are:

HO- C1 = + 48.4, C2 = + 10.1, C3 = - 6.0, C4 = 0.0 ppm

The tables that are provided below illustrate typical chemical shifts observed for a variety of selected compounds containing the -OH group.

---

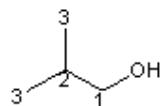
### Alkyl Chemical Shifts



C-6	C-5	C-4	C-3	C-2	C-1	-OH	Solvent
					49.8	-OH	CDCl <sub>3</sub>
				18.2	57.7	-OH	CDCl <sub>3</sub>
			10.3	25.9	64.2	-OH	CDCl <sub>3</sub>
		13.9	19.2	35.0	62.2	-OH	CDCl <sub>3</sub>
	14.1	22.7	28.4	32.6	62.5	-OH	CDCl <sub>3</sub>
R7-	29.9	29.5	26.1	32.9	62.5	-OH	CDCl <sub>3</sub>

---

### Isobutanol

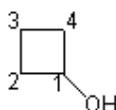


C-3	C-2	C-1	-OH	Solvent
19.1	30.9	69.4	-OH	CDCl <sub>3</sub>

---

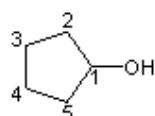
### Alicyclic Alcohols

### Cyclobutanol



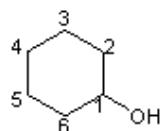
C-3	C-2,4	C-1	-OH	Solvent
12.1	33.4	67.0	-OH	CDCl <sub>3</sub>

### Cyclopentanol



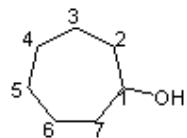
C-3,4	C-2,5	C-1	-OH	Solvent
23.5	35.4	73.6	-OH	CDCl <sub>3</sub>

### Cyclohexanol



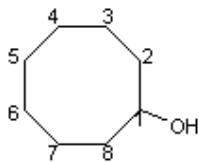
C-4	C-3,5	C-2,6	C-1	-OH	Solvent
25.9	24.5	35.5	70.1	-OH	CDCl <sub>3</sub>

### Cycloheptanol



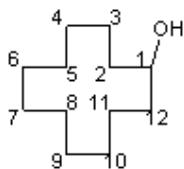
C-4,5	C-3,6	C-2,7	C-1	-OH	Solvent
28.3	22.9	37.6	72.5	-OH	CDCl <sub>3</sub>

### Cyclooctanol



C-5	C-4,6	C-3,7	C-2,8	C-1	-OH	Solvent
25.4	27.6	22.9	34.8	72.0	-OH	CDCl <sub>3</sub>

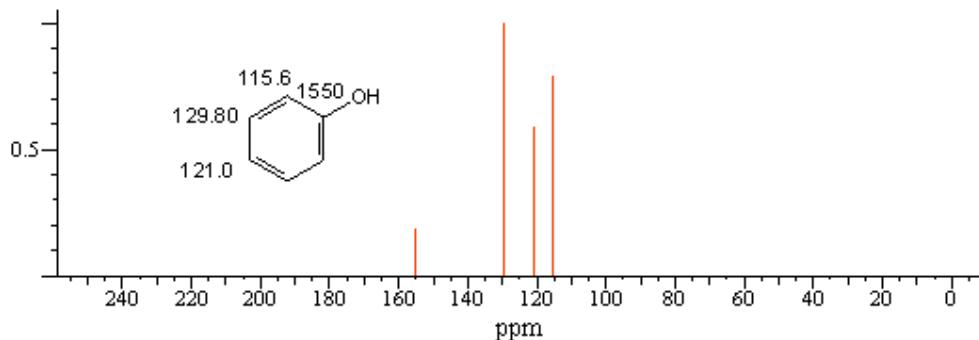
### Cyclododecanol



C-6,7,8	C-5,9	C-4,10	C-3,11	C-2,12	C-1	-OH	Solvent
23.5	24.4	24.0	21.0	32.5	69.1	-OH	CDCl <sub>3</sub>

b□[Aromatic](#)

### Aromatics



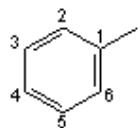
This section contains the carbon-13 NMR chemical shifts of the phenols. The -OH group produces a strongly deshielded chemical shift for the adjacent carbon of both aliphatic and aromatic compounds.

The aromatic additivity constants are:

HO- C1= + 26.6, C2, 6 = -12.8, C3, 5 = + 1.4, C4 = -7.3 ppm

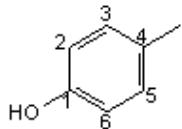
The tables that are provided below illustrate typical chemical shifts observed for a variety of selected compounds containing the -OH group.

## Aromatic Alcohols

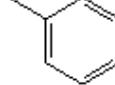
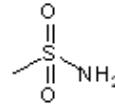
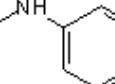
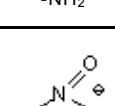
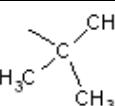


C-4	C-3,5	C-2,6	C-1	-R	Solvent
128.7	128.5	126.4	136.8	-OH	CDCl <sub>3</sub>
126.2	130.5	127.9	138.2	-OH	CDCl <sub>3</sub>
127.2	128.3	126.9	141.0	-OH	CDCl <sub>3</sub>
127.2	128.2	126.5	143.8	-OH	CDCl <sub>3</sub>
127.1	128.3	125.5	146.1	-OH	CDCl <sub>3</sub>
121.1	129.8	115.6	155.0	-OH	CDCl <sub>3</sub>

## 4-Substituted Phenols



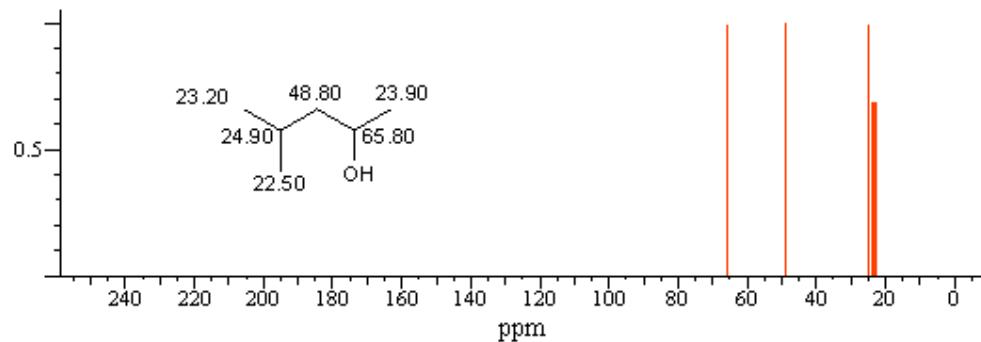
HO-	C-1	C-2,6	C-3,5	C-4	-X	Solvent
HO-	157.1	118.1	137.7	80.4	-I	Polysol
HO-	161.4	116.5	134.0	101.9	-C≡N	Polysol
HO-	153.9	117.2	132.5	113.2	-Br	CDCl <sub>3</sub>
HO-	161.8	115.4	132.1	121.3		Polysol
HO-	153.6	116.9	129.7	126.2	-Cl	CDCl <sub>3</sub>
HO-	155.6	116.3	130.4	127.2	-S-CH <sub>3</sub>	Polysol
HO-	162.2	115.4	130.8	129.0		Polysol
HO-	153.1	115.6	130.2	130.2	-CH <sub>3</sub>	CDCl <sub>3</sub>

HO-	157.2	115.9	127.8	131.7		CDCl <sub>3</sub>
HO-	160.6	115.4	128.0	133.9		Polysol
HO-	152.3	114.6	121.8	134.5		Polysol
HO-	149.1	115.9	115.7	139.6	-NH <sub>2</sub>	Polysol
HO-	164.5	116.3	126.6	140.9		Polysol
HO-	154.7	114.9	125.9	141.6		Polysol
HO-	151.1	116.6	116.3	157.7	-F	Polysol

2□Secondary

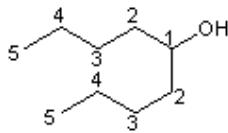
a. [Aliphatic and Alicyclic](#)

## Secondary Alcohols



The -OH group produces a strongly deshielded chemical shift for the adjacent carbon of both aliphatic and aromatic compounds.

### 5-Nonanol

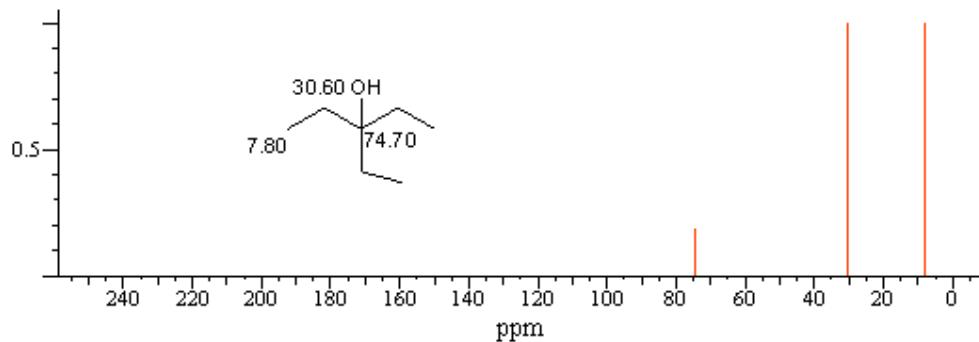


C-5	C-4	C-3	C-2	C-1	-OH	Solvent
14.1	23.0	28.2	37.4	71.8	-OH	CDCl <sub>3</sub>

3□Tertiary

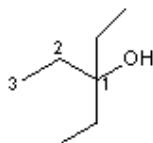
a. [Aliphatic](#)

## Tertiary Alcohols



The -OH group produces a strongly deshielded chemical shift for the adjacent carbon of both aliphatic and aromatic compounds.

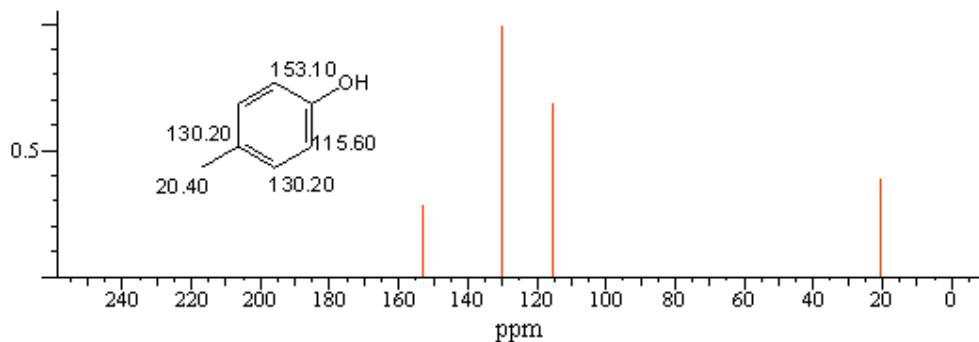
### 3-Ethyl-2-Pentanol



C-3	C-2	C-1	-OH	Solvent
7.8	30.6	74.7	-OH	CDCl <sub>3</sub>

4□[Phenols](#)

## Phenols



This section contains the carbon-13 NMR chemical shifts of the phenols. The -OH group produces a strongly deshielded chemical shift for the adjacent carbon of both aliphatic and aromatic compounds. The aliphatic additivity constants are:

HO- C1 = + 48.4, C2 = + 10.1, C3 = - 6.0, C4 = 0.0 ppm

The aromatic additivity constants are:

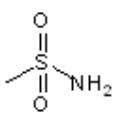
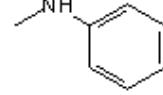
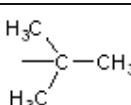
HO- C1 = + 26.6, C2, 6 = -12.8, C3, 5 = + 1.4, C4 = -7.3 ppm

The tables that are provided below illustrate typical chemical shifts observed for a variety of selected compounds containing the -OH group.

---

#### 4-Substituted Phenols

HO-	C-1	C-2,6	C-3,5	C-4	-X	Solvent
HO-	157.1	118.1	137.7	80.4	-I	Polysol
HO-	161.4	116.5	134.0	101.9	-C≡N	Polysol
HO-	153.9	117.2	132.5	113.2	-Br	CDCl <sub>3</sub>
HO-	161.8	115.4	132.1	121.3		Polysol
HO-	153.6	116.9	129.7	126.2	-Cl	CDCl <sub>3</sub>
HO-	155.6	116.3	130.4	127.2	-S-CH <sub>3</sub>	Polysol
HO-	162.2	115.4	130.8	129.0		Polysol
HO-	153.1	115.6	130.2	130.2	-CH <sub>3</sub>	CDCl <sub>3</sub>
HO-	157.2	115.9	127.8	131.7		CDCl <sub>3</sub>

HO-	160.6	115.4	128.0	133.9		Polysol
HO-	152.3	114.6	121.8	134.5		Polysol
HO-	149.1	115.9	115.7	139.6	-NH <sub>2</sub>	Polysol
HO-	164.5	116.3	126.6	140.9		Polysol
HO-	154.7	114.9	125.9	141.6		Polysol
HO-	151.1	116.6	116.3	157.7	-F	Polysol

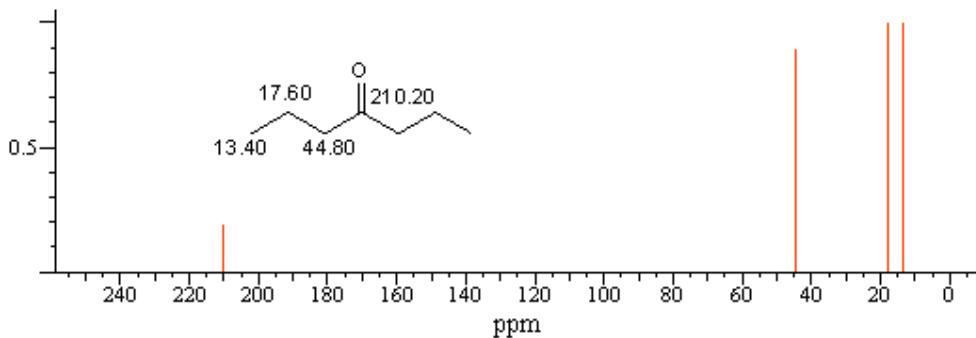
[The Sadler Handbook of Carbon NMR Spectra](#) □ 4 □

## VIII. Compounds Containing Carbon To Oxygen Double Bonds

### A. Ketones (R-C(=O)-R)

## 1. Aliphatic and Alicyclic

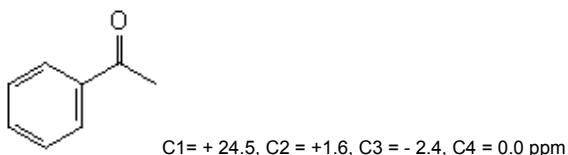
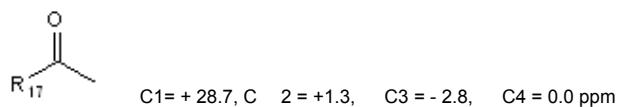
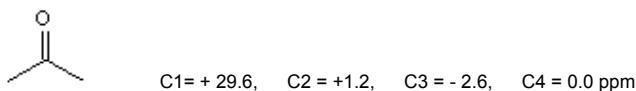
### Aliphatics



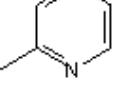
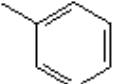
Depending upon their structural environment, the carbonyl (C=O) resonance appears over a chemical shift range of more than 48 ppm (167.8 - 216.7 ppm).

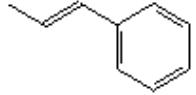
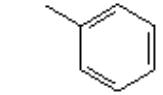
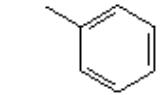
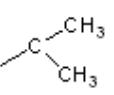
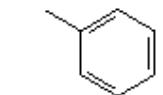
As a substituent, the ketone carbonyl group exerts a moderately strong deshielding effect on adjacent C-1 carbons.

The aliphatic additivity constants are:



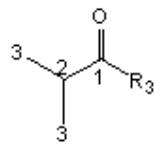
A selection of ketone chemical shifts is provided in the following tables.

C-5	C-4	C-3	C-2	C-1	-C(=O)	-R	Solvent
				25.5	199.6		CDCl <sub>3</sub>
				26.3	197.4		CDCl <sub>3</sub>

				27.4	197.6		CDCl <sub>3</sub>
				29.3	208.7		CDCl <sub>3</sub>
			8.2	31.7	200.1		CDCl <sub>3</sub>
			7.9	36.8	208.7	-CH <sub>3</sub>	CDCl <sub>3</sub>
		13.9	17.9	40.5	199.7		CDCl <sub>3</sub>
		13.8	17.4	42.3	213.5		CDCl <sub>3</sub>
		13.4	17.6	44.8	210.2	-R3	CDCl <sub>3</sub>
	13.9	22.5	26.5	38.2	199.7		CDCl <sub>3</sub>
	14.0	22.6	26.3	43.5	208.2	-CH <sub>3</sub>	CDCl <sub>3</sub>
14.0	22.7	31.7	23.8	42.7	210.3	-R5	CDCl <sub>3</sub>
R3-	29.5	29.3	24.1	42.8	210.5	-R7	CDCl <sub>3</sub>

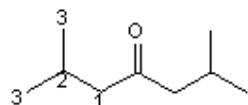
### Branched Alkyl Ketones

#### 2-Methyl-3-Hexanone



C-3	C-2	C-1	-R3	Solvent
18.3	40.8	213.5	-R3	CDCl <sub>3</sub>

#### 2,6-Dimethyl-4-Heptanone

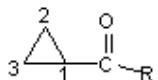


C-3	C-2	C-1	-R	Solvent
22.6	24.5	52.4	209.3	CDCl <sub>3</sub>

---

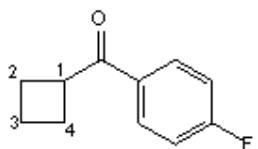
### Alicyclic Ketones

#### Cyclopropyl Ketones



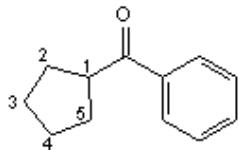
C-2,3	C-1	-C(=O)	-R	Solvent
11.2	16.8	199.8		CDCl <sub>3</sub>
11.6	17.0	200.4		CDCl <sub>3</sub>
10.3	21.1	208.0	-CH <sub>3</sub>	CDCl <sub>3</sub>

#### Cyclobutyl-4-Fluorophenyl Ketone



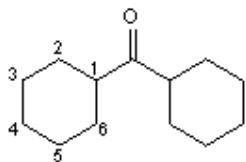
C-3	C-2,4	C-1	-R	Solvent
18.2	25.1	42.2	199.2	CDCl <sub>3</sub>

#### Cyclopentyl Phenyl Ketone



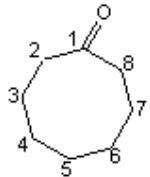
C-3,5	C-2,4	C-1	-R	Solvent
26.4	30.0	46.4	202.5	CDCl <sub>3</sub>

### Dicyclohexyl Ketone



C-4	C-3,5	C-2,6	C-1	-R	Solvent
26.2	25.9	28.8	49.2	215.7	CDCl <sub>3</sub>

### Cyclooctanone



C-5	C-4,6	C-3,7	C-2,8	-C=O	Solvent
24.9	27.3	25.8	41.9	216.7	CDCl <sub>3</sub>

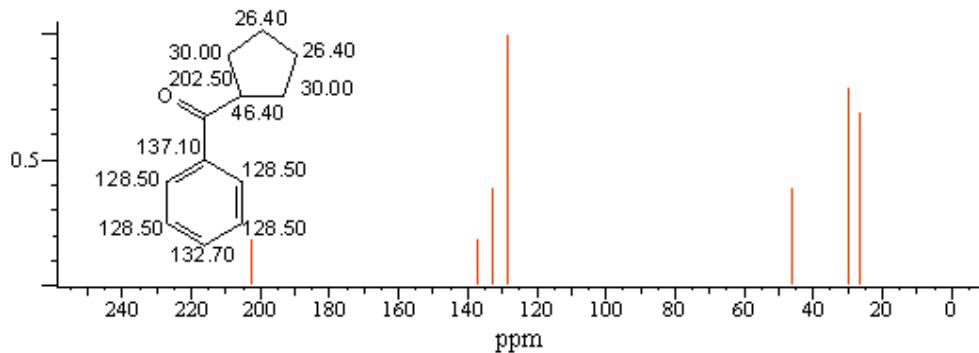
### Carbonyl Chemical Shifts

R-	-C(=O)	-R	Solvent
	167.8	-C≡N	CDCl <sub>3</sub>

	180.8	-CF <sub>3</sub>	CDCl <sub>3</sub>
	183.8		CDCl <sub>3</sub>
	194.5		Polysol
C5-	199.2		CDCl <sub>3</sub>
CH <sub>3</sub> -	199.6		CDCl <sub>3</sub>
	199.7	-R3	CDCl <sub>3</sub>
	202.5	-C5	CDCl <sub>3</sub>
CH <sub>3</sub> -	208.2	-R4	CDCl <sub>3</sub>
R3-	210.2	-R3	CDCl <sub>3</sub>
R7-	210.5	-R7	CDCl <sub>3</sub>
C6-	215.7	-C6	CDCl <sub>3</sub>
	216.7		CDCl <sub>3</sub>

2□[Aromatic](#)

## Aromatics

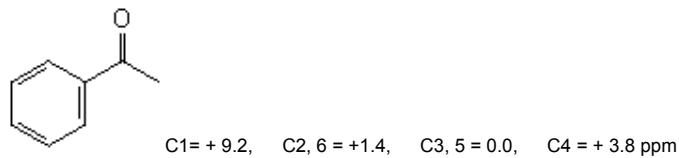


The carbon-13 NMR chemical shifts presented here illustrate typical band intensities of the aromatic ketones. Depending upon their structural environment, the carbonyl ( $\text{C}=\text{O}$ ) resonance appears over a chemical shift range of more than 48 ppm (167.8 - 216.7 ppm).

As a substituent, the ketone carbonyl group exerts a moderately strong deshielding effect on adjacent C-1 carbons.

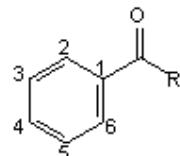
The aromatic additivity constants are:

$\text{R}_4\text{-C}(=\text{O})-$      $\text{C}_1 = +8.9$ ,     $\text{C}_{2,6} = -0.4$ ,     $\text{C}_{3,5} = 0.0$ ,     $\text{C}_4 = +4.3$  ppm

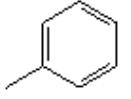
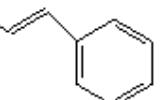


A selection of ketone chemical shifts is provided in the following tables.

### Phenyl Ketones

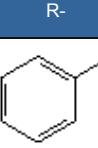
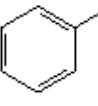
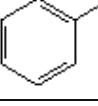
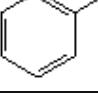
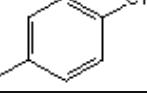
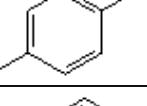
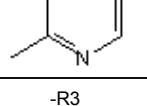
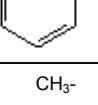


C-4	C-3,5	C-2,6	C-1	$-\text{C}(=\text{O})$	-R	Solvent
132.6	127.6	126.9	129.4	183.8	$-\text{CHCl}_2$	$\text{CDCl}_3$
135.8	129.5	130.4	130.4	180.8	$-\text{CF}_3$	$\text{CDCl}_3$
136.9	129.6	130.3	133.4	167.8	$-\text{C}\equiv\text{N}$	$\text{CDCl}_3$
132.7	128.5	129.6	137.0	194.5		Polysol
132.7	128.5	128.5	137.1	202.5	$-\text{C}_5$	$\text{CDCl}_3$

132.7	128.5	128.0	137.3	199.7	-R4	CDCl <sub>3</sub>
132.2	128.2	129.8	137.6	196.1		CDCl <sub>3</sub>
132.5	128.4	128.4	138.2	189.9		CDCl <sub>3</sub>

---

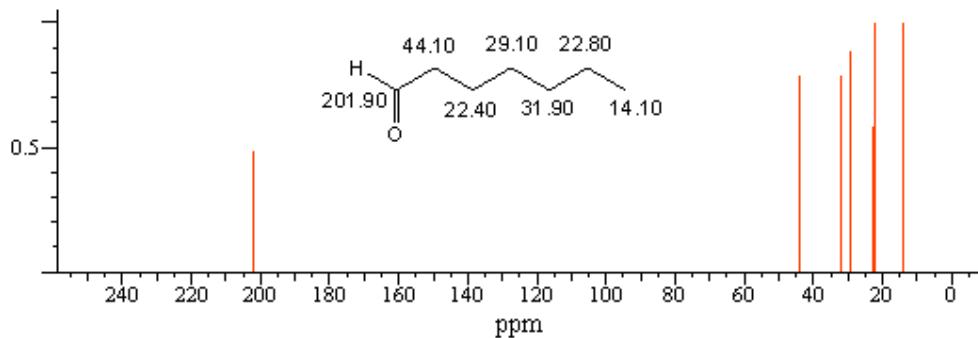
### Carbonyl Chemical Shifts

R-	-C(=O)	-R	Solvent
	167.8	-C≡N	CDCl <sub>3</sub>
	180.8	-CF <sub>3</sub>	CDCl <sub>3</sub>
	183.8	-CHCl <sub>2</sub>	CDCl <sub>3</sub>
	194.5		Polysol
C5-	199.2		CDCl <sub>3</sub>
CH <sub>3</sub> -	199.6		CDCl <sub>3</sub>
	199.7	-R3	CDCl <sub>3</sub>
	202.5	-C5	CDCl <sub>3</sub>
CH <sub>3</sub> -	208.2	-R4	CDCl <sub>3</sub>
R3-	210.2	-R3	CDCl <sub>3</sub>
R7-	210.5	-R7	CDCl <sub>3</sub>

C6-	215.7	-C6	$\text{CDCl}_3$
	216.7		$\text{CDCl}_3$

B □ [Aldehydes](#) ( $\text{R}-\text{C}(=\text{O})-\text{H}$ )

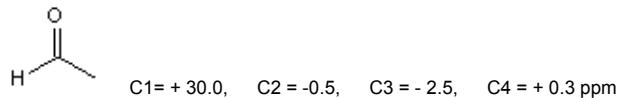
## Aldehydes



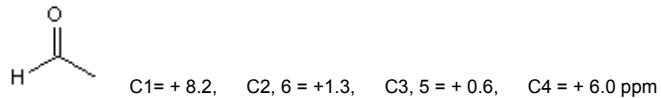
This section deals with the carbon-13 NMR chemical shifts of the carboxaldehydes.

The chemical shifts of adjacent carbon atoms indicate that the carboxaldehyde group exerts a weak to intermediate deshielding effect on both aliphatic and aromatic carbons.

The aliphatic additivity constants are:

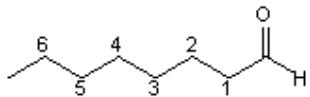


The phenyl additivity constants are:



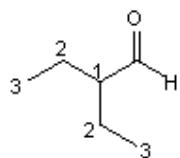
The tables presented below contain the chemical shifts for a variety of carboxaldehyde compounds.

## N-Alkyl Chemical Shifts



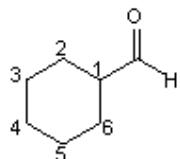
C-6	C-5	C-4	C-3	C-2	C-1	-C(=O)-H	Solvent
		13.8	22.5	24.5	43.7	202.0	CDCl <sub>3</sub>
14.1	22.8	31.9	29.1	22.4	44.1	201.9	CDCl <sub>3</sub>
R6-	29.8	29.8	29.6	22.3	44.1	201.9	CDCl <sub>3</sub>

### 2-Ethylbutyraldehyde



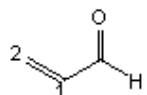
C-3	C-2	C-1	-C(=O)-H	Solvent
11.5	21.7	55.2	204.7	CDCl <sub>3</sub>

### Cyclohexanecarboxaldehyde



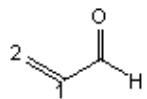
C-4	C-3,5	C-2,6	C-1	-C(=O)-H	Solvent
26.1	25.1	26.1	50.0	204.5	CDCl <sub>3</sub>

### Alkenyl Aldehyde Chemical Shifts

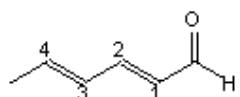


C-2	C-1	-C(=O)-H	Solvent

137.8	138.6	194.4	$\text{CDCl}_3$
-------	-------	-------	-----------------



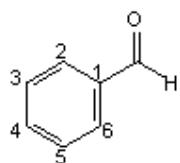
C-3	C-2	C-1	$-\text{C}(=\text{O})-\text{H}$	Solvent
R3-	158.2	133.3	193.5	$\text{CDCl}_3$
	152.3	131.1	193.2	$\text{CDCl}_3$
	148.8	131.8	192.8	$\text{CDCl}_3$



R-	C-4	C-3	C-2	C-1	$-\text{C}(=\text{O})-\text{H}$	Solvent
R2-	148.4	127.9	152.7	130.3	193.4	$\text{CDCl}_3$
R3-	146.7	129.0	152.5	130.2	193.2	$\text{CDCl}_3$
R4-	147.0	128.8	152.5	130.2	193.2	$\text{CDCl}_3$

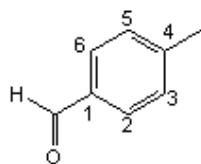
### Aromatic Aldehydes

Benzaldehyde



C-4	C-3,5	C-2,6	C-1	$-\text{C}(=\text{O})-\text{H}$	Solvent
134.4	129.0	129.7	136.6	192.0	$\text{CDCl}_3$

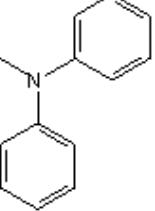
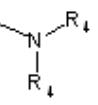
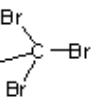
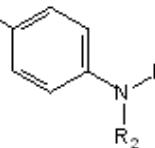
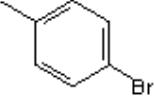
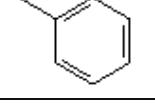
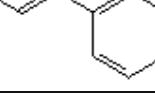
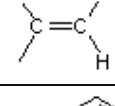
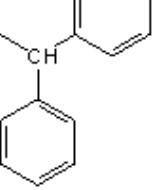
### 4-Substituted Benzaldehydes



H-C(=O)	C-1	C-2,6	C-3,5	C-4	-X	Solvent
189.2	124.9	132.0	110.7	152.2		CDCl3
189.5	125.2	131.6	111.0	154.2		CDCl3
190.8	128.7	132.2	116.1	163.5	-OH	Polysol
190.5	130.2	131.9	114.5	164.6	-O-CH3	CDCl3
191.4	134.4	129.6	129.6	145.3	-CH3	CDCl3
191.3	134.9	129.9	127.1	155.9		CDCl3
190.5	134.9	130.8	129.4	140.7	-Cl	CDCl3
190.6	135.2	130.8	132.3	129.4	-Br	CDCl3
191.3	135.2	130.0	127.3	146.6		CDCl3

### Aldehydic Carbons

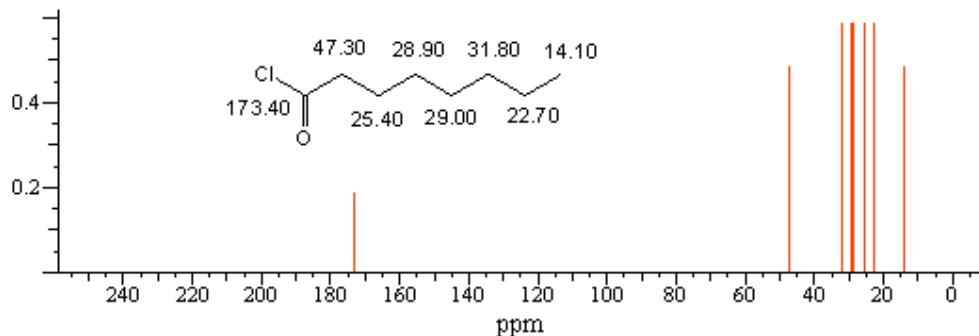
H-C(=O)	-X	Solvent
160.1		CDCl3
161.0	-O-R4	CDCl3

161.6		CDCl <sub>3</sub>
161.9	-NH-CH <sub>2</sub> CH <sub>3</sub>	CDCl <sub>3</sub>
162.5		CDCl <sub>3</sub>
163.2	-NH-CH <sub>3</sub>	CDCl <sub>3</sub>
175.9		CDCl <sub>3</sub>
178.9		CDCl <sub>3</sub>
189.2		CDCl <sub>3</sub>
190.6		CDCl <sub>3</sub>
192.0		CDCl <sub>3</sub>
193.2		CDCl <sub>3</sub>
194.4		CDCl <sub>3</sub>
198.2		CDCl <sub>3</sub>
201.9	-R11	CDCl <sub>3</sub>
204.5	-C6	CDCl <sub>3</sub>

204.7		CDCl <sub>3</sub>
-------	---	-------------------

C  [Acid Halides](#) (R-C(=O)-X)

## Acid Halides

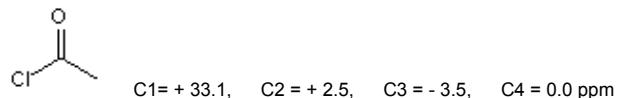


This section contains carbon-13 NMR chemical shifts which are representative for this class of compounds. Although most of the chemical shifts available are of acid chlorides, the chemical shifts observed for several acid bromides indicate that the C(=O)-Br group has a more strongly deshielding effect on adjacent aliphatic groups than does the C(=O)-Cl group.

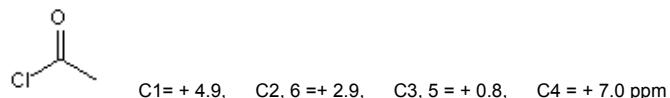
All members of this class react rapidly with traces of moisture to form the corresponding carboxylic acids.

Additivity constants for the acid chloride group are given below.

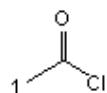
The aliphatic additivity constants are:



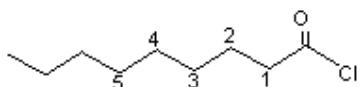
The aromatic additivity constants are:



## Alkyl Chemical Shifts



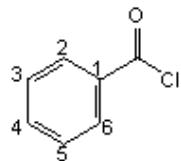
C-1	-X	Solvent
33.7		CDCl <sub>3</sub>
39.1		CDCl <sub>3</sub>



R	C-5	C-4	C-3	C-2	C-1	-X	Solvent
R2-	31.8	29.0	28.7	25.4	47.3		CDCl <sub>3</sub>
R4-	29.4	29.4	28.7	25.4	47.2		CDCl <sub>3</sub>
R7-	29.6	29.3	28.6	25.3	47.2		CDCl <sub>3</sub>

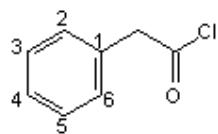
### Aromatic Chemical Shifts

#### Benzoyl Chloride



C-4	C-3,5	C-2,6	C-1	-C(=O)-Cl	Solvent
135.4	129.2	131.3	133.3	168.0	CDCl <sub>3</sub>

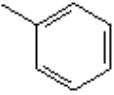
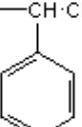
#### Phenyl Acetyl Chlorides



C-4	C-3,5	C-2,6	C-1	-R	Solvent
128.1	128.9	129.5	131.4		CDCl3
130.2	128.4	129.3	133.2		CDCl3
128.3	129.1	128.3	136.0		CDCl3
126.7	128.4	128.2	139.4		Polysol

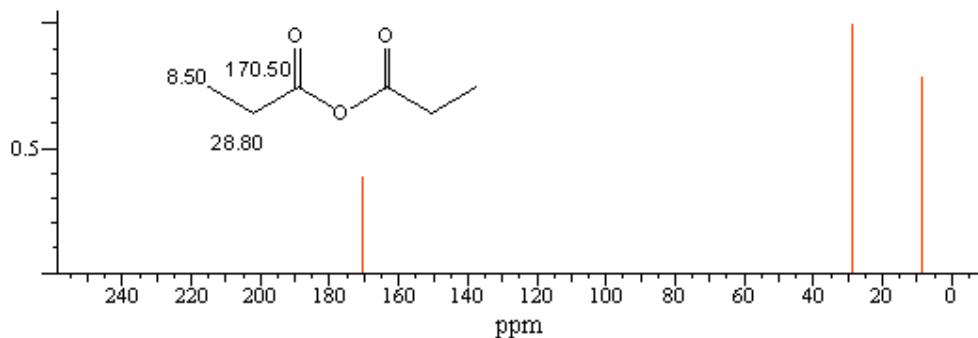
### Carbonyl Halide Chemical Shifts

X-	C(=O)	-R	Solvent
Br-	165.3	-CH3	CDCl3
Cl-	167.1		CDCl3
Cl-	167.1		CDCl3
Cl-	167.7		CDCl3

Cl-	168.0		CDCl <sub>3</sub>
Cl-	168.9		CDCl <sub>3</sub>
Cl-	170.3	-CH <sub>3</sub>	CDCl <sub>3</sub>
Cl-	173.2	-R12	CDCl <sub>3</sub>
Cl-	173.4	-R7	CDCl <sub>3</sub>

D □ [Anhydrides](#) (R-C(=O)-O-C(=O)-R)

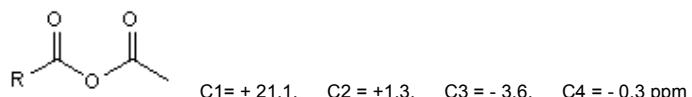
## Anhydrides



This section deals with the chemical shifts of the carboxylic anhydrides. As a group, the anhydrides are very reactive and readily decompose to the corresponding carboxylic acid in the presence of the traces of water found in DMSO-d<sub>6</sub>, polysol and acetone-d<sub>6</sub>. In general, the carbonyl chemical shift of the anhydride resonates at a higher field than that of the carboxylic acid.

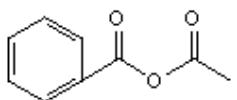
The deshielding effect of the anhydride group in relation to adjacent aliphatic carbons is that of a weakly deshielding substituent.

The aliphatic additivity constants are:



The anhydride group exerts an intermediate additivity effect on the C1 carbon of phenyl ring carbons as indicated below.

The aromatic additivity constants are:

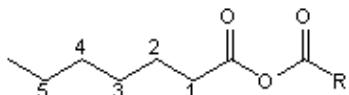


C1 = + 6.1, C2,6 = + 2.1, C3, 5 = + 0.5, C4 = + 6.1 ppm

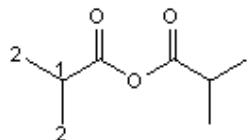
The chemical shifts of a selection of anhydride molecules are presented in the tables which follow.

---

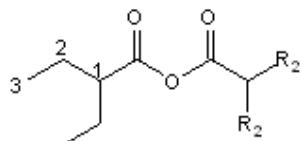
### Alkyl Anhydrides



C-5	C-4	C-3	C-2	C-1	$-\text{C}(=\text{O})\text{-O-C}(=\text{O})\text{-R}$	Solvent
				21.9	166.9	$\text{CDCl}_3$
			8.5	28.8	170.5	$\text{CDCl}_3$
13.9	22.5	31.2	24.1	35.3	169.6	$\text{CDCl}_3$



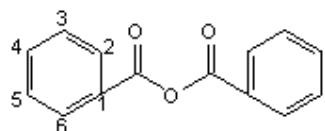
C-2	C-1	$-\text{C}(=\text{O})\text{-O-C}(=\text{O})\text{-CH}(\text{CH}_3)_2$	Solvent
18.3	35.2	172.7	$\text{CDCl}_3$



C-3	C-2	C-1	$-\text{C}(=\text{O})\text{-O-C}(=\text{O})\text{-CH(R2)}_2$	Solvent
11.5	24.6	49.9	171.6	$\text{CDCl}_3$

---

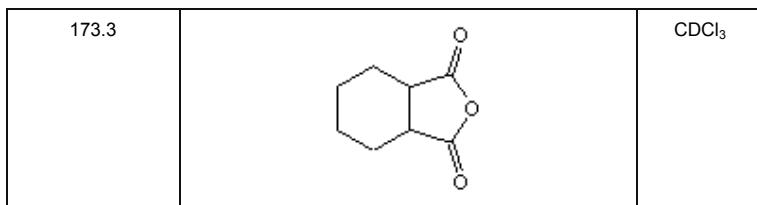
### Benzoic Anhydride



C-4	C-3,5	C-2,6	C-1	$-\text{C}(=\text{O})\text{-O-C}(=\text{O})\text{-R}$	Solvent
134.5	128.9	130.5	134.5	162.3	$\text{CDCl}_3$

### Carbonyl Chemical Shifts

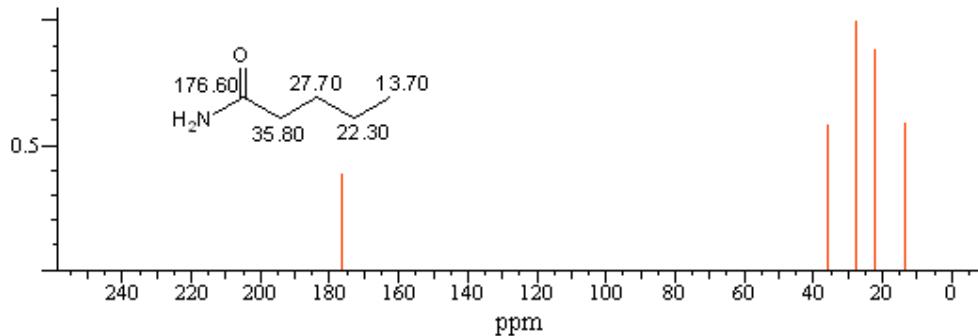
R-C(=O)-O-C(=O)	Compound	Solvent
161.8		$\text{CDCl}_3$
166.3		$\text{CDCl}_3$
166.9		$\text{CDCl}_3$
167.1		$\text{CDCl}_3$
169.6		$\text{CDCl}_3$
170.5		$\text{CDCl}_3$
171.6		$\text{CDCl}_3$
171.7		$\text{CDCl}_3$



### E□Amides

1. [Primary](#) ( $\text{R}-\text{C}(=\text{O})-\text{NH}_2$ )

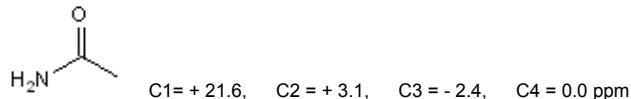
## Primary Amides



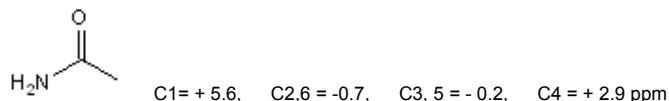
This section concerns itself with the carbon-13 NMR chemical shifts of compounds containing the primary amide group (- $\text{C}(=\text{O})-\text{NH}_2$ ).

The primary amide group exerts an intermediate deshielding effect on the adjacent aliphatic and aromatic carbons as shown by the additivity constants provided below.

The aliphatic additivity constants are:

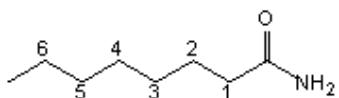


The phenyl additivity constants are:



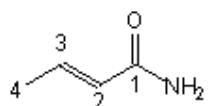
As indicated in the following chemical shift tables, the primary amide compounds are not readily soluble in  $\text{CDCl}_3$  and usually require the use of  $\text{DMSO-d}_6$  or  $\text{DMSO-d}_6/\text{CDCl}_3$  mixture (polysol) in order to obtain high quality carbon-13 spectra.

## Alkyl Chemical Shifts



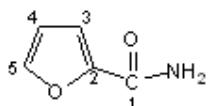
C-6	C-5	C-4	C-3	C-2	C-1	$-\text{C}(=\text{O})\text{-NH}_2$	Solvent
					22.3		Polysol
				9.7	29.0		$\text{CDCl}_3$
		13.7	22.3	27.7	35.8		$\text{CDCl}_3$
R3-	29.1	29.1	29.1	25.4	35.5		Polysol

## Crotonamide



C-4	C-3	C-2	C-1	$-\text{C}(=\text{O})\text{-NH}_2$	Solvent
17.3	138.2	126.1	167.2		Polysol

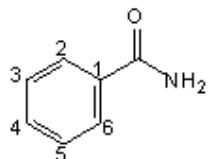
## 2-Furamide



C-5	C-4	C-3	C-2	-C(=O)-NH <sub>2</sub>	Solvent
144.6	111.7	113.9	148.0	160.1	Polysol

---

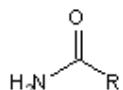
### Phenyl Amides



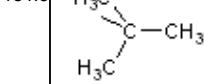
C-4	C-3,5	C-2,6	C-1	-X	Solvent
126.3	129.0	128.2	136.2		Polysol
131.3	128.2	127.7	134.0		Polysol

---

### Carbonyl Chemical Shifts

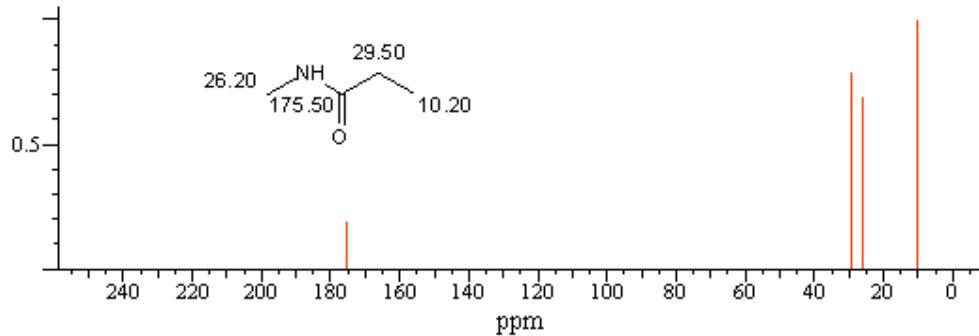


H <sub>2</sub> N-C(=O)	-R	Solvent
160.1		Polysol
167.2		Polysol
172.6	-CH <sub>3</sub>	Polysol
175.3	-R8	Polysol

176.5	-R6	CDCl <sub>3</sub>
177.5	-R2	CDCl <sub>3</sub>
181.3		Polysol

2□Secondary (R-C(=O)-NH-R)

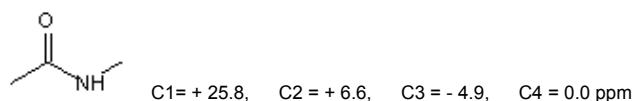
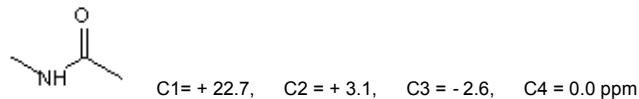
## Secondary Amides



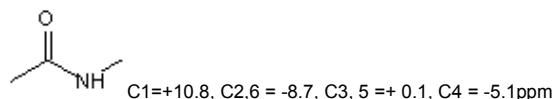
The data contained in this section deal with the N-substituted secondary amides (R-C(=O)-NH-R'). Due to the presence of the N-substituent, the range of chemical shifts is larger than that observed for the primary amides.

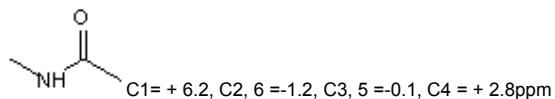
The additivity effect of either side of the -C(=O)-NH- group is that of an intermediate deshielding group as they also are with the adjacent carbons of phenyl groups.

The alkyl additivity constants are:



The phenyl additivity constants are:

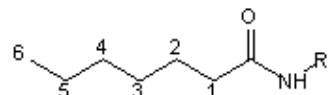




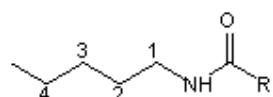
The tables provided below display the chemical shifts for a selection of secondary amide compounds.

---

### Alkyl Chemical Shifts



C-6	C-5	C-4	C-3	C-2	C-1	-NH-C(=O)-R	Solvent
					22.8		CDCl <sub>3</sub>
				10.2	29.5		CDCl <sub>3</sub>
				9.9	30.4		CDCl <sub>3</sub>
			13.7	19.1	39.1		Polysol
R12-	29.7	29.5	29.5	25.9	36.8		CDCl <sub>3</sub>

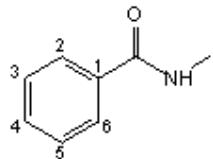


C-4	C-3	C-2	CH <sub>3</sub>	-NH-C(=O)-R	Solvent
			26.3		CDCl <sub>3</sub>

			26.7		CDCl <sub>3</sub>
		14.6	34.4		CDCl <sub>3</sub>
	11.5	23.0	41.4		CDCl <sub>3</sub>
13.6	20.3	31.6	39.6		CDCl <sub>3</sub>

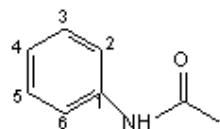
### Aromatic Chemical Shifts

#### N-Substituted Benzamides



C-4	C-3,5	C-2,6	C-1	-C(=O)-NH-R	Solvent
131.2	128.3	127.2	134.6		CDCl <sub>3</sub>
131.2	128.2	127.7	135.3		Polysol
130.9	128.3	126.8	136.0		CDCl <sub>3</sub>

#### N-Phenyl Amides



C-4	C-3,5	C-2,6	C-1	-NH-C(=O)-R	Solvent
125.1	128.9	118.7	137.0	(syn)	CDCl3
124.7	129.6	120.3	137.2	(anti)	CDCl3
124.2	128.8	120.5	138.4		CDCl3
123.3	128.5	119.7	139.2		Polysol
123.6	128.4	120.6	139.3		Polysol

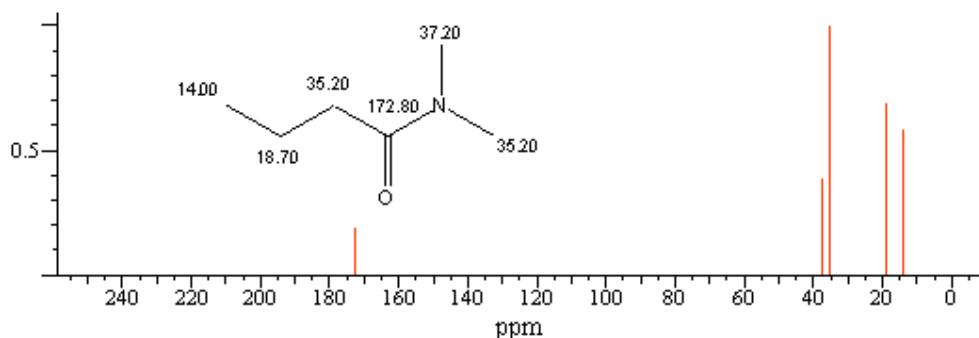
### Carbonyl Chemical Shifts

R-	C(=O)-NH	-R	Solvent
H-	160.1		CDCl3
	165.8		Polysol
	168.8	-CH3	CDCl3
CH3-	171.0	-R2	CDCl3
CH3-	171.2	-R4	CDCl3

R2-	173.3		CDCl <sub>3</sub>
R17-	174.0	-CH <sub>3</sub>	CDCl <sub>3</sub>

3□ **Tertiary** (R-C(=O)-N-R<sub>2</sub>)

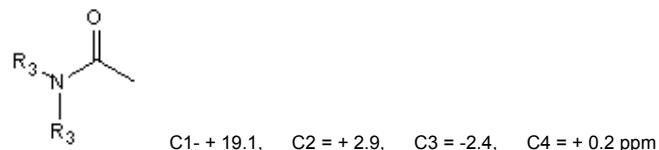
## Tertiary Amides



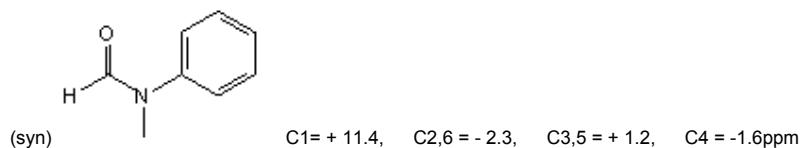
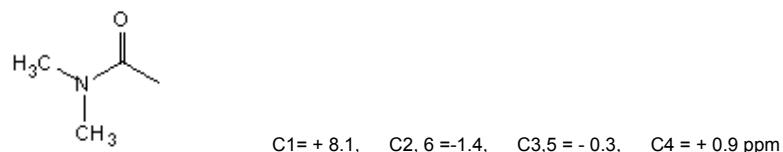
With a wider range of possible substituent combinations, the chemical shift ranges observed for the tertiary amides are generally larger than those of the secondary amides.

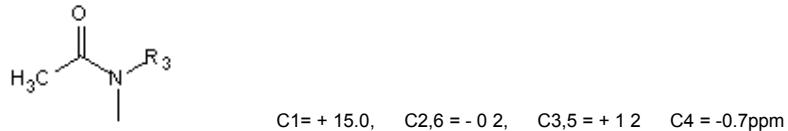
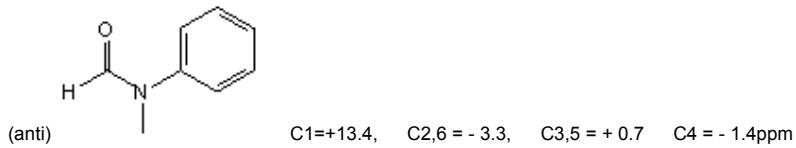
A selection of additivity constants for aliphatic and aromatic tertiary amides is provided below.

The aliphatic additivity constants are:



The aromatic additivity constants are:

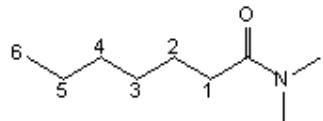




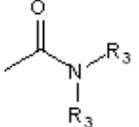
The following tables contain the chemical shifts from a selection of aliphatic and aromatic compounds.

---

### Alkyl Chemical Shifts

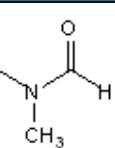
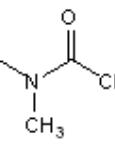
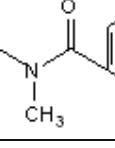
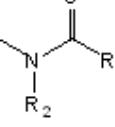
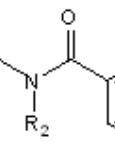
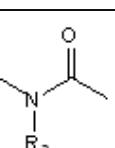
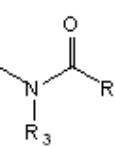


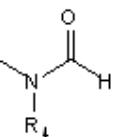
C-6	C-5	C-4	C-3	C-2	C-1	$-\text{C}(=\text{O})\text{-N}(\text{R},\text{R})$	Solvent
					21.4		CDCl <sub>3</sub>
					21.4		CDCl <sub>3</sub>
					22.6		CDCl <sub>3</sub>
				9.6	26.2		CDCl <sub>3</sub>
			14.0	18.7	35.2		CDCl <sub>3</sub>

R4-	29.7	29.7	29.7	25.7	33.2		CDCl <sub>3</sub>
-----	------	------	------	------	------	---	-------------------

---

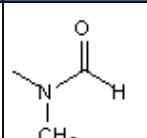
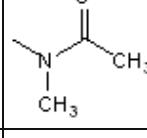
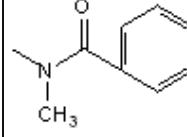
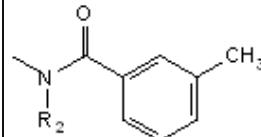
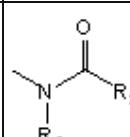
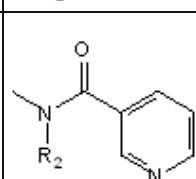
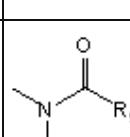
### Higher Field (syn) Isomers

C-4	C-3	C-2	C-1	-N(R)-C(=O)-R'	Solvent
			31.1		CDCl <sub>3</sub>
			34.8		CDCl <sub>3</sub>
			35.2		CDCl <sub>3</sub>
		13.2	40.2		CDCl <sub>3</sub>
		13.5	40.2		CDCl <sub>3</sub>
	11.2	21.0	47.4		CDCl <sub>3</sub>
	11.4	21.2	47.6		CDCl <sub>3</sub>

13.8	19.8	29.7	41.9		CDCl <sub>3</sub>
------	------	------	------	---	-------------------

---

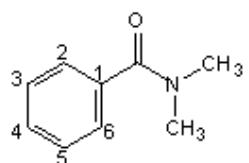
### Lower Field (anti) Isomers

C-4	C-3	C-2	C-1	-N(R)-C(=O)-R'	Solvent
			36.1		CDCl <sub>3</sub>
			37.9		CDCl <sub>3</sub>
			38.9		CDCl <sub>3</sub>
		13.5	41.0		CDCl <sub>3</sub>
		14.4	42.0		CDCl <sub>3</sub>
		13.5	42.5		CDCl <sub>3</sub>
	11.4	22.6	49.8		CDCl <sub>3</sub>

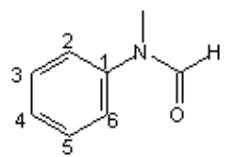
	11.2	22.2	50.6		CDCl3
13.8	20.3	31.1	47.1		CDCl3

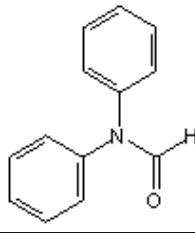
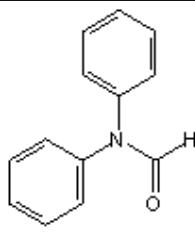
---

### Phenyl Chemical Shifts

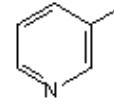


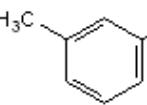
C-4	C-3,5	C-2,6	C-1	-C(=O)-N(R) <sub>2</sub>	Solvent
130.1	128.4	127.6	135.4		CDCl3
129.3	128.1	127.0	136.5		CDCl3
129.1	128.3	126.7	136.6		CDCl3



C-4	C-3,5	C-2,6	C-1	Compound	Solvent
126.8	129.6		126.1	 (syn)	CDCl <sub>3</sub>
127.0	129.1	125.1	141.8	 (anti)	CDCl <sub>3</sub>
127.7	129.6	128.2	143.4		CDCl <sub>3</sub>

### Carbonyl Chemical Shifts

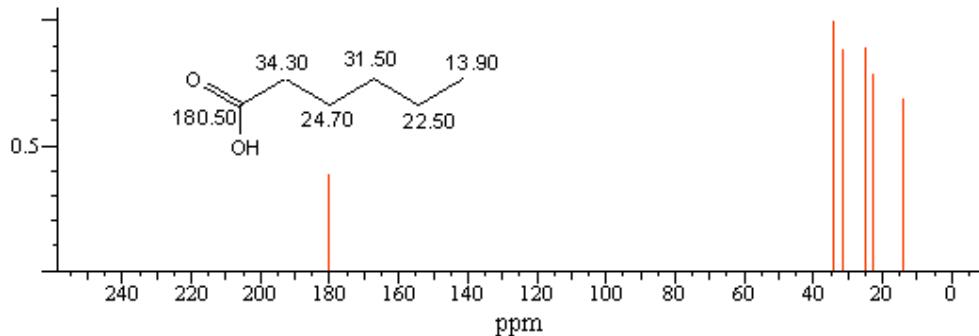
R-	C(=O)	-N(R,R')	Solvent
H-	161.6		CDCl <sub>3</sub>
H-	162.5		CDCl <sub>3</sub>
	168.3		CDCl <sub>3</sub>
CH <sub>3</sub> -	169.4		CDCl <sub>3</sub>

<chem>CH3-</chem>	170.1		<chem>CDCl3</chem>
	171.0		<chem>CDCl3</chem>
R9-	172.4		<chem>CDCl3</chem>
R2-	172.5		<chem>CDCl3</chem>
R3-	172.8		<chem>CDCl3</chem>

## F□Carboxylic Acids (R-C(=O)-OH)

### 1. Aliphatic and Alicyclic

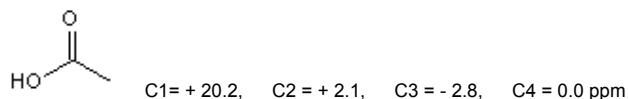
## Aliphatics



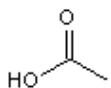
The carbon-13NMR chemical shifts covered in this section contain the carboxylic acid group (- C(=O)- OH) as a common denominator. Because many of these compounds present solubility problems, a significant difference in chemical shifts of the carboxylic acid group is observed depending upon the solvent employed in preparing the spectrogram.

The chemical shift effect of the carboxylic acid group is that of an intermediate deshielding substituent in its effect on aliphatic groups and a weakly deshielding moiety in its effect on adjacent aromatic carbons.

The aliphatic additivity constants are:



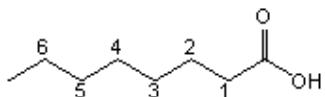
The aromatic additivity constants are:



C1=+1.1, C2, 6 = + 1.9, C3, 5 = + 0.1 C 4 = + 5.4 ppm

The overall chemical shift range for the carbonyl resonance is more than 29ppm (156.5- 185.8ppm) as shown in the chemical shift tables given below.

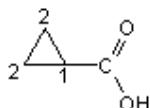
### Alkyl Chemical Shifts



C-6	C-5	C-4	C-3	C-2	C-1	-C(=O)-OH	Solvent
					20.7	177.7	CDCl <sub>3</sub>
				8.9	27.7	181.2	CDCl <sub>3</sub>
			13.7	18.6	36.3	180.5	CDCl <sub>3</sub>
		13.7	22.5	27.1	34.0	180.5	CDCl <sub>3</sub>
	13.9	22.5	31.5	24.7	34.3	180.5	CDCl <sub>3</sub>
14.0	22.7	31.7	28.9	24.9	34.3	180.8	CDCl <sub>3</sub>
R3-	29.5	29.5	29.3	24.9	34.3	180.6	CDCl <sub>3</sub>
R9-	29.7	29.7	29.4	25.0	34.2	175.8	Polysol
R11-	29.7	29.7	29.3	25.0	34.3	176.3	Polysol

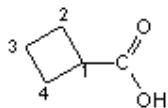
### Alicyclic Chemical Shifts

#### Cyclopropanecarboxylic Acid



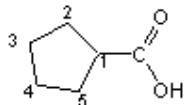
C-2,3	C-1	-C(=O)-OH	Solvent
9.2	13.1	181.9	CDCl <sub>3</sub>

#### Cyclobutanecarboxylic Acid



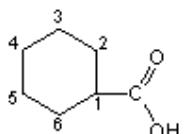
C-3	C-2,4	C-1	-C(=O)-OH	Solvent
18.6	25.4	38.4	181.9	CDCl <sub>3</sub>

Cyclopentanecarboxylic Acid



C-3,4	C-2,5	C-1	-C(=O)-OH	Solvent
26.0	30.1	43.9	183.5	CDCl <sub>3</sub>

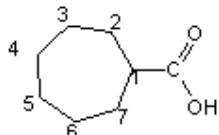
Cyclohexanecarboxylic Acid



C-4	C-3,5	C-2,6	C-1	-C(=O)-OH	Solvent
25.9	25.5	29.0	43.1	183.0	CDCl <sub>3</sub>

C-4	C-3,5	C-2,6	C-1	-CH <sub>2</sub>	-C(=O)-OH	Solvent
26.3	26.2	33.2	34.9	42.0	179.7	CDCl <sub>3</sub>

Cycloheptanecarboxylic Acid



C-4,5	C-3,6	C-2,7	C-1	-C(=O)-OH	Solvent
28.5	26.5	30.7	45.0	183.8	CDCl <sub>3</sub>

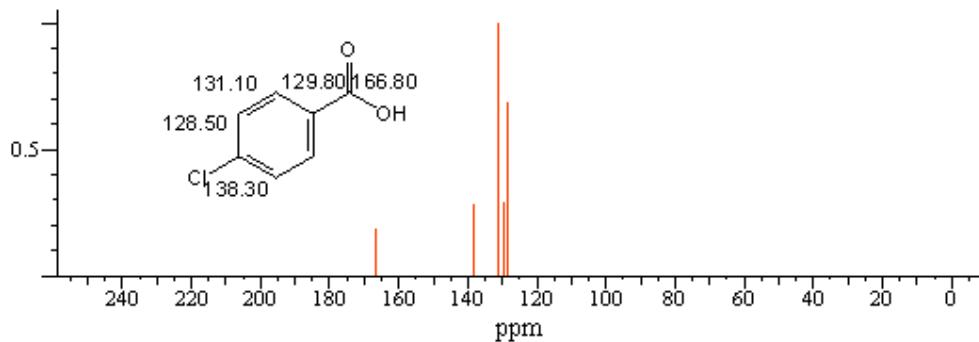
## Carbonyl Chemical Shifts

HO-C(=O)-	-R	Solvent
156.5	-C≡C-H	CDCl <sub>3</sub>
166.2		Polysol
166.9		Polysol
167.1		Polysol
168.2		Polysol
169.1		Polysol
170.4		D <sub>2</sub> O
172.3		CDCl <sub>3</sub>
172.4		CDCl <sub>3</sub>
172.7		CDCl <sub>3</sub>
175.5		D <sub>2</sub> O
175.8	-R15	Polysol
178.4		CDCl <sub>3</sub>

179.7		CDCl <sub>3</sub>
180.6	-R8	CDCl <sub>3</sub>
181.2		CDCl <sub>3</sub>
183.0		CDCl <sub>3</sub>
183.8		CDCl <sub>3</sub>
185.8		CDCl <sub>3</sub>

2□[Aromatic](#)

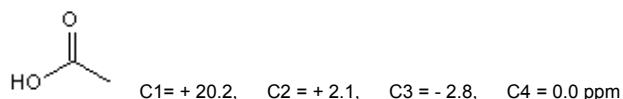
## Aromatics



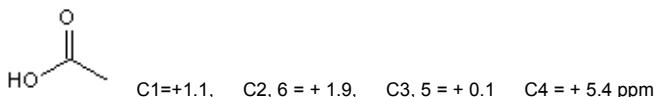
The carbon-13NMR chemical shifts covered in this section contain the carboxylic acid group (- C(=O)- OH) as a common denominator. Because many of these compounds present solubility problems, a significant difference in chemical shifts of the carboxylic acid group is observed depending upon the solvent employed in preparing the spectrogram.

The chemical shift effect of the carboxylic acid group is that of an intermediate deshielding substituent in its effect on aliphatic groups and a weakly deshielding moiety in its effect on adjacent aromatic carbons.

The aliphatic additivity constants are:



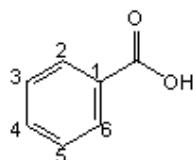
The aromatic additivity constants are:



The overall chemical shift range for the carbonyl resonance is more than 29ppm (156.5- 185.8ppm) as shown in the chemical shift tables given below.

---

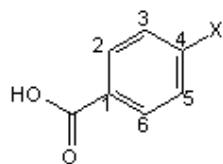
### Phenyl Chemical Shifts



C-4	C-3,5	C-2,6	C-1	-X	Solvent
133.8	128.5	130.3	129.5		CDCl <sub>3</sub>
135.6	130.8	129.0	131.8		CDCl <sub>3</sub>
127.3	129.4	128.6	133.3		CDCl <sub>3</sub>
127.4	128.7	127.7	139.9		CDCl <sub>3</sub>
126.5	130.1	127.5	143.3		Polysol

---

### 4-Substituted Benzoic Acids



HO-C(=O)-	C-1	C-2,6	C-3,6	C-4	-X	Solvent
168.2	117.4	131.1	110.6	153.1		Polysol
169.1	121.3	132.1	115.4	161.8	-OH	Polysol
167.4	123.3	131.5	113.5	162.9	-O-CH <sub>3</sub>	Polysol
167.1	127.6	132.3	115.4	165.5	-F	Polysol
166.8	129.8	131.1	128.5	138.3	-Cl	Polysol
166.9	130.2	131.2	131.5	127.1	-Br	Polysol
171.4	134.6	129.3	129.3	134.6		Polysol
166.2	135.1	130.0	132.2	115.5	-C≡N	Polysol
166.8	136.0	130.1	129.3	139.0		Polysol

### Carbonyl Chemical Shifts

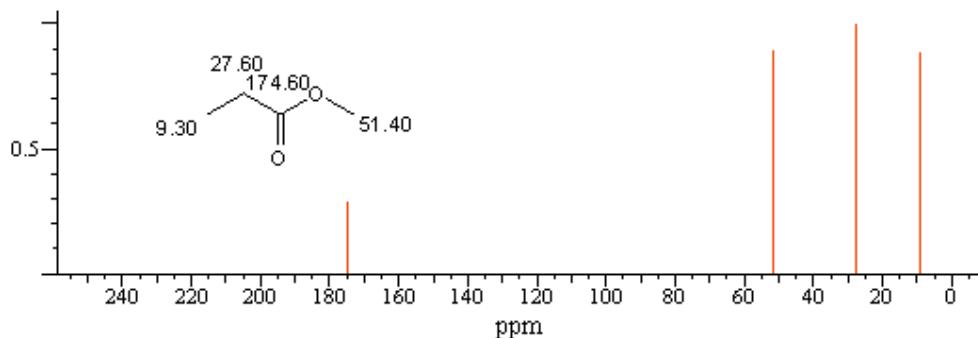
HO-C(=O)-	-R	Solvent
156.5	-C≡C-H	CDCl <sub>3</sub>
166.2		Polysol
166.9		Polysol
167.1		Polysol

168.2		Polysol
169.1		Polysol
170.4		D <sub>2</sub> O
172.3		CDCl <sub>3</sub>
172.4		CDCl <sub>3</sub>
172.7		CDCl <sub>3</sub>
175.5		D <sub>2</sub> O
175.8	-R15	Polysol
178.4		CDCl <sub>3</sub>
179.7		CDCl <sub>3</sub>
180.6	-R8	CDCl <sub>3</sub>
181.2		CDCl <sub>3</sub>
183.0		CDCl <sub>3</sub>
183.8		CDCl <sub>3</sub>
185.8		CDCl <sub>3</sub>

## G□Esters

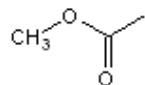
### 1. Aliphatic Esters of Aliphatic Acids

## Aliphatics

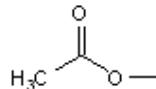


The carbon-13 chemical shifts contained in this section display the chemical shifts and spectrum patterns produced by the carboxylic acid ester functional group ( $\text{R}-\text{C}(=\text{O})-\text{O}-\text{R}'$ ). The carbonyl side of the bond exerts a weak to intermediate deshielding effect on the adjacent (C1) carbons of both aliphatic and aromatic compounds. The oxygen side of the bond, on the other hand, has a strongly deshielding effect on these carbons.

The aliphatic additivity constants are:

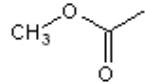


C1 = + 20.1, C2 = + 2.4, C3 = - 2.6, C4 = 0.0 ppm

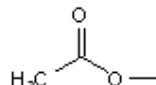


C1 = + 50.5, C2 = + 6.0, C3 = - 6.0, C4 = 0.0 ppm

The aromatic additivity constants are:



C1 = + 2.1, C2, 6 = + 1.3, C3, 5 = + 0.1, C4 = + 4.5 ppm

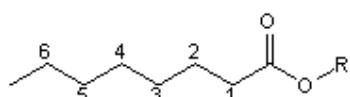


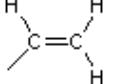
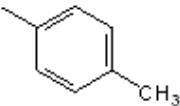
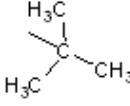
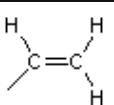
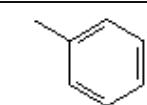
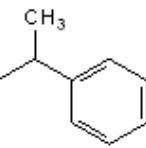
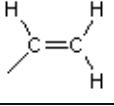
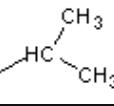
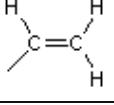
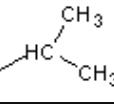
C1 = + 22.7, C2, 6 = - 6.7, C3, 5 = + 1.0, C4 = - 2.8 ppm

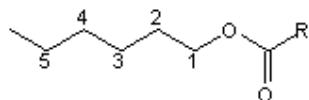
The chemical shift tables presented below contain the shifts for a selected group of carboxylic acid esters.

---

### Alkyl Chemical Shifts

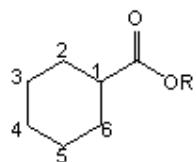


C-5	C-4	C-3	C-2	C-1	-C(=O)	-O-R	Solvent
				19.4	170.6	-R4	CDCl <sub>3</sub>
				20.4	167.7		CDCl <sub>3</sub>
				20.7	169.1		CDCl <sub>3</sub>
				22.3	170.0		CDCl <sub>3</sub>
			8.8	27.3	171.3		CDCl <sub>3</sub>
			9.3	27.6	174.6	-CH <sub>3</sub>	CDCl <sub>3</sub>
			9.0	27.7	172.6		CDCl <sub>3</sub>
			9.0	27.8	173.1		CDCl <sub>3</sub>
		13.6	18.4	35.9	170.5		CDCl <sub>3</sub>
		13.7	18.6	36.1	173.9	-CH <sub>3</sub>	CDCl <sub>3</sub>
		13.7	18.7	36.6	172.7		CDCl <sub>3</sub>
		13.7	18.8	36.7	172.5	-C6	CDCl <sub>3</sub>
	13.8	22.5	27.3	34.2	173.5		CDCl <sub>3</sub>
	13.7	22.5	27.2	34.4	172.6	-3-Cholesterol	CDCl <sub>3</sub>
R5-	29.4	29.3	24.8	34.0	170.4		CDCl <sub>3</sub>
R15-	29.5	29.5	25.2	34.2	174.1	-CH <sub>3</sub>	CDCl <sub>3</sub>
R9-	29.5	29.3	25.2	34.7	172.8		CDCl <sub>3</sub>

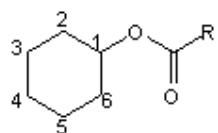


C-5	C-4	C-3	C-2	C-1	-O-C(=O)	-R	Solvent
				51.2	173.8	-R5	CDCl <sub>3</sub>
				51.5	166.5		CDCl <sub>3</sub>
				51.6	171.6		CDCl <sub>3</sub>
				52.0	165.9		CDCl <sub>3</sub>
			14.4	59.9	175.7	-C6	CDCl <sub>3</sub>
			14.3	60.4	170.7	-CH <sub>3</sub>	CDCl <sub>3</sub>
			14.3	62.0	164.5		CDCl <sub>3</sub>
			14.4	63.7	155.5	-O-R2	CDCl <sub>3</sub>
			14.0	68.6	150.5	-Cl	CDCl <sub>3</sub>
		10.4	22.4	65.6	161.2	-H	CDCl <sub>3</sub>
		10.5	22.2	66.4	166.4		CDCl <sub>3</sub>
		10.4	22.4	66.9	154.2		CDCl <sub>3</sub>
	13.7	19.4	31.0	63.7	161.0	-H	CDCl <sub>3</sub>
	13.8	19.5	31.1	64.7	166.3		CDCl <sub>3</sub>
	13.7	19.1	30.7	72.4	150.6	-Cl	CDCl <sub>3</sub>
R14-	29.5	26.1	28.8	64.6	170.8	-CH <sub>3</sub>	CDCl <sub>3</sub>

### Cyclohexyl Ester Chemical Shifts



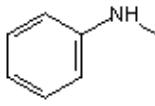
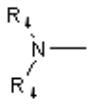
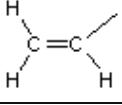
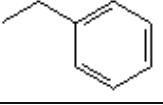
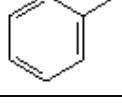
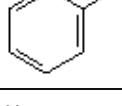
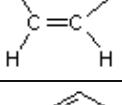
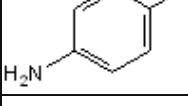
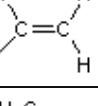
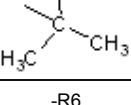
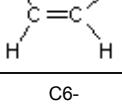
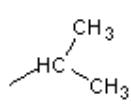
C-4	C-3,5	C-2,6	C-1	$-\text{C}(=\text{O})\text{-O}$	-R	Solvent
26.0	25.7	29.2	43.2	176.2	$-\text{CH}_3$	$\text{CDCl}_3$
26.1	25.7	29.2	43.5	175.3		$\text{CDCl}_3$
26.1	25.8	29.3	43.5	175.7		$\text{CDCl}_3$

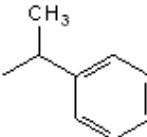
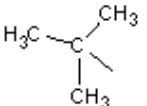


C-4	C-3,5	C-2,6	C-1	$-\text{O-C}(=\text{O})$	-R	Solvent
25.8	24.0	32.0	72.7	172.5	$-\text{R}_3$	$\text{CDCl}_3$
25.6	23.7	31.7	72.3	167.6		$\text{CDCl}_3$
25.7	23.9	31.9	72.5	170.1	$-\text{CH}_3$	$\text{CDCl}_3$

### Carbonyl Chemical Shifts

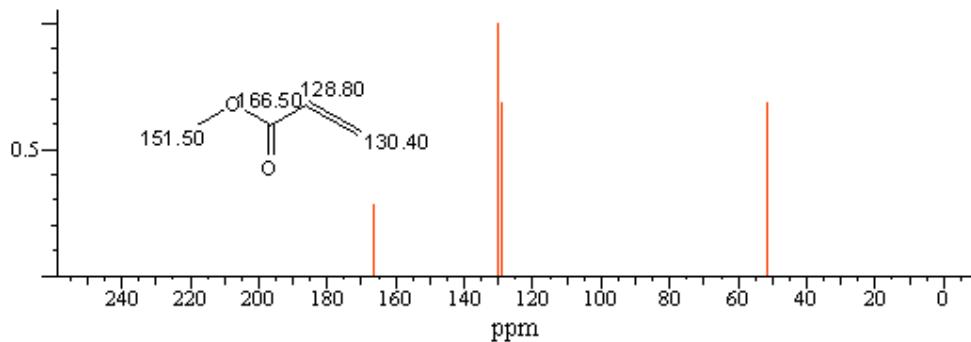
R-	$-\text{C}(=\text{O})\text{-O}$	-R	Solvent
$\text{Cl}^-$	149.3		$\text{CDCl}_3$
$\text{Cl}^-$	150.6	$-\text{R}_4$	$\text{CDCl}_3$
	152.0		$\text{CDCl}_3$

H-C≡C-	152.8		CDCl <sub>3</sub>
	154.2	-R3	CDCl <sub>3</sub>
R6-0-	155.6	-R6	CDCl <sub>3</sub>
	156.5		CDCl <sub>3</sub>
CH <sub>3</sub> -0-	157.1	-CH <sub>3</sub>	CDCl <sub>3</sub>
NH <sub>2</sub> -	157.6	-R12	CDCl <sub>3</sub>
NH <sub>2</sub> -	158.4	-CH <sub>3</sub>	Polysol
H-	161.2		CDCl <sub>3</sub>
H-	161.9	-CH <sub>3</sub>	CDCl <sub>3</sub>
	165.9		CDCl <sub>3</sub>
	166.3		CDCl <sub>3</sub>
	166.4	-R3	CDCl <sub>3</sub>
	166.5	-CH <sub>3</sub>	CDCl <sub>3</sub>
	167.0	-CH <sub>3</sub>	Polysol
CH <sub>3</sub> -	167.7		CDCl <sub>3</sub>
CH <sub>3</sub> -	170.0		CDCl <sub>3</sub>
	170.4	-R6	CDCl <sub>3</sub>
C6-	172.5	-R3	CDCl <sub>3</sub>
R3-	172.7		CDCl <sub>3</sub>

R2-	173.1		CDCl <sub>3</sub>
R5-	173.8	-CH <sub>3</sub>	CDCl <sub>3</sub>
C4-	175.4		CDCl <sub>3</sub>
C6-	175.7		CDCl <sub>3</sub>
	178.6	-CH <sub>3</sub>	CDCl <sub>3</sub>

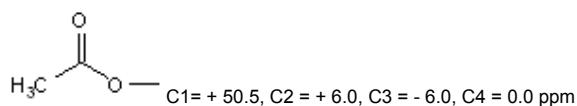
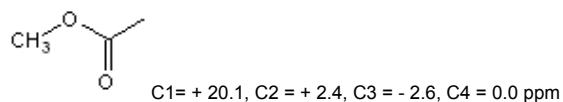
## 2□Olefinic Esters of Aliphatic Acids

### Olefins

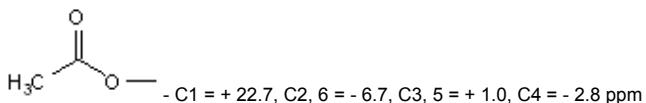
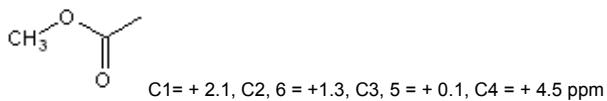


The carbon-13 chemical shifts contained in this section display the chemical shifts and spectrum patterns produced by the carboxylic acid ester functional group (R-C(=O)-O-R'). The carbonyl side of the bond exerts a weak to intermediate deshielding effect on the adjacent (C1) carbons of both aliphatic and aromatic compounds. The oxygen side of the bond, on the other hand, has a strongly deshielding effect on these carbons.

The aliphatic additivity constants are:



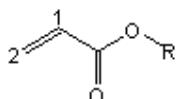
The aromatic additivity constants are:



The chemical shift tables presented below contain the shifts for a selected group of carboxylic acid esters.

---

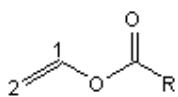
### Acrylate Chemical Shifts



CH <sub>2</sub> -	CH	-C(=O)-O	-R	Solvent
130.4	128.8	166.5	-CH <sub>3</sub>	CDCl <sub>3</sub>
130.7	128.2	165.9		CDCl <sub>3</sub>
129.8	129.2	165.9	-R4	CDCl <sub>3</sub>

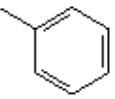
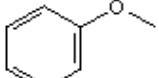
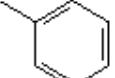
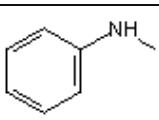
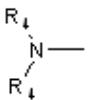
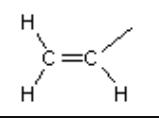
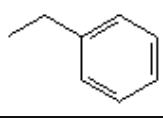
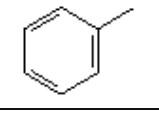
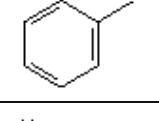
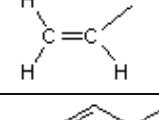
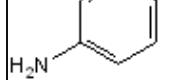
---

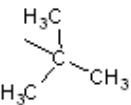
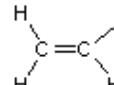
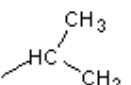
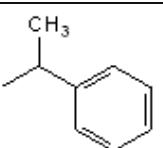
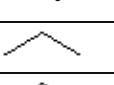
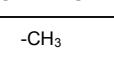
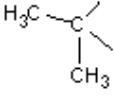
### Vinyl Ester Chemical Shifts



CH <sub>2</sub> -	CH	-C(=O)-O	-R	Solvent
97.0	141.5	170.4	-R9	CDCl <sub>3</sub>
97.0	141.7	171.3		CDCl <sub>3</sub>
97.2	141.6	167.7	-CH <sub>3</sub>	CDCl <sub>3</sub>

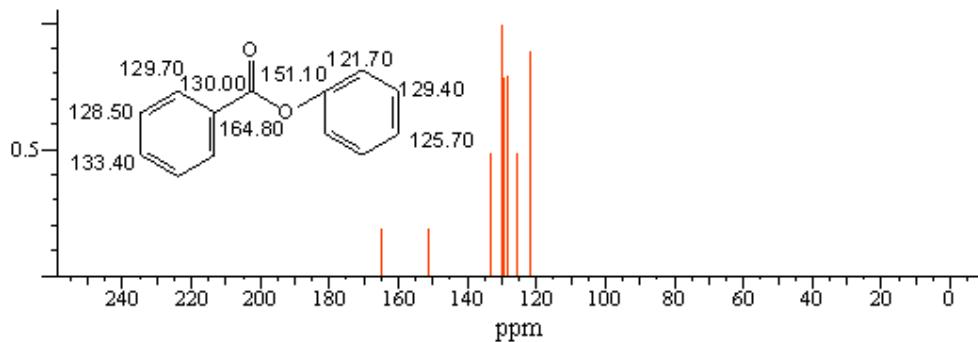
## Carbonyl Chemical Shifts

R-	-C(=O)-O	-R	Solvent
Cl-	149.3		CDCl <sub>3</sub>
Cl-	150.6	-R4	CDCl <sub>3</sub>
	152.0		CDCl <sub>3</sub>
H-C≡C-	152.8		CDCl <sub>3</sub>
	154.2	-R3	CDCl <sub>3</sub>
R6-0-	155.6	-R6	CDCl <sub>3</sub>
	156.5		CDCl <sub>3</sub>
CH <sub>3</sub> -0-	157.1	-CH <sub>3</sub>	CDCl <sub>3</sub>
NH <sub>2</sub> -	157.6	-R12	CDCl <sub>3</sub>
NH <sub>2</sub> <sup>+</sup>	158.4	-CH <sub>3</sub>	Polysol
H-	161.2		CDCl <sub>3</sub>
H-	161.9	-CH <sub>3</sub>	CDCl <sub>3</sub>
	165.9		CDCl <sub>3</sub>
	166.3		CDCl <sub>3</sub>
	166.4	-R3	CDCl <sub>3</sub>
	166.5	-CH <sub>3</sub>	CDCl <sub>3</sub>
	167.0	-CH <sub>3</sub>	Polysol

CH <sub>3</sub> -	167.7		CDCl <sub>3</sub>
CH <sub>3</sub> -	170.0		CDCl <sub>3</sub>
	170.4	-R6	CDCl <sub>3</sub>
C6-	172.5	-R3	CDCl <sub>3</sub>
R3-	172.7		CDCl <sub>3</sub>
R2-	173.1		CDCl <sub>3</sub>
R5-	173.8	-CH <sub>3</sub>	CDCl <sub>3</sub>
C4-	175.4		CDCl <sub>3</sub>
C6-	175.7		CDCl <sub>3</sub>
	178.6	-CH <sub>3</sub>	CDCl <sub>3</sub>

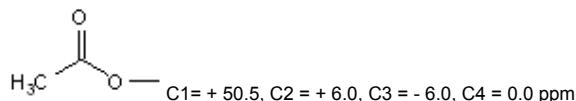
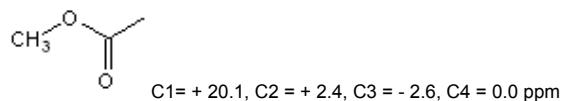
### 3 □ [Aromatic Esters of Aliphatic Acids](#)

#### Aromatics

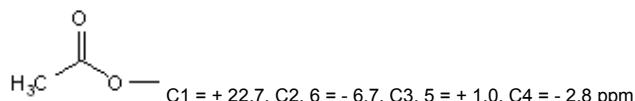
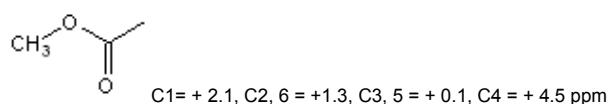


The carbon-13 chemical shifts contained in this section display the chemical shifts and spectrum patterns produced by the carboxylic acid ester functional group (R-C(=O)-O-R'). The carbonyl side of the bond exerts a weak to intermediate deshielding

effect on the adjacent (C1) carbons of both aliphatic and aromatic compounds. The oxygen side of the bond, on the other hand, has a strongly deshielding effect on these carbons. The aliphatic additivity constants are:



The aromatic additivity constants are:

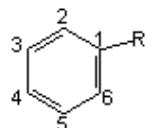


The chemical shift tables presented below contain the shifts for a selected group of carboxylic acid esters.

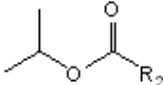
---

### Aromatic Chemical Shifts

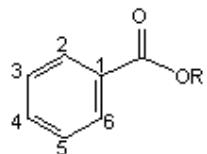
#### Benzyl Compounds

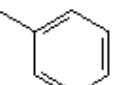


C-4	C-3,5	C-2,6	C-1	-R	Solvent
127.1	129.4	128.6	134.4		CDCl <sub>3</sub>
128.5	128.5	128.2	136.0		CDCl <sub>3</sub>

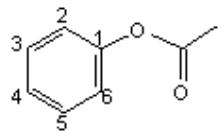
127.8	128.5	126.1	142.2		CDCl <sub>3</sub>
-------	-------	-------	-------	---	-------------------

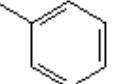
### Benzoates



C-4	C-3,5	C-2,6	C-1	-C(=O)-O-	-R	Solvent
133.4	128.5	129.7	130.0	164.8		CDCl <sub>3</sub>
132.8	128.4	129.6	130.9	166.3	-CH <sub>2</sub> CH <sub>3</sub>	CDCl <sub>3</sub>
132.7	128.3	129.6	130.9	166.4	-R3	CDCl <sub>3</sub>

### Phenyl Esters

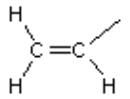
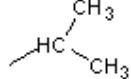
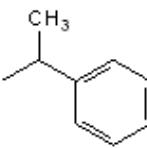
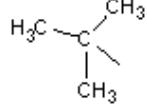


C-4	C-3,5	C-2,6	C-1	-O-C(=O)-	-R	Solvent
125.6	129.4	121.7	151.1	169.2	- CH <sub>3</sub>	CDCl <sub>3</sub>
125.7	129.4	121.7	151.1	164.8		CDCl <sub>3</sub>
124.9	129.0	121.8	151.2	155.3	-NH <sub>2</sub>	Polysol
127.2	129.9	120.5	151.8	149.	-Cl	CDCl <sub>3</sub>

### Carbonyl Chemical Shifts

R-	-C(=O)-O-	-R	Solvent
----	-----------	----	---------

Cl-	149.3		CDCl <sub>3</sub>
Cl-	150.6	-R4	CDCl <sub>3</sub>
	152.0		CDCl <sub>3</sub>
H-C≡C-	152.8		CDCl <sub>3</sub>
	154.2	-R3	CDCl <sub>3</sub>
R6-0-	155.6	-R6	CDCl <sub>3</sub>
	156.5		CDCl <sub>3</sub>
CH <sub>3</sub> -0-	157.1	-CH <sub>3</sub>	CDCl <sub>3</sub>
NH <sub>2</sub> -	157.6	-R12	CDCl <sub>3</sub>
NH <sub>2</sub> -	158.4	-CH <sub>3</sub>	Polysol
H-	161.2		CDCl <sub>3</sub>
H-	161.9	-CH <sub>3</sub>	CDCl <sub>3</sub>
	165.9		CDCl <sub>3</sub>
	166.3		CDCl <sub>3</sub>
	166.4	-R3	CDCl <sub>3</sub>
	166.5	-CH <sub>3</sub>	CDCl <sub>3</sub>
	167.0	-CH <sub>3</sub>	Polysol
CH <sub>3</sub> -	167.7		CDCl <sub>3</sub>
CH <sub>3</sub> -	170.0		CDCl <sub>3</sub>

	170.4	-R6	CDCl <sub>3</sub>
C6-	172.5	-R3	CDCl <sub>3</sub>
R3-	172.7		CDCl <sub>3</sub>
R2-	173.1		CDCl <sub>3</sub>
R5-	173.8	-CH <sub>3</sub>	CDCl <sub>3</sub>
C4-	175.4		CDCl <sub>3</sub>
C6-	175.7		CDCl <sub>3</sub>
	178.6	-CH <sub>3</sub>	CDCl <sub>3</sub>