CÁLCULO DO DESLOCAMENTO QUÍMICO

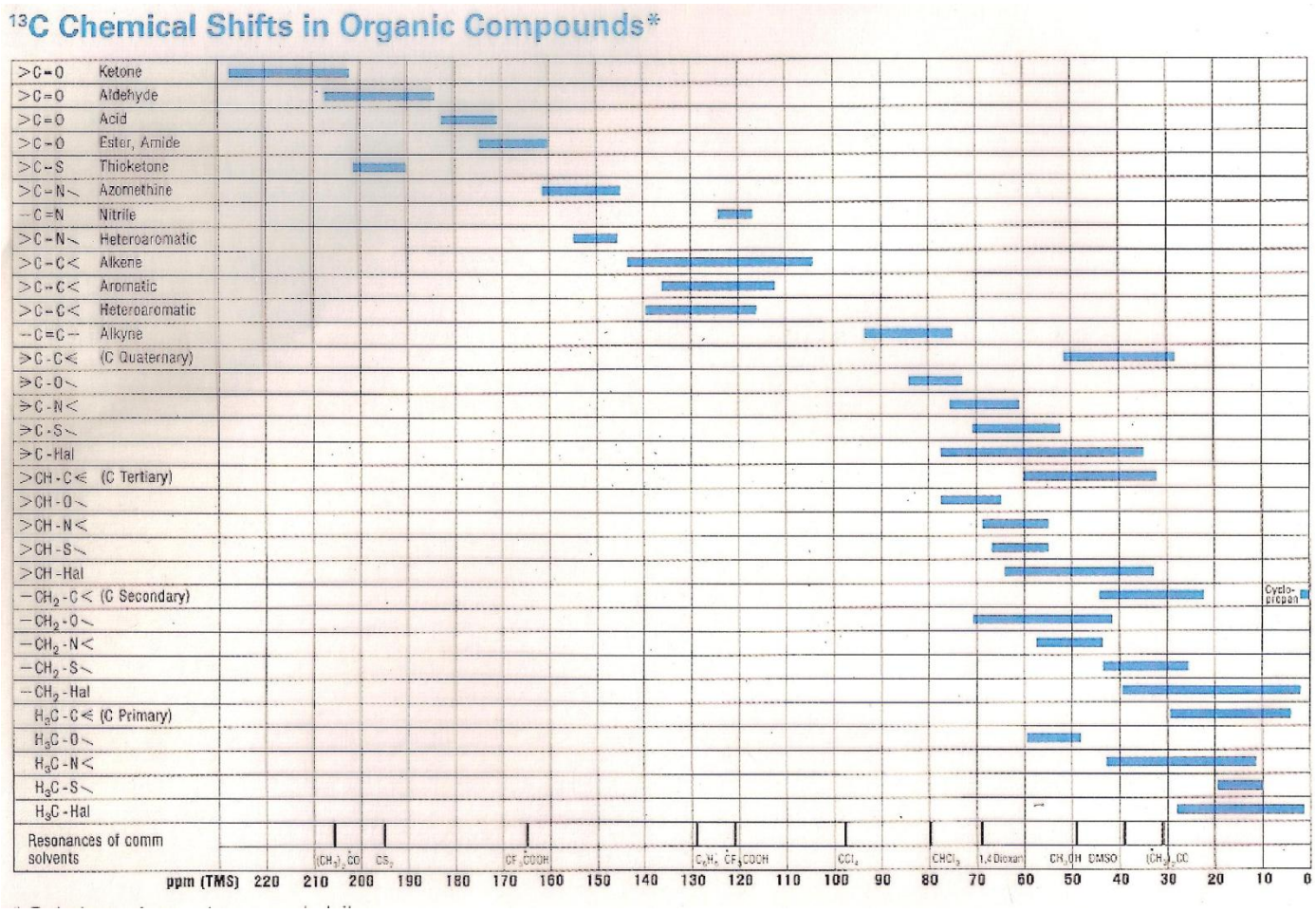
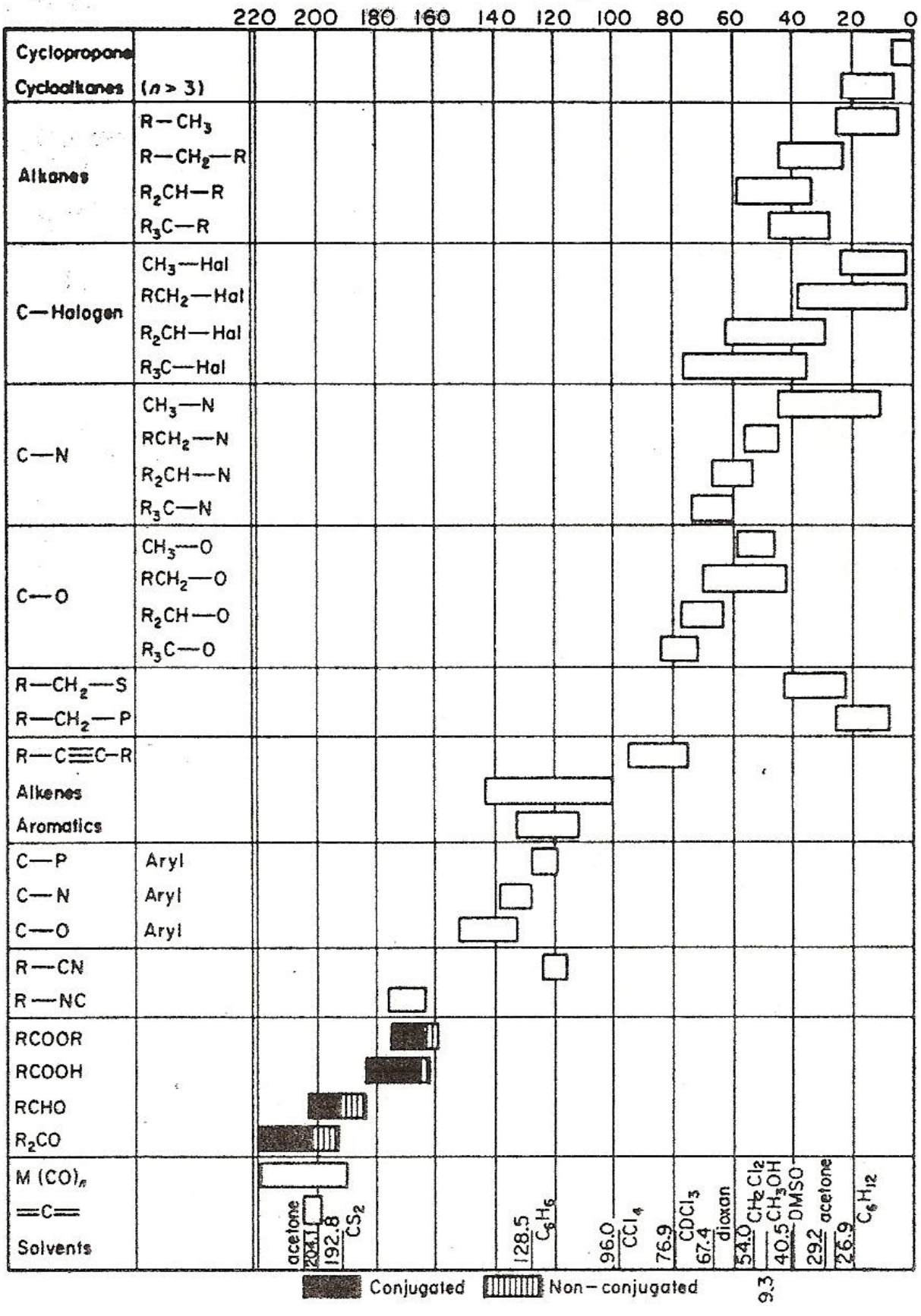
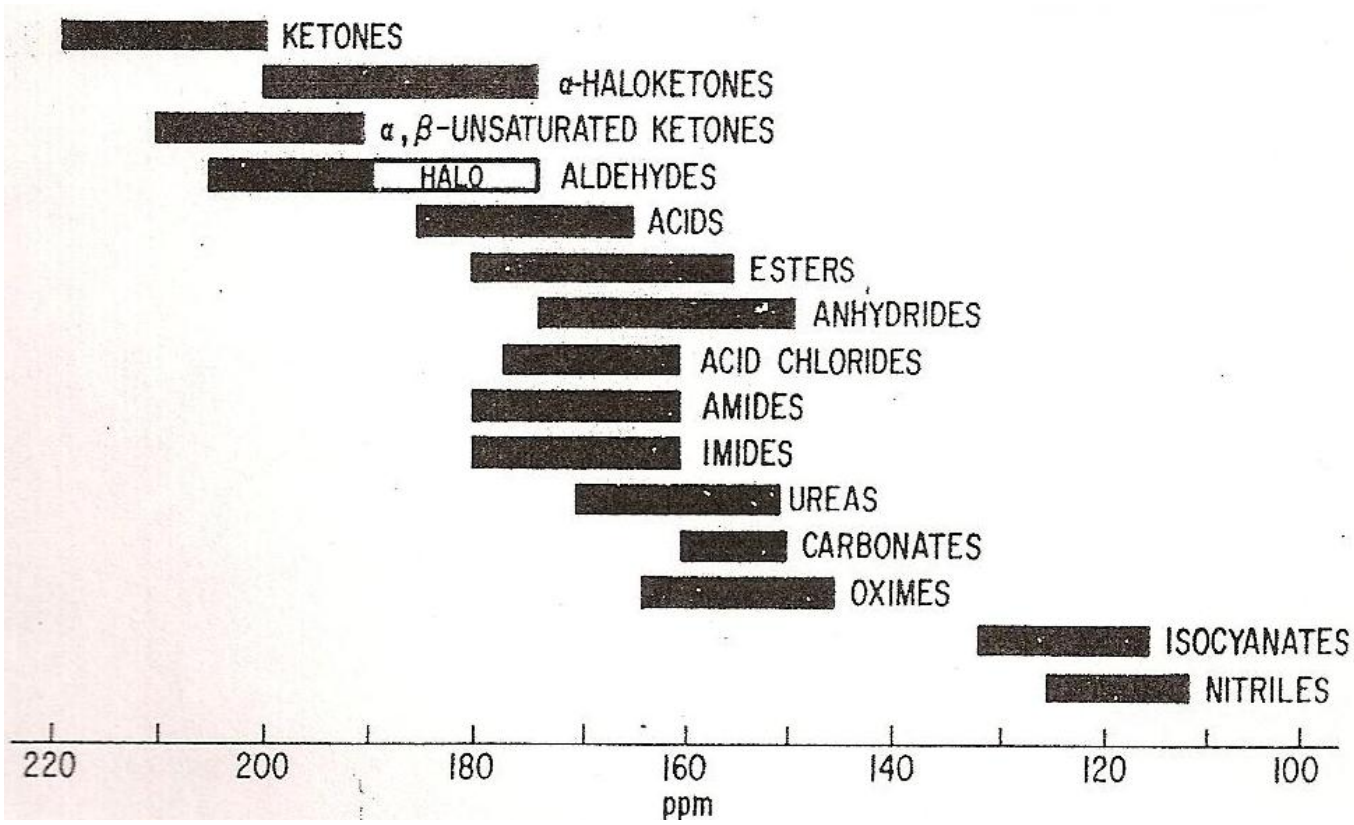


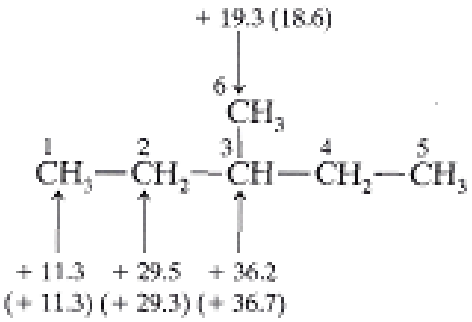
TABELA DE DESLOCAMENTOS QUÍMICOS



DESLOCAMENTOS QUÍMICOS DE COMPOSTOS CARBONÍLICOS



DESLOCAMENTO QUÍMICO EM ALCANOS



The ^{13}C Shift Parameters in Some Linear and Branched Hydrocarbons

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

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

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

$$\delta_3 = -2.5 + (9.1 \times 3) + (9.4 \times 2) + (-3.7 \times 2) = 36.2.$$

$$\delta_6 = -2.5 + (9.1 \times 1) + (9.4 \times 2) + (-2.5 \times 2) + (-1.1 \times 1) = 19.3$$

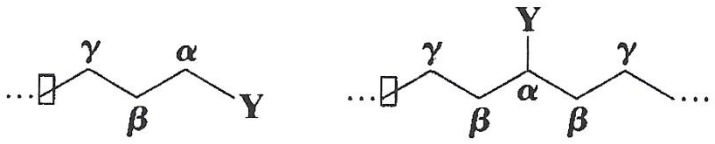
DESLOCAMENTO QUÍMICO EM ALCANOS

TABLE 4.5 The ^{13}C Shifts for Some Linear and Branched-Chain Alkanes (ppm from TMS)

Compound	C-1	C-2	C-3	C-4	C-5
Methane	−2.3				
Ethane	5.7				
Propane	15.8	16.3			
Butane	13.4	25.2			
Pentane	13.9	22.8	34.7		
Hexane	14.1	23.1	32.2		
Heptane	14.1	23.2	32.6	29.7	
Octane	14.2	23.2	32.6	29.9	
Nonane	14.2	23.3	32.6	30.0	30.3
Decane	14.2	23.2	32.6	31.1	30.5
Isobutane	24.5	25.4			
Isopentane	22.2	31.1	32.0	11.7	
Isohexane	22.7	28.0	42.0	20.9	14.3
Neopentane	31.7	28.1			
2,2-Dimethylbutane	29.1	30.6	36.9	8.9	
3-Methylpentane	11.5	29.5	36.9	(18.8, 3-CH_3)	
2,3-Dimethylbutane	19.5	34.3			
2,2,3-Trimethylbutane	27.4	33.1	38.3	16.1	
2,3-Dimethylpentane	7.0	25.3	36.3	(14.6, 3-CH_3)	

DESLOCAMENTO QUÍMICO EM ALCANOS SUBSTITUIDOS

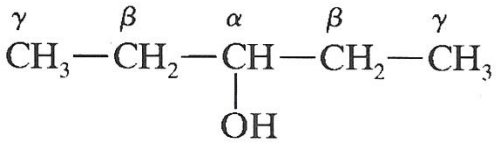
TABLE 4.6 Incremental Substituent Effects (ppm) on Replacement of H by Y in Alkanes. Y is Terminal or Internal[a]



Terminal **Internal**

	α		β		γ
Y	**Terminal**	**Internal**	**Terminal**	**Internal**	
CH_3	9	6	10	8	−2
$CH{=}CH_2$	20		6		−0.5
$C{\equiv}CH$	4.5		5.5		−3.5
COOH	21	16	3	2	−2
COO^-	25	20	5	3	−2
COOR	20	17	3	2	−2
COCl	33	28		2	
$CONH_2$	22		2.5		−0.5
COR	30	24	1	1	−2
CHO	31				−2
Phenyl	23	17	9	7	−2
OH	48	41	10	8	−5
OR	58	51	8	5	−4
OCOR	51	45	6	5	−3
NH_2	29	24	11	10	
NH_3^+	26	24	8	6	−5
NHR	37	31	8	6	−4
NR_2	42		6		−3
NR_3^+	31		5		−7
NO_2	63	57	4	4	
CN	4	1	3	3	−3
SH	11	11	12	11	−4
SR	20		7		−3
F	68	63	9	6	−4
Cl	31	32	11	10	−4
Br	20	25	11	10	−3
I	−6	4	11	12	−1

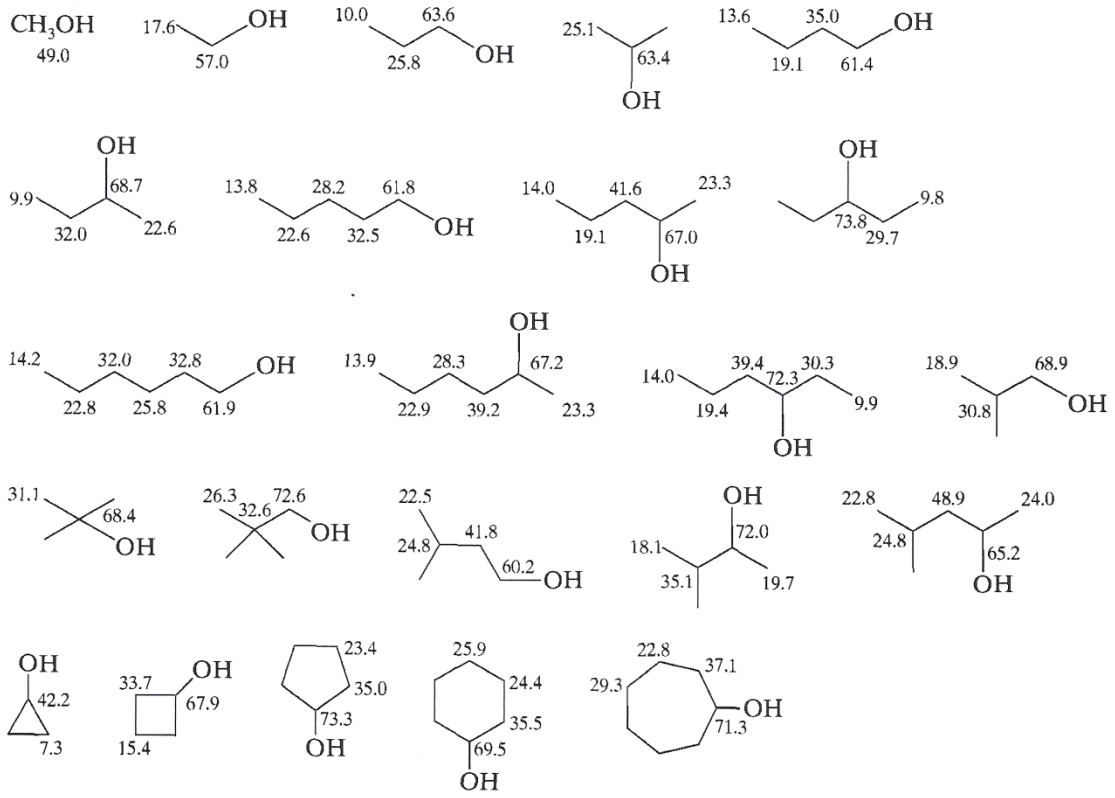
DESLOCAMENTO QUÍMICO EM ALCANOS SUBSTITUIDOS



	Calculated	Experimental (See Table 4.14)
C_α	34.7 + 41 = 75.7	73.8
C_β	22.8 + 8 = 30.8	29.7
C_γ	13.9 − 5 = 8.9	9.8

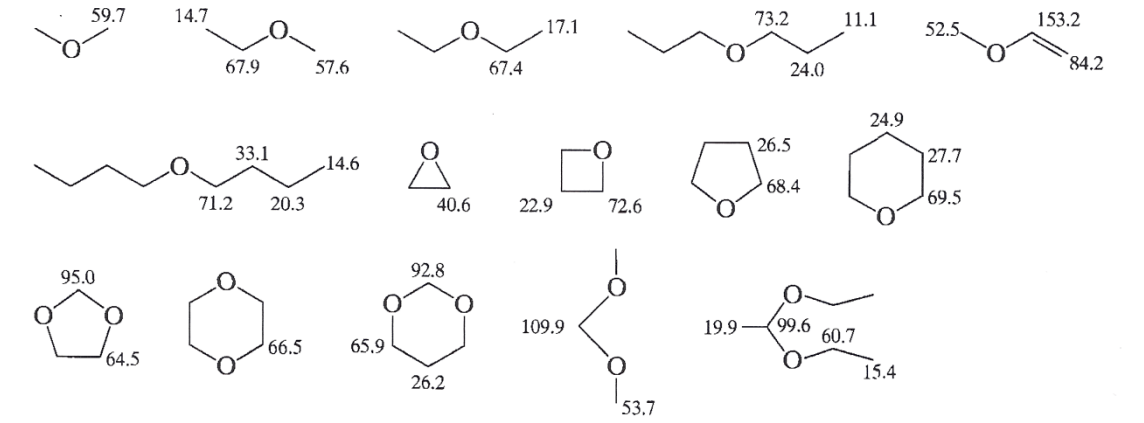
DESLOCAMENTO QUÍMICO EM ÁLCOOIS

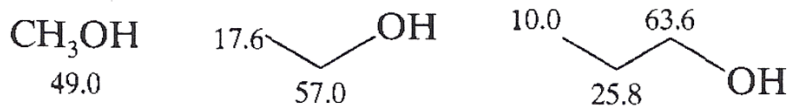
Chemical Shift of Alcohols (ppm from TMS)

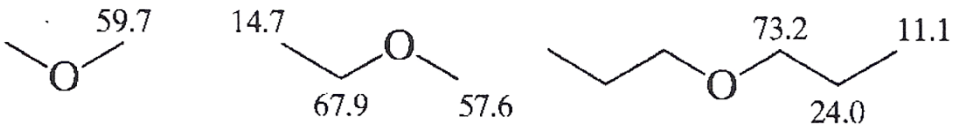


DESLOCAMENTO QUÍMICO EM ÉTERES

Chemical Shift of Ethers, Acetals, and Epoxides (ppm from TMS)







DESLOCAMENTO QUÍMICO EM AMINAS

Efeito de um NH_2 ligado ao carbono:

$R\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}NH_2$
3 2 1

Desblinda o C1 ~ 30 ppm
Desblinda o C2 ~ 11 ppm
Blinda o C3 ~ 4ppm

A alquilação no N desblinda o C1 de aprox. 10 ppm

Composto	C1	C2	C3	C4
CH_3NH_2	26,9			
$CH_3CH_2NH_2$	35,9	17,7		
$CH_3CH_2CH_2NH_2$	44,9	27,3	11,2	
$(CH_3)_2CHNH_2$	42,8	26,2		
$CH_3CH_2CH_2CH_2NH_2$	42,3	36,7	20,4	14,0
$(CH_3)_3CNH_2$	47,5			
$CH_3CH_2NH(CH_3)_2$	58,2	13,8		
Cycloexilamina	50,4	36,7	25,7	25,7
N-Metilcicloexilamina	58,7	33,3	25,1	26,3

DESLOCAMENTO QUÍMICO EM HALOALCANOS

O efeito dos haletos no δ é complexo:

- F e Cl apresentam desblindagem sucessivas com a substituição geminal

-I apresenta blindagem do Cα com sucessivas substituição geminais

Br apresenta desblindagem com 1 e 2 substituições, mas blindagem com 3 e 4 substituições

Shift Position of Alkyl Halides

Compound	C-1	C-2	C-3
CH_4	−2.3		
CH_3F	75.4		
CH_3Cl	24.9		
CH_2Cl_2	54.0		
$CHCl_3$	77.5		
CCl_4	96.5		
CH_3Br	10.0		
CH_2Br_2	21.4		
$CHBr_3$	12.1		
CBr_4	−28.5		
CH_3I	−20.7		
CH_2I_2	−54.0		
CHI_3	−139.9		
CI_4	−292.5		
CH_3CH_2F	79.3	14.6	
CH_3CH_2Cl	39.9	18.7	
CH_3CH_2Br	28.3	20.3	
CH_3CH_2I	−0.2	21.6	
$CH_3CH_2CH_2Cl$	46.7	26.5	11.5
$CH_3CH_2CH_2Br$	35.7	26.8	13.2
$CH_3CH_2CH_2I$	10.0	27.6	16.2

DESLOCAMENTOS QUÍMICOS CALCULADOS (CH_3-X)

Substituent X	δ_{CH_3-X}	Substituent X	δ_{CH_3-X}
-H	-2.3	-cyclopentyl	20.5
$-CH_3$	7.3	-cyclohexyl	23.1
$-CH_2CH_3$	15.4	$-CH=CH_2$	18.7
$-CH(CH_3)_2$	24.1	$-C\equiv CH$	3.7
$-C(CH_3)_3$	31.3	-phenyl	21.4
$-(CH_2)_6CH_3$	14.1	-α-naphthyl	19.1
$-CH_2$phenyl	15.7	-β-naphthyl	21.5
$-CH_2F$	15.8	C -2-pyridyl	24.2
$-CH_2Cl$	18.7	-3-pyridyl	18.0
$-CH_2Br$	19.1	-4-pyridvl	20.6
$-CH_2I$	20.4	-2-furyl	13.7
$-CHCl_2$	31.6	-2-thienyl	14.7
$-CHBr_2$	31.8	-2-pyrrolyl	11.8
$-CCl_3$	46.3	-2-indolyl	13.4
C $-CBr_3$	49.4	-3-indolyl	9.8
$-CH_2OH$	18.2	-4-indolyl	21.6
$-CH_2OCH_3$	14.7	-5-indolyl	21.5
$-CH_2OCH_2CH_3$	15.4	-6-indolyl	21.7
$-CH_2OCH=CH_2$	14.6	-7-indolyl	16.6
$-CH_2O$phenyl	14.9	H -F	71.6
$-CH_2OCOCH_3$	14.4	A -Cl	25.6
$-CH_2NH_2$	19.0	L -Br	9.6
$-CH_2NHCH_3$	14.3	-I	-24.0
$-CH_2N(CH_3)_2$	12.8	-OH	50.2
$-CH_2NO_2$	12.3	$-OCH_3$	60.9
$-CH_2SH$	19.7	$-OCH_2CH_3$	57.6
$-CH_2SO_2CH_3$	6.7	$-OCH(CH_3)_2$	54.9
$-CH_2SO_3H$	8.0	O $-OC(CH_3)_3$	49.4
$-CH_2CHO$	5.2	$-OCH_2CH=CH_2$	57.4
$-CH_2COCH_3$	7.0	-Ocyclohexyl	55.1
$-CH_2COOH$	9.6	$-OCH=CH_2$	52.5
-Ophenyl	54.8	$-SO_2CH_2CH_3$	39.3
$-OCOOCH_3$	54.9	$-SO_2Cl$	52.6
$-OCOCH_3$	51.5	S $-SO_3H$	39.6
O -OCOcyclohexyl	51.2	$-SO_3Na$	41.1
$-OCOCH=CH_2$	51.5	-CHO	31.2
-OCOphenyl	51.8	$-COCH_3$	30.7
$-OSO_2OCH_3$	59.1	$-COCH_2CH_3$	27.5
$-OSO_2$ptoluyl	56.3	$-COCCl_3$	21.1
$-NH_2$	28.3	$-COCH=CH_2$	25.7
$-NH_3^+$	26.5	-COcyclohexyl	27.6
$-NHCH_3$	38.2	O -COphenyl	25.7
-NHcyclohexyl	33.5	II -COOH	21.7
-NHphenyl	30.2	C $-COO^-$	24.4
$-N(CH_3)_2$	47.5	/\ $-COOCH_3$	20.6
-N-pyrrolidinyl	42.7	$-COOCOCH_3$	21.8
N -N-piperidinyl	47.7	$-CONH_2$	22.3
$-N(CH_3)$phenyl	39.9	$-CON(CH_3)_2$	21.5
-1-pyrrolyl	35.9	-COSH	32.6
-1-imidazolyl	32.2	$-COSCH_3$	30.2
-1-pyrazolyl	38.4	$-COCOCH_3$	23.2
-1-indolyl	32.1	-COCl	33.6
$-NHCOCH_3$	26.1	-COBr	39.1
$-N(CH_3)CHO$	36.5;31.5	$-COSi(CH_3)_3$	35.7
-NC	26.8	-CN	1.7
-NCS	29.1		
$-NO_2$	61.2		
-SH	6.5		
$-SCH_3$	19.3		
S $-SC_8H_{17}$	15.5		
-Sphenyl	15.6		
$-SSCH_3$	22.0		
$-SOCH_3$	40.1		
$-SO_2CH_3$	42.6		

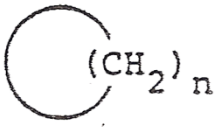
DESLOCAMENTOS QUÍMICOS CALCULADOS

	Substituent	Methyl	Ethyl		n-Propyl			Isopropyl		t-Butyl	
		$-CH_3$	$-CH_2$	$-CH_3$	$-CH_2$	$-CH_2$	$-CH_3$	$-CH$	$-CH_3$	$-C$	$-CH_3$
	-H	- 2.3	7.3	7.3	15.4	15.9	15.4	15.9	15.4	25.0	24.1
C	$-CH=CH_2$	18.7	27.4	13.4	36.2	22.4	13.6	32.3	22.1	33.8	29.4
	$-C\equiv CH$	3.7	12.3	13.8	20.6	22.2	13.4	20.3	22.8	27.4	31.1
	-phenyl	21.4	29.1	15.8	38.3	24.8	13.8	34.3	24.0	34.6	31.4
H	-F	71.6	80.1	15.8	85.2	23.6	9.2	87.3	22.6	93.5	28.3
A	-Cl	25.6	39.9	18.9	46.8	26.3	11.6	53.7	27.3	66.7	34.6
L	-Br	9.6	27.6	19.4	35.6	26.4	13.0	44.8	28.5	62.1	36.4
	-I	-24.0	- 1.6	20.6	9.1	27.0	15.3	20.9	31.2	43.0	40.4
	-OH	50.2	57.8	18.2	64.2	25.9	10.3	64.0	25.3	68.9	31.2
O	$-OCH_3$	60.9	67.7	14.7	74.5	23.2	10.5	72.6	21.4	72.7	27.0
	$-OCH_2CH_3$	57.6	66.0	15.4	72.5	23.2	10.7				
	$-OCH(CH_3)_2$	54.9						68.5	23.0	73.0	28.5
	$-OC(CH_3)_3$	49.4						63.5	25.2	76.3	33.8
	-O-phenyl	54.8	63.2	14.9	69.4	22.8	10.6	69.3	22.0		
	$-OCOCH_3$	51.5	60.4	14.4	66.2	22.4	10.5	67.5	21.9	79.9	28.1
	-OCO-phenyl	51.8	60.8	14.4	66.4	22.2	10.5	68.2	21.9	80.7	28.2
	$-OSO_2$-p-toluyl	56.3	66.9	14.7							
	$-NH_2$	28.3	36.9	19.0	44.6	27.4	11.5	43.0	26.5	47.2	32.9
	$-NHCH_3$	38.2	45.9	14.3	54.0	23.2	12.5	50.5	22.5	50.4	28.2
N	$-N(CH_3)_2$	47.6	53.6	12.8	61.8	20.6	11.9	55.5	18.7	53.6	25.4
	$-NHCOCH_3$	26.1	34.4	14.6	40.7	22.5	11.1	40.5	22.3	49.9	28.6
	-NC	26.8	36.4	15.3	43.4	22.9	11.0	45.5	23.4	54.0	30.7
	$-NO_2$	61.2	70.8	12.3	77.4	21.2	10.8	78.8	20.8	85.2	26.9
	-SH	6.5	19.1	19.7	26.4	27.6	12.6	29.9	27.4	41.1	35.0
	$-SCH_3$	19.3									
S	$-SSCH_3$	22.0	31.8	14.7							
	$-SOCH_3$	40.1									
	$-SO_2CH_3$	42.6	48.2	6.7	56.3	16.3	13.0	53.5	15.2	57.6	22.7
	$-SO_2Cl$	52.6	60.2	9.1	67.1	18.4	12.1	67.6	17.1	74.2	24.5
	$-SO_3H$	39.6	46.7	8.0	53.7	18.8	13.7	52.9	16.8	55.9	25.0
	-CHO	31.3	36.7	5.2	45.7	15.7	13.3	41.1	15.5	42.4	23.4
	$-COCH_3$	30.7	35.2	7.0	45.2	17.5	13.5	41.6	18.2	44.3	26.5
O	-CO-phenyl	25.7	31.7	8.3	40.4	17.7	13.8	35.2	19.1	43.5	27.9
‖	-COOH	21.7	28.5	9.6	36.2	18.7	13.7	34.1	18.8	38.7	27.1
C	$-COOCH_3$	20.6	27.2	9.2	35.6	18.9	13.8	34.1	19.1	38.7	27.3
/ \	$-CONH_2$	22.3	29.0	9.7				34.9	19.5		
	$-COCl$	33.6	41.0	9.3	48.9	18.8	13.0	46.5	19.0	49.4	27.1
	-CN	1.7	10.8	10.6	19.3	19.0	13.3	19.8	19.9	28.1	28.5

DESLOCAMENTOS QUÍMICOS EM *n*-OCTANOS

Substituent X	X-CH_2	-CH_2	-CH_2	-CH_2	-CH_2	-CH_2	-CH_2	-CH_3
-H	14.1	22.8	32.1	29.5	29.5	32.1	22.8	14.1
C -$CH=CH_2$	34.5	~29.6	~29.6	~29.6	~29.6	32.2	23.0	13.9
-phenyl	36.2	31.7	~29.6	~29.6	~29.6	32.1	22.8	14.1
-F[1])	84.2	30.6	25.3	29.3	29.3	31.9	22.7	14.1
H -Cl	45.1	32.8	27.0	29.0	29.2	31.9	22.8	14.1
A -Br	33.8	33.0	28.3	28.8	29.2	31.8	22.7	14.1
L -I	6.9	33.7	30.6	28.6	29.1	31.8	22.6	14.1
-OH	63.1	32.9	25.9	29.5	29.4	31.9	22.8	14.1
O -OC_8H_{17}	71.1	30.0	26.3	29.6	29.4	32.0	22.8	14.1
-ONO	68.3	29.2	26.0	29.3	29.3	31.9	22.7	14.0
-NH_2	42.4	34.1	27.0	29.6	29.4	31.9	22.7	14.1
N -$N(CH_3)_2$	60.1	29.5*	~27.9*	~27.7*	29.7*	32.0	22.8	14.1
-NO_2	75.8	26.2	27.9	~29.6	~29.6	31.4	22.6	
-SH	24.7	34.2	28.5	29.2	29.1	31.9	22.7	
S -SCH_3	34.5	29.0	29.4	29.4	29.4	31.9	22.8	
-SOC_8H_{17}	52.6	~29.1	~29.1	~29.1	~29.1	31.8	22.7	
-CHO	44.0	22.2	~29.3	~29.3	~29.3	31.9	22.7	14.1
O -$COCH_3$	43.7	24.1	~29.5	~29.5	~29.5	32.0	22.8	14.1
‖ -CO-phenyl	38.6	24.4	29.5	29.5	29.5	31.9	22.7	14.0
C -COOH	34.2	24.8	~29.3	~29.3	~29.3	31.9	22.7	14.1
/ \ -$COOCH_3$	34.2	25.1	29.3	29.3	29.3	31.9	22.8	14.1
-$CONH_2$	35.6	25.4	29.1	29.1	~29.1	~29.1	22.6	14.1
-COCl	47.2	25.1	28.5	29.1				
-CN	17.2	25.5	~29.9	~29.9				

DESLOCAMENTOS QUÍMICOS EM CICLOALCANOS



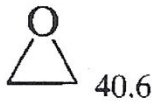
n	δ
3	- 2.8
4	22.9
5	25.6
6	27.1
7	28.8
8	26.8
9	26.0
10	25.1
11	26.3

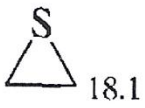
n	δ
12	23.8
13	26.2
14	25.2
15	27.0
16	26.9
18	27.5
20	28.0
30	29.3
40	29.4
72	29.7

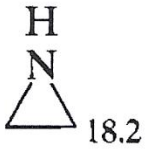
DESLOCAMENTOS QUÍMICOS EM HETEROCICLOS SATURADOS

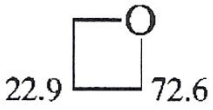
Chemical Shifts for Saturated Heterocyclics

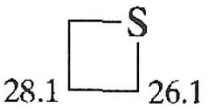
Unsubstituted

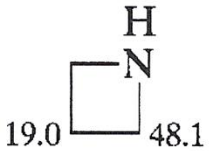


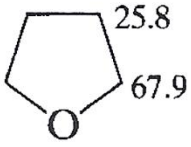


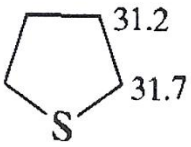


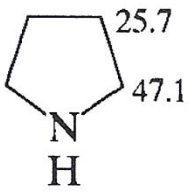


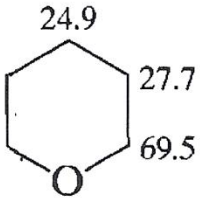


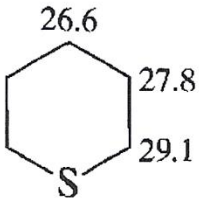


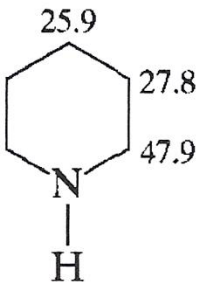




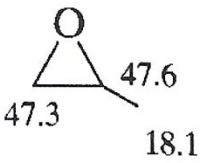


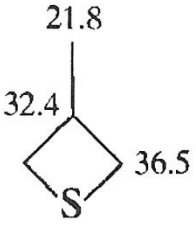


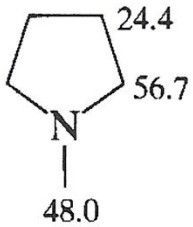




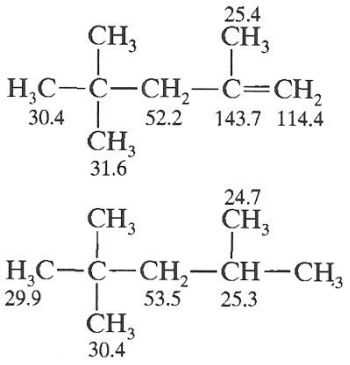
Substituted



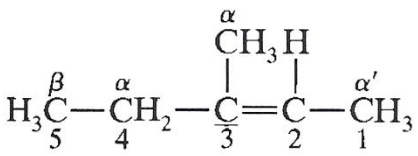


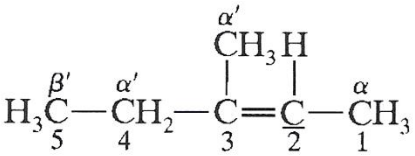


DESLOCAMENTO QUÍMICO EM ALCENOS



Constantes de blindagem	
α	10.6
β	7.2
γ	−1.5
α'	−7.9
β'	−1.8
γ'	−1.5
$Z(cis)$ correction	−1.1





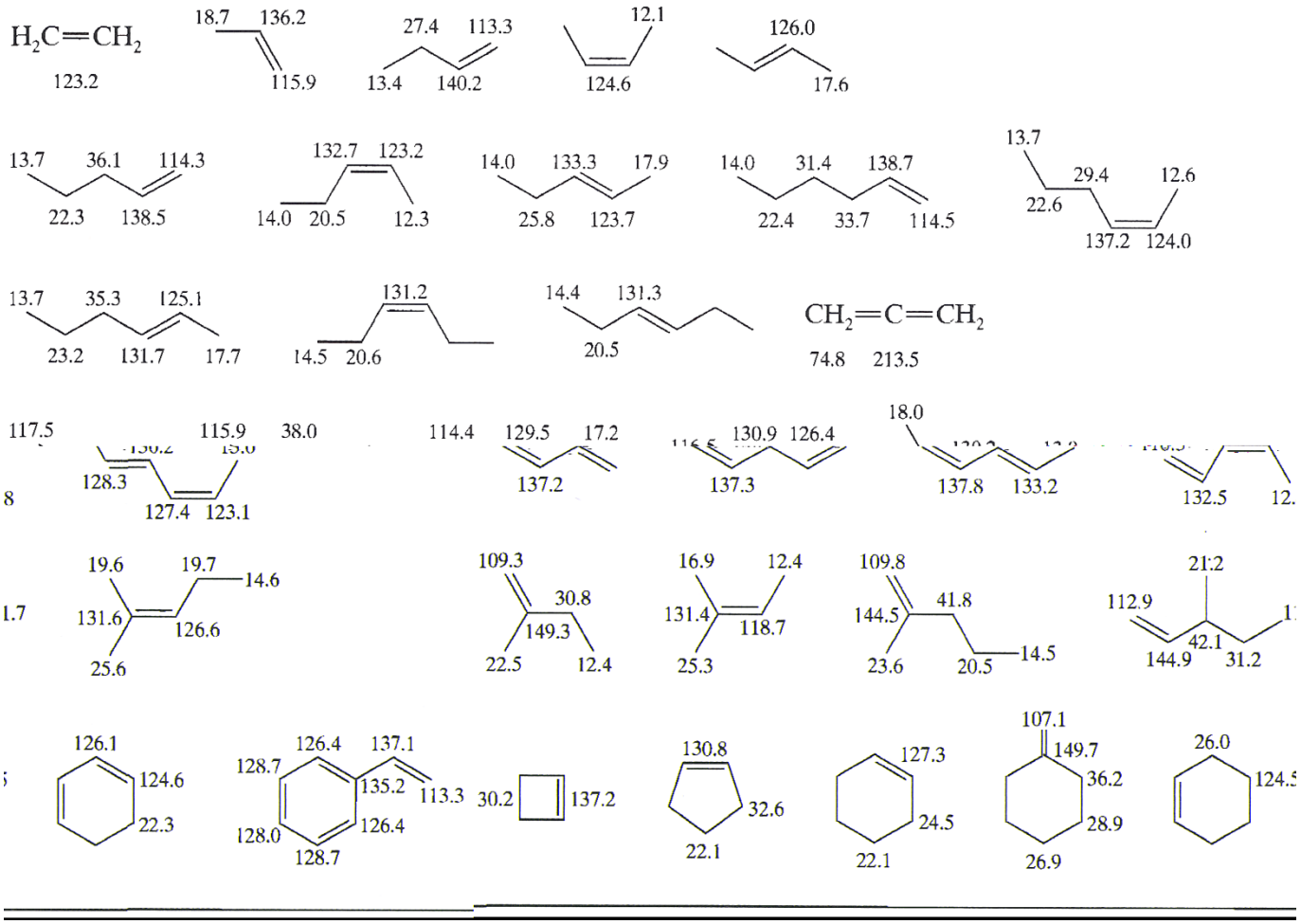
$$\delta_3 = 123.3 + (2 \times 10.6) + (1 \times 7.2) + (1 \times -7.9) - 1.1 = 142.7 \text{ ppm}$$

$$\delta_2 = 123.3 + (1 \times 10.6) + (2 \times -7.9) + (1 \times 1.8) - 1.1 = 115.2 \text{ ppm}$$

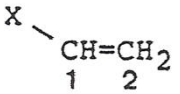
The measured values are C-3 = 137.2 and C-2 = 116.8. The agreement is fair.

DESLOCAMENTO QUÍMICO EM ALCENOS

Alkene and Cycloalkene Chemical Shift (ppm from TMS)



DESLOCAMENTO QUÍMICO EM COMPOSTOS VINÍLICOS



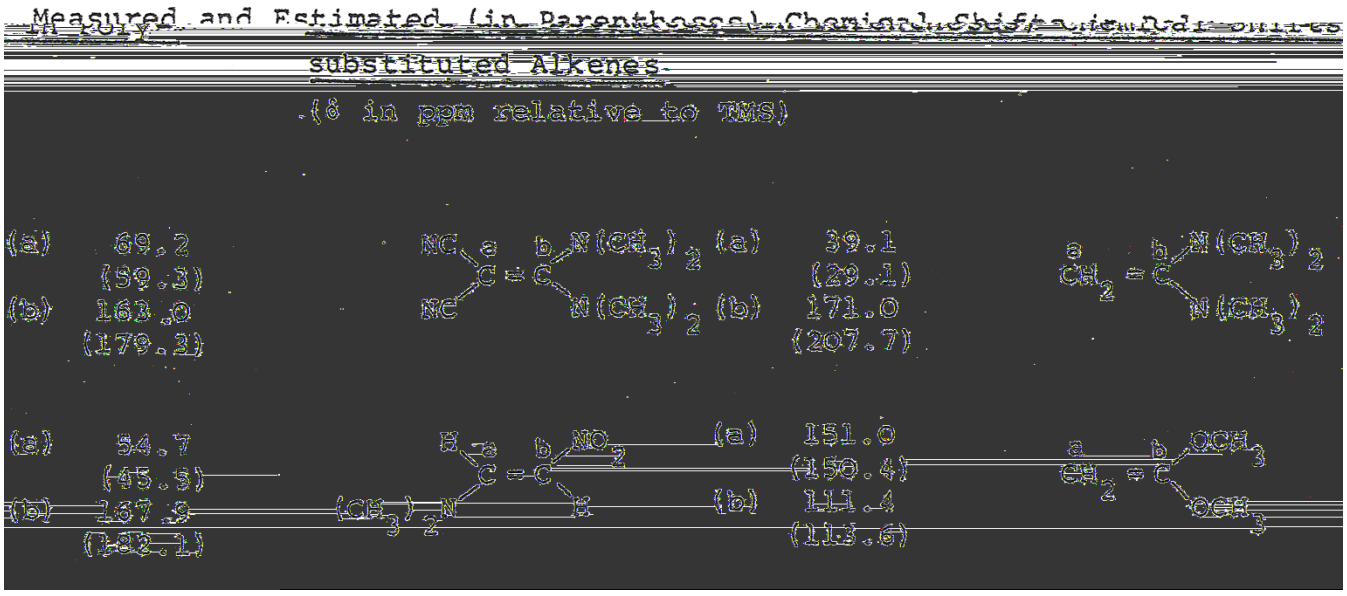
$\delta_{C_i} = 123.3 + Z_i$

	Substituent X	Z_1	Z_2
C	-H	0.0	0.0
	$-CH_3$	12.9	- 7.4
	$-CH_2CH_3$	17.2	- 9.8
	$-CH_2CH_2CH_3$	15.7	- 8.8
	$-CH(CH_3)_2$	22.7	-12.0
	$-CH_2CH_2CH_2CH_3$	14.6	- 8.9
	$-C(CH_3)_3$	26.0	-14.8
	$-CH_2Cl$	10.2	- 6.0
	$-CH_2Br$	10.9	- 4.5
	$-CH_2I$	14.2	- 4.0
	$-CH_2OH$	14.2	- 8.4
	$-CH_2OCH_2CH_3$	12.3	- 8.8
	$-CH=CH_2$	13.6	- 7.0
	$-C\equiv CH$	- 6.0	5.9
	-phenyl	12.5	-11.0
H	-F	24.9	-34.3
A	-Cl	2.8	- 6.1
L	-Br	- 8.6	- 0.9
	-I	-38.1	7.0
	$-OCH_3$	29.4	-38.9
O	$-OCH_2CH_3$	28.8	-37.1
	$-OCH_2CH_2CH_2CH_3$	28.1	-40.4
	$-OCOCH_3$	18.4	-26.7
	$-N(CH_3)_2$	28.0*	-32.0*
	$-N^+(CH_3)_3$	19.8	-10.6
N	-N-pyrrolidonyl	6.5	-29.2
	$-NO_2$	22.3	- 0.9
	-NC	- 3.9	- 2.7
S	$-SCH_2$-phenyl	18.5	-16.4
	$-SO_2CH=CH_2$	14.3	7.9
	-CHO	15.3	14.5
O	$-COCH_3$	13.8	4.7
=	-COOH	5.0	9.8
C	$-COOCH_2CH_3$	6.3	7.0
^	-COCl	8.1	14.0
	-CN	-15.1	14.2
	$-Si(CH_3)_3$	16.9	6.7
	$-SiCl_3$	8.7	16.1

DESLOCAMENTO QUÍMICO EM COMPOSTOS VINÍLICOS

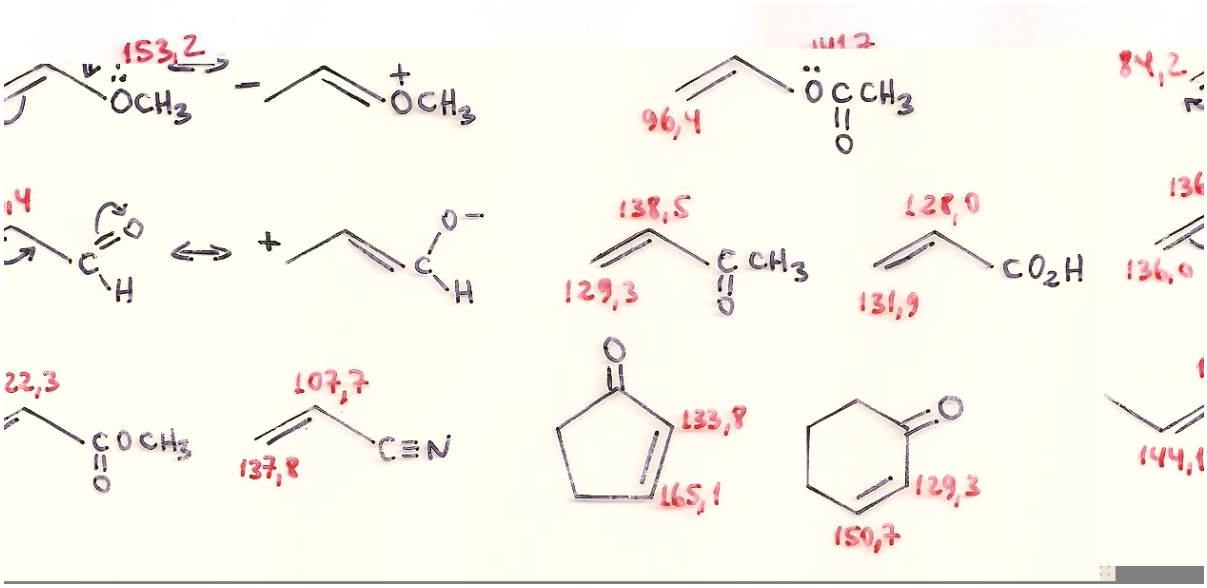
$$Br-\underset{a}{CH}=\underset{b}{CH}-CH_3$$

(a)	base value:	123.3		(b)	base value:	123.3	
	Z_1 (Br)	-8.6			Z_2 (Br)	-0.9	
	Z_2 (CH_3)	-7.4			Z_1 (CH_3)	12.9	
	estimated:	107.3			estimated:	135.3	
	determined:	108.9	(cis)		determined:	129.4	(cis)
		104.7	(trans)			132.7	(trans)



DESLOCAMENTO QUÍMICO EM COMPOSTOS VINÍLICOS

Pode-se prever o Deslocamento químico de alcenos substituídos através de regras empíricas do efeito do substituinte.



DESLOCAMENTO QUÍMICO EM ALCINOS

-Triplas substituídas somente por grupos alquilas: 60-95 ppm

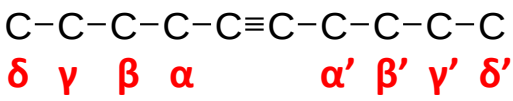
-Carbono terminal da tripla ligação posiciona-se em campo mais alto do que o interno.

-Os carbonos ligados a tripla são deslocados de 5-15 ppm para campo alto relativo ao carbono do alcano correspondente.

Tabela de incrementos

α	**6,93**	**α'**	**-5,69**
β	**4,75**	**β'**	**2,32**
γ	**-0,13**	**γ'**	**-1,31**
δ	**0,51**	**δ'**	**0,50**

Valor base do acetileno = 71,9 ppm

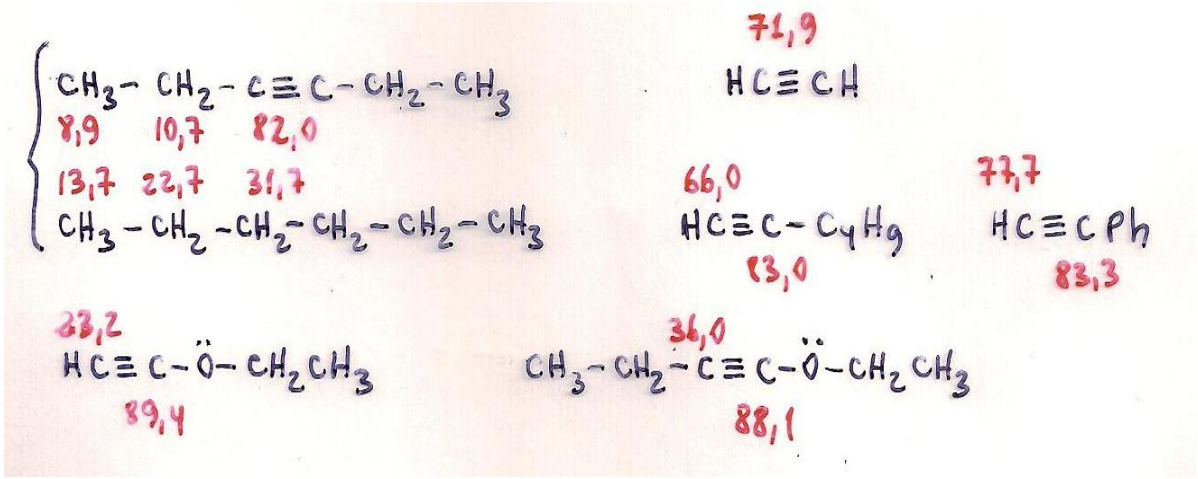


DESLOCAMENTO QUÍMICO EM ALCINOS

$$\underset{a}{X}-C\equiv C-\underset{b}{H}$$

X	a	b
-H	71.9	71.9
$-CH_3$	80.4	68.3
$-CH_2CH_3$	85.5	67.1
$-CH_2CH_2CH_3$	84.0	68.7
$-CH_2CH_2CH_2CH_3$	83.0	66.0
$-CH(CH_3)_2$	89.2	67.6
$-C(CH_3)_3$	92.6	66.8
-cyclohexyl	88.7	68.3
$-CH_2OH$	83.0	73.8
$-CH=CH_2$	82.8	80.0
$-C\equiv C-CH_3$	68.8	64.7
-phenyl	84.6	78.3
$-OCH_2CH_3$	88.2	22.0
$-SCH_2CH_3$	72.6	81.4
-CHO	81.8	83.1
$-COCH_3$	81.9	78.1
-COOH	74.0	78.6
$-COOCH_3$	74.8	75.6

DESLOCAMENTO QUÍMICO EM ALCINOS



DESLOCAMENTO QUÍMICO EM BENZENOS SUBSTITUÍDOS

Incremental Shifts of the Aromatic Carbon Atoms of Monosubstituted Benzenes (ppm from Benzene at 128.5 ppm). Carbon Atom of Substituents in parts per million from TMS[a]

Substituent	C-1 (Attachment)	C-2	C-3	C-4	C of Substituent (ppm from TMS)
H	0.0	0.0	0.0	0.0	
CH_3	9.3	0.7	−0.1	−2.9	21.3
CH_2CH_3	15.6	−0.5	0.0	−2.6	29.2 (CH_2), 15.8 (CH_3)
$CH(CH_3)_2$	20.1	−2.0	0.0	−2.5	34.4 (CH), 24.1 (CH_3)
$C(CH_3)_3$	22.2	−3.4	−0.4	−3.1	34.5 (C), 31.4 (CH_3)
$CH{=}CH_2$	9.1	−2.4	0.2	−0.5	137.1 (CH), 113.3 (CH_2)
$C{\equiv}CH$	−5.8	6.9	0.1	0.4	84.0 (C), 77.8 (CH)
C_6H_5	12.1	−1.8	−0.1	−1.6	
CH_2OH	13.3	−0.8	−0.6	−0.4	64.5
$CH_2O(C{=}O)CH_3$	7.7	~0.0	~0.0	~0.0	20.7 (CH_3), 66.1 (CH_2), 170.5 (C=O)
OH	26.6	−12.7	1.6	−7.3	
OCH_3	31.4	−14.4	1.0	−7.7	54.1
OC_6H_5	29.0	−9.4	1.6	−5.3	
$O(C{=}O)CH_3$	22.4	−7.1	−0.4	−3.2	23.9 (CH_3), 169.7 (C=O)
$(C{=}O)H$	8.2	1.2	0.6	5.8	192
$(C{=}O)CH_3$	7.8	−0.4	−0.4	2.8	24.6 (CH_3), 195.7 (C=O)
$(C{=}O)C_6H_5$	9.1	1.5	−0.2	3.8	196.4 (C=O)
$(C{=}O)F_3$	−5.6	1.8	0.7	6.7	
$(C{=}O)OH$	2.9	1.3	0.4	4.3	168
$(C{=}O)OCH_3$		2.0	1.2	−0.1	4.8
$(C{=}O)Cl$		4.6	2.9	0.6	7.0
$(C{=}O)NH_2$		5.0	−1.2	0.0	3.4
$C{\equiv}N$		−16	3.6	0.6	4.3
NH_2		19.2	−12.4	1.3	−9.5
$N(CH_3)_2$		22.4	−15.7	0.8	−11.8
$NH(C{=}O)CH_3$		11.1	−9.9	0.2	−5.6
NO_2		19.6	−5.3	0.9	6.0
$N{=}C{=}O$		5.7	−3.6	1.2	−2.8
F		35.1	−14.3	0.9	−4.5
Cl		6.4	0.2	1.0	−2.0
Br		−5.4	3.4	2.2	−1.0
I		−32.2	9.9	2.6	−7.3
CF_3		2.6	−3.1	0.4	3.4
SH		2.3	0.6	0.2	−3.3
SCH_3		10.2	−1.8	0.4	−3.6
SO_2NH_2		15.3	−2.9	0.4	3.3
$Si(CH_3)_3$		13.4	4.4	−1.1	−1.1

(CH_3), 166.8 (C=O)
168.5
119.5
40.3
129.5
15.9

benzenes.

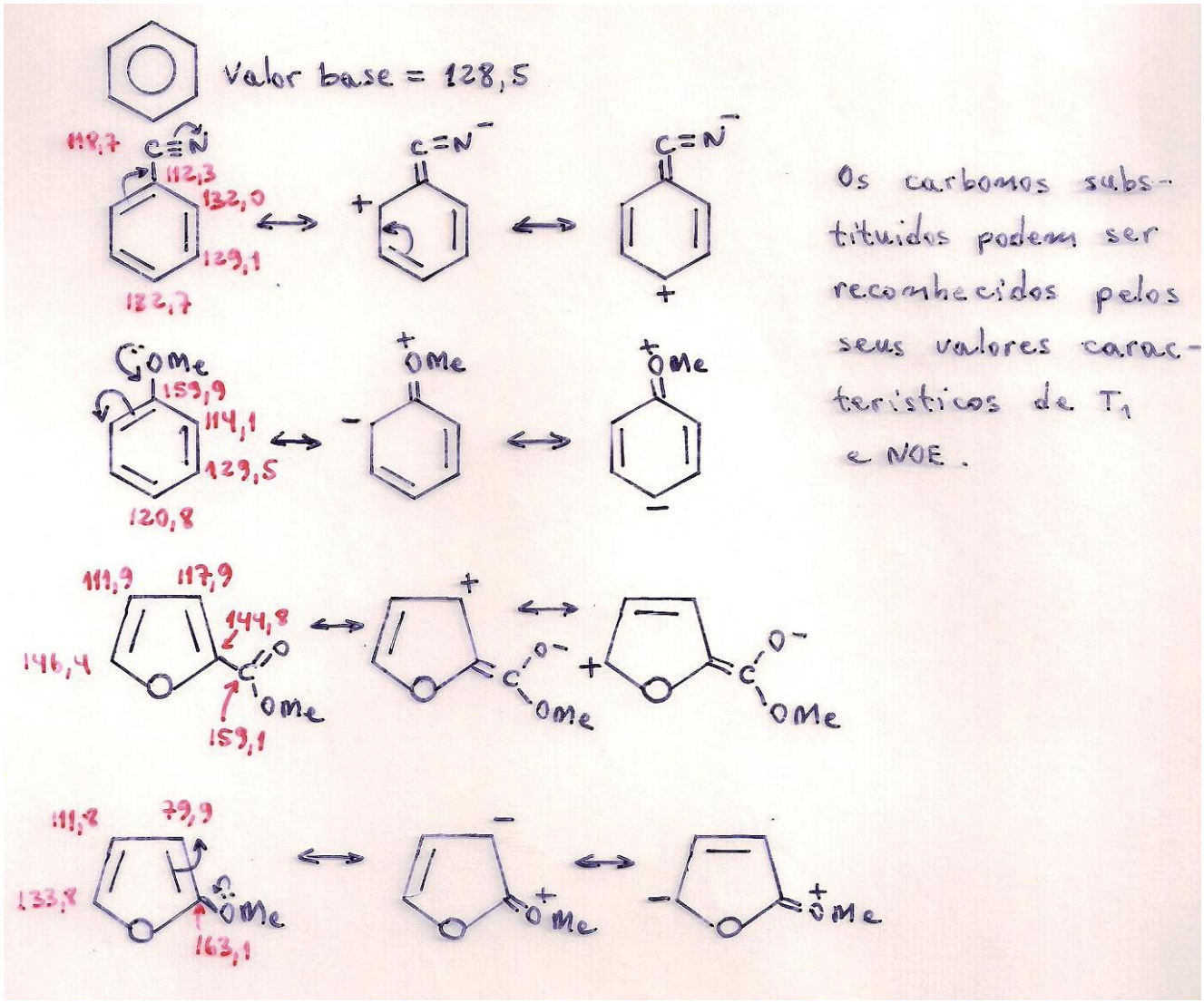
[a] See Ewing, D.E., (1979). *Org. Magn. Reson.*, **12,** 499, for 709 chemical shifts of monosubstitute

DESLOCAMENTO QUÍMICO EM BENZENOS SUBSTITUÍDOS

$\delta_{C_i} = 128.5 + Z_i$

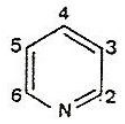
	Substituent X	Z_1	Z_2	Z_3	Z_4
	-H	0.0	0.0	0.0	0.0
	$-CH_3$	9.2	0.7	-0.1	-3.0
	$-CH_2CH_3$	15.7	-0.6	-0.1	-2.8
	$-CH(CH_3)_2$	20.2	-2.2	-0.3	-2.8
	$-CH_2CH_2CH_2CH_3$	14.2	-0.2	-0.2	-2.8
	$-C(CH_3)_3$	22.4	-3.3	-0.4	-3.1
	-cyclopropyl	15.1	-3.3	-0.6	-3.6
	$-CH_2Cl$	9.3	0.3	0.2	0.0
	$-CH_2Br$	9.5	0.7	0.3	0.2
C	$-CF_3$	2.5	-3.2	0.3	3.3
	$-CCl_3$	16.3	-1.7	-0.1	1.8
	$-CH_2OH$	12.4	-1.2	0.2	-1.1
	$-CHOCH_2$	9.2	-3.1	-0.1	-0.5
	$-CH_2NH_2$	14.9	-1.4	-0.2	-2.0
	$-CH_2SCH_3$	9.8	0.4	-0.1	-1.6
	$-CH_2SOCH_3$	0.8	1.5	0.4	-0.2
	$-CH_2CN$	1.6	0.5	-0.8	-0.7
	$-CH=CH_2$	8.9	-2.3	-0.1	-0.8
	$-C\equiv CH$	-6.2	3.6	-0.4	-0.3
	-phenyl	13.1	-1.1	0.5	-1.1
H	-F	34.8	-13.0	1.6	-4.4
A	-Cl	6.3	0.4	1.4	-1.9
L	-Br	-5.8	3.2	1.6	-1.6
	-I	-34.1	8.9	1.6	-1.1
	-OH	26.9	-12.8	1.4	-7.4
	-ONa	39.6	-8.2	1.9	-13.6
	$-OCH_3$	31.4	-14.4	1.0	-7.7
O	$-OCH=CH_2$	28.2	-11.5	0.7	-5.8
	-Ophenyl	27.6	-11.2	-0.3	-6.9
	$-OCOCH_3$	22.4	-7.1	0.4	-3.2
	$-OSi(CH_3)_3$	26.8	-8.4	0.9	-7.1
	$-OPO(Ophenyl)_2$	21.9	-8.4	1.2	-3.0
	-OCN	25.0	-12.7	2.6	-1.0
	$-NH_2$	18.2	-13.4	0.8	-10.0
	$-NHCH_3$	21.4	-16.2	0.8	-11.6
	$-N(CH_3)_2$	22.5	-15.4	0.9	-11.5
	-NHphenyl	14.7	-10.6	0.9	-10.5
	$-N(phenyl)_2$	19.8	-7.0	0.9	-5.6
	$-NH_3^+$	0.1	-5.8	2.2	2.2
N	$-N^+(CH_3)_3$	19.5	-7.3	2.5	2.4
	$-NHCOCH_3$	9.7	-8.1	0.2	-4.4
	$-NHNH_2$	22.8	-16.5	0.5	-9.6
	$-N(CH_3)NO$	13.7	-9.5	0.8	-1.4
	-N=N-phenyl	24.0	-5.8	0.3	2.2
	$-N^+\equiv N$	-12.7	6.0	5.7	16.0
	-NC	-1.8	-2.2	1.4	0.9
	-NCO	5.1	-3.7	1.1	-2.8
	-NCS	3.0	-2.7	1.3	-1.0
	-NO	37.4	-7.7	0.8	7.0
	$-NO_2$	19.9	-4.9	0.9	6.1
	-SH	2.1	0.7	0.3	-3.2
	$-SCH_3$	10.0	-1.9	0.2	-3.6
	$-SC(CH_3)_3$	4.5	9.0	-0.3	0.0
S	-Sphenyl	7.3	2.5	0.6	-1.5
	$-SOCH_3$	17.6	-5.0	1.1	2.4
	$-SO_2CH_3$	12.3	-1.4	0.8	5.1
	$-SO_2Cl$	15.6	-1.7	1.2	6.8
	$-SO_3H$	15.0	-2.2	1.3	3.8
	$-SO_2OCH_3$	6.4	-0.6	1.5	5.9
	-SCN	-3.7	2.5	2.2	2.2
	-CHO	8.2	1.2	0.5	5.8
	$-COCH_3$	8.9	0.1	-0.1	4.4
O	$-COCF_3$	-5.6	1.8	0.7	6.7
‖	-COphenyl	9.3	1.6	-0.3	3.7
C	-COOH	2.1	1.6	-0.1	5.2
^	$-COO^-$	9.7	4.6	2.2	4.6
	$-COOCH_3$	2.0	1.2	-0.1	4.3
	$-CONH_2$	5.0	-1.2	0.1	3.4
	$-CON(CH_3)_2$	8.0	-1.5	-0.2	1.0
	-COCl	4.7	2.7	0.3	6.6
	-CSphenyl	18.7	1.0	-0.6	2.4
	-CN	-15.7	3.6	0.7	4.3
	$-P(CH_3)_2$	13.6	1.6	-0.6	-1.0
	$-P(phenyl)_2$	8.9	5.2	0.0	0.1
	$-PO(OCH_2CH_3)_2$	1.6	3.6	-0.2	3.4
	$-PS(OCH_2CH_3)_2$	6.1	2.8	-0.4	3.4
	$-SiH_3$	-0.5	7.3	-0.4	1.3
	$-Si(CH_3)_3$	11.6	4.9	-0.7	0.4
	$-Sn(CH_3)_3$	13.4	7.4	-0.2	-0.3
	$-Pb(CH_3)_3$	20.1	8.0	-0.1	-1.0

DESLOCAMENTO QUÍMICO EM BENZENOS SUBSTITUÍDOS



DESLOCAMENTO QUÍMICO EM NAFTALENOS

DESLOCAMENTO QUÍMICO EM PIRIDINAS

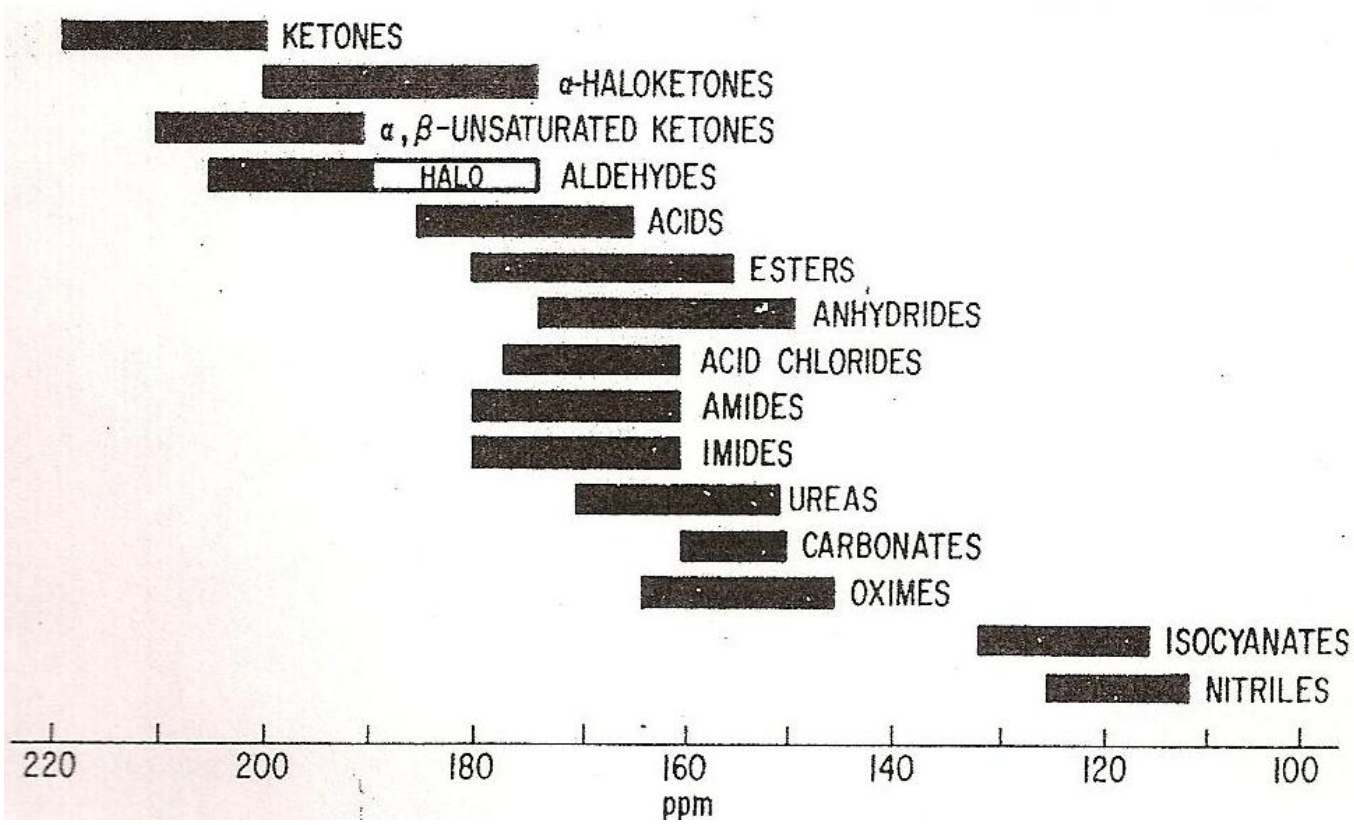


$$\delta_{C-2} = 149.8 + z_{i2}$$
$$\delta_{C-3} = 123.6 + z_{i3}$$
$$\delta_{C-4} = 135.7 + z_{i4}$$
$$\delta_{C-5} = 123.6 + z_{i5}$$
$$\delta_{C-6} = 149.8 + z_{i6}$$

2- or 6-substituent (i = 2 or 6)	$z_{22}=z_{66}$	$z_{23}=z_{65}$	$z_{24}=z_{64}$	$z_{25}=z_{63}$	$z_{26}=z_{62}$
$-CH_3$	8.8	-0.6	0.2	-3.0	-0.4
$-CH_2CH_3$	13.6	-1.8	0.4	-2.9	-0.7
-F	14.4	-13.1	6.1	-1.5	-1.5
-Cl	2.3	0.7	3.3	-1.2	0.6
-Br	-6.7	4.8	3.3	-0.5	1.4
-OH	15.5	-3.5	-0.9	-16.9	-8.2
$-OCH_3$	15.3	-7.5	2.1	-13.1	-2.2
$-NH_2$	11.3	-14.7	2.3	-10.6	-0.9
$-NO_2$	8.0	-5.1	5.5	6.6	0.4
-CHO	3.5	-2.6	1.3	4.1	0.7
$-COCH_3$	4.3	-2.8	0.7	3.0	-0.2
$-CONH_2$	0.1	-1.2	1.5	2.8	-1.4
-CN	-15.9	5.0	1.6	3.6	1.4
$-Si(CH_3)_3$	17.6	3.8	-2.9	-2.0	-0.5
$-Sn(CH_3)_3$	22.5	6.8	-3.2	-2.5	-0.2
3e5 Subst.	z_{32}/z_{56}	z_{33}/z_{55}	z_{34}/z_{54}	z_{35}/z_{53}	z_{36}/z_{52}
$-CH_3$	1.3	9.0	0.2	-0.8	-2.3
$-CH_2CH_3$	-0.4	15.5	-0.6	-0.4	-2.7
-F	-11.5	36.2	-13.0	0.9	-3.9
-Cl	-0.3	8.2	-0.2	0.7	-1.4
-Br	2.1	-2.6	2.9	1.2	-0.9
-I	7.1	-28.4	9.1	2.4	0.3
-OH	-10.7	31.4	-12.2	1.3	-8.6
$-OCH_3$	-12.5	31.6	-15.7	0.2	-8.4
$-NH_2$	-11.9	21.5	-14.2	0.9	-10.8
-CHO	2.4	7.9	0.0	0.6	5.4
$-COCH_3$	3.5	8.6	-0.5	-0.1	0.0
$-COOCH_3$	-0.6	1.1	-0.3	-1.7	1.8
$-CONH_2$	2.7	6.0	1.3	1.3	-1.5
-CN	3.6	-13.7	4.4	0.6	4.2
$-Si(CH_3)_3$	1.9	8.3	2.5	-3.1	-0.9
$-Sn(CH_3)_3$	5.1	12.2	6.6	-0.7	-1.2

4-substituent (i = 4)	$z_{42}=z_{46}$	$z_{43}=z_{45}$	z_{44}
$-CH_3$	0.5	0.8	10.8
$-CH_2CH_3$	-0.1	-0.4	17.0
$-CH(CH_3)_2$	0.4	-1.8	21.4
$-C(CH_3)_3$	0.1	-3.4	23.4
$-CH=CH_2$	0.3	-2.9	8.6
-F	2.7	-11.8	33.0
-Br	3.0	3.4	-3.0
$-OCH_3$	0.9	-13.8	29.2
$-NH_2$	0.9	-13.8	19.6
-CHO	1.7	-0.6	5.5
$-COCH_3$	1.6	-2.6	6.8
$-COOCH_3$	1.0	-0.7	1.6
$-CONH_2$	0.4	-0.8	6.4
-CN	2.1	2.2	-15.7
$-Si(CH_3)_3$	-3.6	1.6	11.4
$-Sn(CH_3)_3$	-1.9	6.5	15.7

DESLOCAMENTOS QUÍMICOS DE COMPOSTOS CARBONÍLICOS



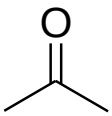
DESLOCAMENTOS QUÍMICOS EM CETONAS E ALDEÍDOS

-Substituintes em α desblinda a carbonila de 2-3 ppm

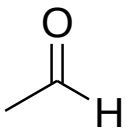
-Efeito da carbonila na cadeia carbônica:

C(α) → desblinda de 10 a 14 ppm

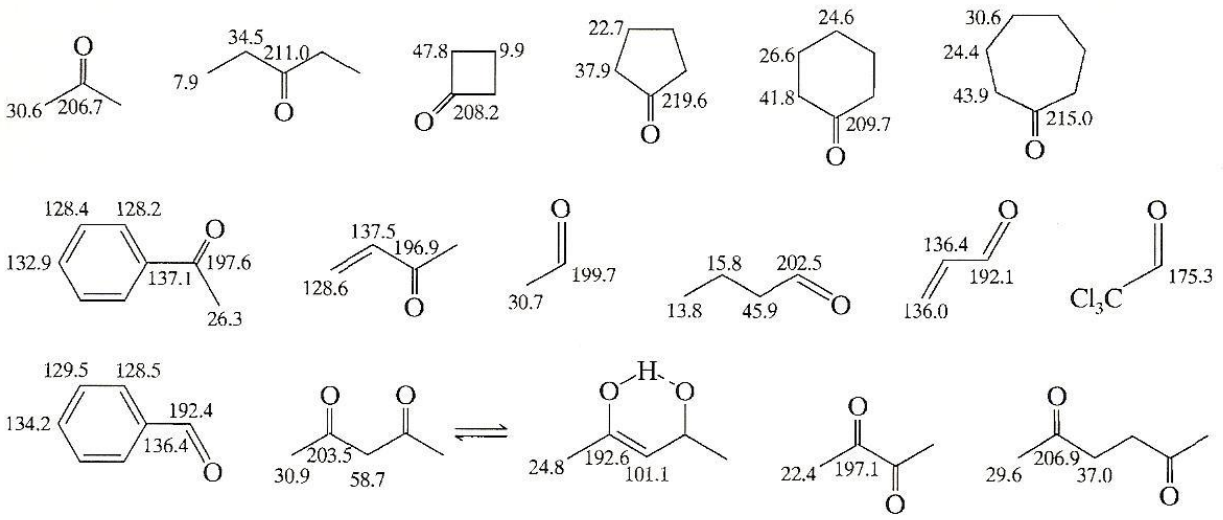
C(β) → blinda de alguns ppm



203,8



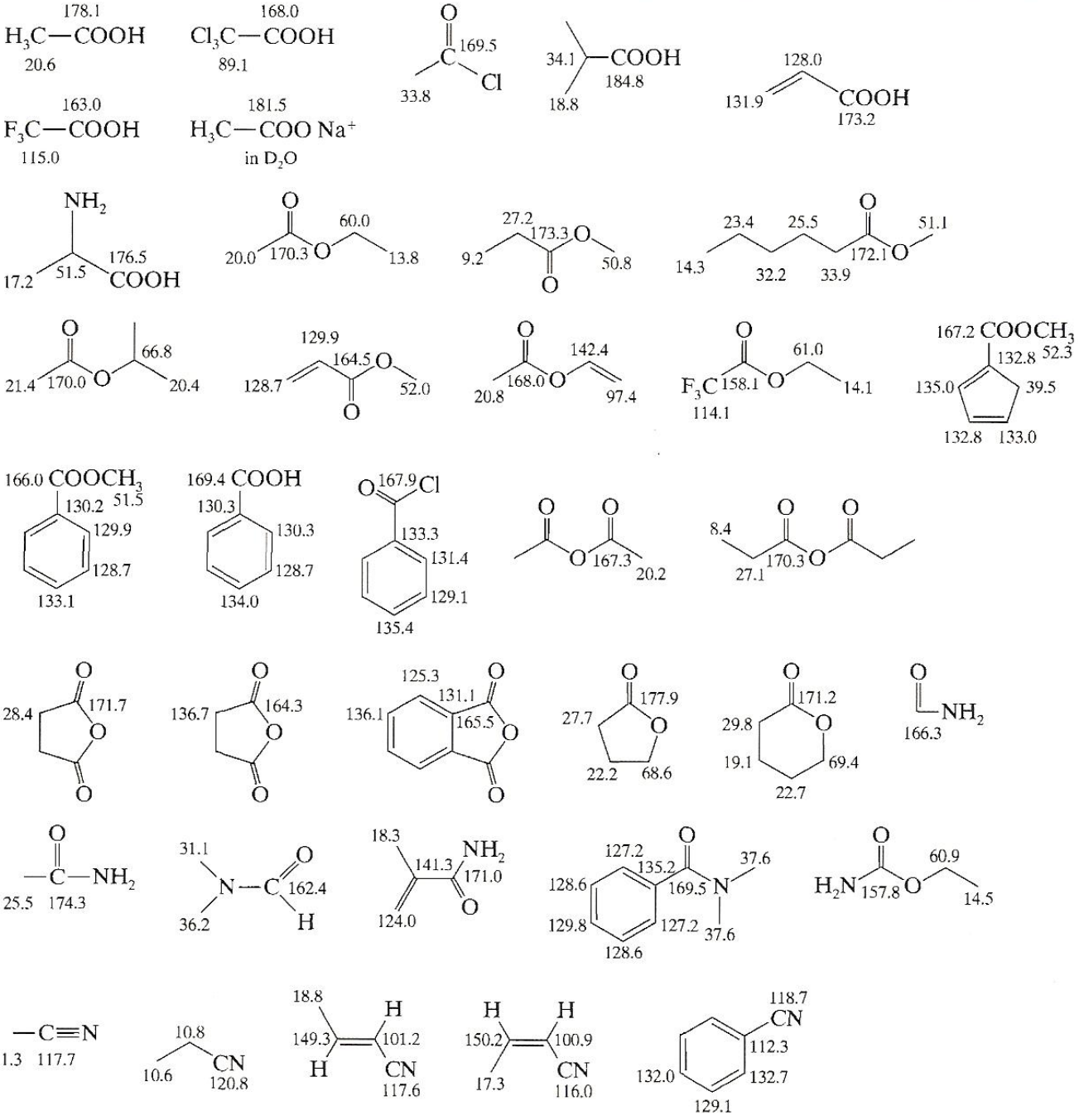
199,3



DESLOCAMENTO QUÍMICO DE C-13 DE SOLVENTES COMUNS

		$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
solvent signals		77.16 ± 0.06	29.84 ± 0.01 206.26 ± 0.13	39.52 ± 0.06	128.06 ± 0.02	1.32 ± 0.02 118.26 ± 0.02	49.00 ± 0.01	
acetic acid	CO	175.99	172.31	171.93	175.82	173.21	175.11	177.21
	CH_3	20.81	20.51	20.95	20.37	20.73	20.56	21.03
acetone	CO	207.07	205.87	206.31	204.43	207.43	209.67	215.94
	CH_3	30.92	30.60	30.56	30.14	30.91	30.67	30.89
acetonitrile	CN	116.43	117.60	117.91	116.02	118.26	118.06	119.68
	CH_3	1.89	1.12	1.03	0.20	1.79	0.85	1.47
benzene	CH	128.37	129.15	128.30	128.62	129.32	129.34	
tert-butyl alcohol	C	69.15	68.13	66.88	68.19	68.74	69.40	70.36
	CH_3	31.25	30.72	30.38	30.47	30.68	30.91	30.29
tert-butyl methyl	OCH_3	49.45	49.35	48.70	49.19	49.52	49.66	49.37
ether	C	72.87	72.81	72.04	72.40	73.17	74.32	75.62
	CCH_3	26.99	27.24	26.79	27.09	27.28	27.22	26.60
BHT	C(1)	151.55	152.51	151.47	152.05	152.42	152.85	
	C(2)	135.87	138.19	139.12	136.08	138.13	139.09	
	CH(3)	125.55	129.05	127.97	128.52	129.61	129.49	
	C(4)	128.27	126.03	124.85	125.83	126.38	126.11	
	CH_3Ar	21.20	21.31	20.97	21.40	21.23	21.38	
	CH_3C	30.33	31.61	31.25	31.34	31.50	31.15	
	C	34.25	35.00	34.33	34.35	35.05	35.36	
chloroform	CH	77.36	79.19	79.16	77.79	79.17	79.44	
cyclohexane	CH_2	26.94	27.51	26.33	27.23	27.63	27.96	
1,2-dichloroethane	CH_2	43.50	45.25	45.02	43.59	45.54	45.11	
dichloromethane	CH_2	53.52	54.95	54.84	53.46	55.32	54.78	
diethyl ether	CH_3	15.20	15.78	15.12	15.46	15.63	15.46	14.77
	CH_2	65.91	66.12	62.05	65.94	66.32	66.88	66.42
diglyme	CH_3	59.01	58.77	57.98	58.66	58.90	59.06	58.67
	CH_2	70.51	71.03	69.54	70.87	70.99	71.33	70.05
	CH_2	71.90	72.63	71.25	72.35	72.63	72.92	71.63
1,2-dimethoxyethane	CH_3	59.08	58.45	58.01	58.68	58.89	59.06	58.67
	CH_2	71.84	72.47	17.07	72.21	72.47	72.72	71.49
dimethylacetamide	CH_3	21.53	21.51	21.29	21.16	21.76	21.32	21.09
	CO	171.07	170.61	169.54	169.95	171.31	173.32	174.57
	NCH_3	35.28	34.89	37.38	34.67	35.17	35.50	35.03
	NCH_3	38.13	37.92	34.42	37.03	38.26	38.43	38.76
dimethylformamide	CH	162.62	162.79	162.29	162.13	163.31	164.73	165.53
	CH_3	36.50	36.15	35.73	35.25	36.57	36.89	37.54
	CH_3	31.45	31.03	30.73	30.72	31.32	31.61	32.03
dimethyl sulfoxide	CH_3	40.76	41.23	40.45	40.03	41.31	40.45	39.39
dioxane	CH_2	67.14	67.60	66.36	67.16	67.72	68.11	67.19
ethanol	CH_3	18.41	18.89	18.51	18.72	18.80	18.40	17.47
	CH_2	58.28	57.72	56.07	57.86	57.96	58.26	58.05
ethyl acetate	CH_3CO	21.04	20.83	20.68	20.56	21.16	20.88	21.15
	CO	171.36	170.96	170.31	170.44	171.68	172.89	175.26
	CH_2	60.49	60.56	59.74	60.21	60.98	61.50	62.32
	CH_3	14.19	14.50	14.40	14.19	14.54	14.49	13.92
ethyl methyl ketone	CH_3CO	29.49	29.30	29.26	28.56	29.60	29.39	29.49
	CO	209.56	208.30	208.72	206.55	209.88	212.16	218.43
	CH_2CH_3	36.89	36.75	35.83	36.36	37.09	37.34	37.27
	CH_2CH_3	7.86	8.03	7.61	7.91	8.14	8.09	7.87
ethylene glycol	CH_2	63.79	64.26	62.76	64.34	64.22	64.30	63.17
"grease"	CH_2	29.76	30.73	29.20	30.21	30.86	31.29	

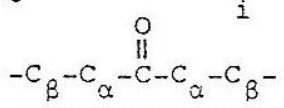
DESLOCAMENTOS QUÍMICOS EM COMPOSTOS CARBONÍLICOS



CÁLCULO DO DESLO. QUÍMICO DE CARBONILAS

Aldehydes and Ketones

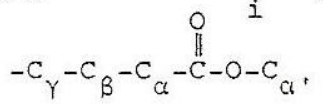
$$\delta_{C=O} = 193.0 + \sum_i Z_i$$



Substituent i	Z_α	Z_β
-C≲	6.5	2.6
$-CH=CH_2$	-0.8	0.0
$-CH=CH-CH_3$	0.2	0.0
-phenyl	-1.2	0.0

Carboxylic Acids and Esters

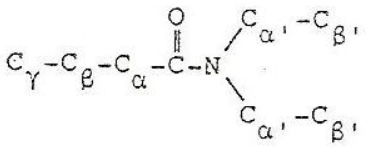
$$\delta_{C=O} = 166.0 + \sum_i Z_i$$



Substituent i	Z_α	Z_β	Z_γ	$Z_{\alpha'}$
-C≲	11.0	3.0	-1.0	-5.0
$-CH=CH_2$	5.0			-9.0
-phenyl	6 0	1.0		-8.0

Amides

$$\delta_{C=O} = 165.0 + \sum_i Z_i$$



Substituent i	Z_α	Z_β	Z_γ	$Z_{\alpha'}$	$Z_{\beta'}$
-C≲	7.7	4.5	-0.7	-1.5	-0.3
$-CH=CH_2$	3.3				
-phenyl	4.7			-4.5	