| Tipo de carbono | Deslocamento químico (ppm) |
|---|---|
| C=O (cetonas) | 205 - 220 |
| C=O (aldeídos) | 190 - 200 |
| C=O (ácidos e ésteres) | 160 - 185 |
| C (anéis aromáticos) | 125 - 150 |
| C=C (alcenos) | 115 - 140 |
| $RCH_2O$- | 50 - 90 |
| $RCH_2Cl$ | 30 - 60 |
| $RCH_2NH_2$ | 30 - 65 |
| $R_3CH$ | 25 - 35 |
| $CH_3CO$- | 20 - 50 |
| $R_2CH_2$ | 16 - 25 |
| $RCH_3$ | 10 - 15 |

R = pode conter outros elementos ligados a carbono  Ex : R = $CH_2OH$

## PARÂMENTROS DE GRANT-PAUL

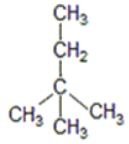
$\delta_c = -2,1 + \Sigma n_i A_i = \Sigma$ (correções devidas às ramificações)  $\delta_c$ com relação ao TMS

| | $A_i$ |
|---|---|
| α | +9.1 |
| β | +9.4 |
| γ | -2.5 |
| δ | +0.3 |
| ε | +0.1 |

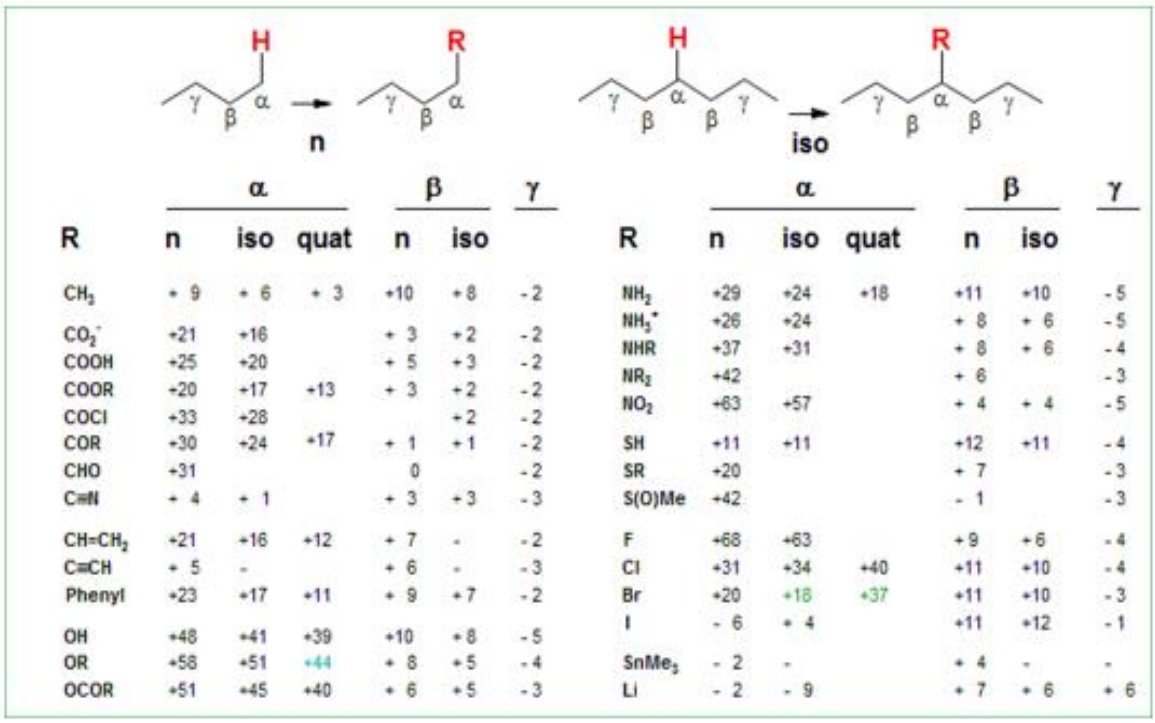
**CORREÇÕES**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 1°(1°) | 0 | 2°(1°) | 0 | 3°(1°) | 0 | 4°(1°) | -1.5 |
| 1°(2°) | 0 | 2°(2°) | 0 | 3°(2°) | -3.7 | 4°(2°) | -8.4 |
| 1°(3°) | -1.1 | 2°(3°) | -2.5 | 3°(3°) | -9.5 | 4°(3°) | -15.0 |
| 1°(4°) | -3.4 | 2°(4°) | -7.5 | 3°(4°) | -15.0 | 4°(4°) | -25.0 |

Correções devidas às ramificações ex: 1°(3°) = $CH_3$ (1°) ligado a um grupo $R_2C$ (3°)

| experimental | | calculado | desvio |
|---|---|---|---|
| 8.5 |  | -2.1 + α + β + 3γ + 1°(2°) = -2.1 + 9.1 + 9.4 - 7.5 + 0 = 8.9 | +0.4 |
| 36.5 | | -2.1 + 2α + 3β + 2°(1°) + 2°(4°) = -2.1 + 18.2 + 28.2 + 0 - 7.5 = 36.8 | +0.3 |
| 30.3 | | -2.1 + 4α + β + 4°(2°) + 3[4°(1°)] = -2.1 + 36.4 + 9.4 - 8.4 - 4.5 = 30.8 | +0.5 |
| 28.7 | | -2.1 + α + 3β + γ + 1°(4°) = -2.1 + 9.1 + 28.2 - 2.5 - 3.4 = 29.3 | +0.6 |

www2.chem.wisc.edu/areas/reich/nmr/06-crm-03-shift-effect.htm

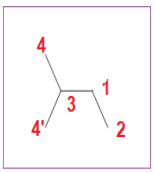



| R | α n | α iso | α quat | β n | β iso | γ |
|---|---|---|---|---|---|---|
| $CH_3$ | + 9 | + 6 | + 3 | +10 | + 8 | - 2 |
| $CO_2^-$ | +21 | +16 | | + 3 | + 2 | - 2 |
| COOH | +25 | +20 | | + 5 | + 3 | - 2 |
| COOR | +20 | +17 | +13 | + 3 | + 2 | - 2 |
| COCl | +33 | +28 | | | + 2 | - 2 |
| COR | +30 | +24 | +17 | + 1 | + 1 | - 2 |
| CHO | +31 | | | 0 | | - 2 |
| C≡N | + 4 | + 1 | | + 3 | + 3 | - 3 |
| $CH=CH_2$ | +21 | +16 | +12 | + 7 | - | - 2 |
| C≡CH | + 5 | - | | + 6 | - | - 3 |
| Phenyl | +23 | +17 | +11 | + 9 | + 7 | - 2 |
| OH | +48 | +41 | +39 | +10 | + 8 | - 5 |
| OR | +58 | +51 | +44 | + 8 | + 5 | - 4 |
| OCOR | +51 | +45 | +40 | + 6 | + 5 | - 3 |

| R | α n | α iso | α quat | β n | β iso | γ |
|---|---|---|---|---|---|---|
| $NH_2$ | +29 | +24 | +18 | +11 | +10 | - 5 |
| $NH_3^+$ | +26 | +24 | | + 8 | + 6 | - 5 |
| NHR | +37 | +31 | | + 8 | + 6 | - 4 |
| $NR_2$ | +42 | | | + 6 | | - 3 |
| $NO_2$ | +63 | +57 | | + 4 | + 4 | - 5 |
| SH | +11 | +11 | | +12 | +11 | - 4 |
| SR | +20 | | | + 7 | | - 3 |
| S(O)Me | +42 | | | - 1 | | - 3 |
| F | +68 | +63 | | + 9 | + 6 | - 4 |
| Cl | +31 | +34 | +40 | +11 | +10 | - 4 |
| Br | +20 | +18 | +37 | +11 | +10 | - 3 |
| I | - 6 | + 4 | | +11 | +12 | - 1 |
| $SnMe_3$ | - 2 | - | | + 4 | - | - |
| Li | - 2 | - 9 | | + 7 | + 6 | + 6 |

www2.chem.wisc.edu/areas/reich/nmr/06-crm-03-shift-effect.htm

Exemplo de uso das tabelas anteriores:

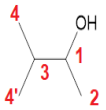
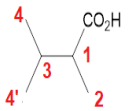
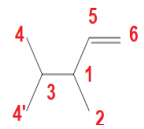



1 = 2α + 2β + 2°(1°) + 2°(3°) = 34,5

2 = 1α + 1β + 2γ + 1°(2°) = 19,1

3 = 3α + 1β + 2x 3°(1°) + 3°(1°) = 33

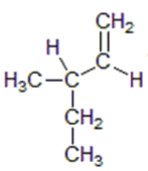
4 = 1α + 2β + 1γ + 1°(3°) = 27,1

| | | calculado | | experimental | |
|---|---|---|---|---|---|
|  | 1 | 34,5 + 41 = | 75 | 72,69 | 1 |
| | 2 | 19,1 + 8 = | 27 | 19,93 | 2 |
| | 3 | 33 + 8 = | 41 | 35,08 | 3 |
| | 4 | 27,1 - 5 = | 22 | 18,15 e 18,06 | 4 |
|  | 1 | 34,5 + 24 = | 58 | 52,29 | 1 |
| | 2 | 19,1 + 10 = | 19 | 20,57 | 2 |
| | 3 | 33 + 10 = | 43 | 35,25 | 3 |
| | 4 | 27,1 - 5 = | 22 | 18,29 e 18,60 | 4 |
|  | 1 | 34,5 + 20 = | 54 | 46,7 | 1 |
| | 2 | 19,1 + 3 = | 22 | 21,5 | 2 |
| | 3 | 33 + 3 = | 36 | 31,7 | 3 |
| | 4 | 27,1 - 2 = | 25 | 19,5 e 14,0 | 4 |
|  | 1 | 34,1 + 16 = | 50 | 45 | 1 |
| | 2 | 19,1 + 0 = | 19 | 16 | 2 |
| | 3 | 33 + 0 = | 33 | 32 | 3 |
| | 4 | 27,1 - 2 = | 25 | 20 e 20 | 4 |

$C_\gamma$-$C_\beta$-$C_\alpha$-**C**=C-$C_\alpha$'-$C_\beta$'-$C_\gamma$'

$\delta_c$(olefin) = 123.3 + $A_i$ + correções

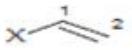
| $A_i$ | | correções | |
|---|---|---|---|
| α | 10.6 | α,α' (trans) | 0 |
| β | 7.2 | α,α' (cis) | -1.1 |
| γ | -1.5 | α,α | -4.8 |
| α' | -7.9 | α',α' | +2.5 |
| β' | -1.8 | β,β | +2.3 |
| γ' | +1.5 | | |




| | Obs | Calculated |
|---|---|---|
| | 112.9 | $\delta_{calc}$ = 123.3 + α' +2β' + γ' = 113.3 |
| | 144.9 | $\delta_{calc}$ = 123.3 + α + 2β + γ = 146.8 |

F.W. Wehrli & T.Wirthlin " Interpretation of C-13NMR Spectra", Wiley, 1974, p.41

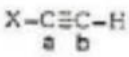
## Efeito dos substituintes em ALCENOS



(δ (X=H) = 123.3 ppm)

| X | $C_1$ | $C_2$ | | X | $C_1$ | $C_2$ | |
|---|---|---|---|---|---|---|---|
| F- | 24.9 | -34.3 | | HC(O)- | 13.6 | 13.1 | |
| Cl- | 3.3 | -5.4 | | MeC(O)- | 14.2 | 5.5 | |
| Br- | -7.2 | -3.3 | | HOC(O)- | 5.2 | 9.1 | |
| I- | -37.4 | 7.7 | | EtOC(O)- | 6.3 | 7.0 | |
| HO- | 25.7 | -35.3 | CC-72-724 | $H_2NC(O)$- | 7.1 | 4.3 | |
| MeO- | 30.3 | -37.3 | | N≡C- | -15.1 | 15.1 | |
| PhO- | 24.9 | -28.6 | ZOK-81-1143 | Ph- | 14.4 | -9.5 | |
| AcO- | 17.9 | -27.6 | | $CH_2$=CH- | 14.8 | -5.0 | |
| PhS- | 8.5 | -8.4 | ZOK-81-1143 | HC≡C- | -6.0 | 5.9 | |
| PhSe- | 4.3 | -4.7 | ZOK-81-1143 | $Me_3Si$- | 15.7 | 6.6 | MRC-89-72 |
| PhTe- | -12.4 | 4.0 | ZOK-81-1143 | $Cl_3Si$- | 8.7 | 16.1 | |
| C≡N- | -3.9 | -2.7 | | $Me_3Ge$- | 17.7 | 6.0 | MRC-89-72 |
| $O_2N$- | 22.3 | -0.9 | | $Vi_3Sn$- | 12.0 | -5.4 | |
| $Bu_3P$- | -4.3 | 17.9 | | $(BuO)_2B$- | 4.5 | 10.8 | |
| $Ph_2P$- | -3.6 | 22.4 | JA-75-2946 | $(Vi)_2B$- | - | 14.7 | JA-75-4527 |
| $Ph_2P(O)$- | 8.1 | 11.1 | | $Br_2B$- | - | 23.2 | JA-75-4527 |
| $H_2As$ | 2.9 | 8.2 | OM-94-1525 | Vi-Hg- | 34.9 | 11.0 | |
| $CH_3$- | 9.8 | -8.3 | | $(THFLi)_4$- | 59.7 | 9.4 | JA-93-10871 |
| $CH_3CH_2$- | 17.4 | -10.1 | | $(THFLi)_2$- | 67.5 | 5.6 | JA-93-10871 |
| $(CH_3)_2CH$- | 22.7 | -11.2 | | | | | |
| $(CH_3)_3C$- | 26.0 | -15.3 | | | | | |
| $HOCH_2$- | 14.2 | -5.4 | | | | | |
| $H_2NCH_2$- | 16.7 | -9.7 | | | | | |
| $ClCH_2$- | 11.7 | -4.7 | | | | | |
| $BrCH_2$- | 12.2 | -3.5 | | | | | |
| $ICH_2$- | 14.2 | -4.0 | | | | | |

## EFEITO DOS SUBSTITUINTES EM ALCINOS




| 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 |

Acesso em: http://coral.ufsm.br/quimica_organica/images/cnmr_calc_deslocqui.pdf

# EFEITO DOS SUBSTITUINTES DE UM ANEL AROMÁTICO RMN de C-13

## deslocamento padrão = 128,5 ppm

| Substituent | Ipso** | Orto | Meta | Para |
|---|---|---|---|---|
| H | 0.0 | 0.0 | 0.0 | 0.0 |
| $CH_3$ | 8.9 | 0.7 | -0.1 | -2.9 |
| $C_2H_5$ | 15.6 | -0.4 | 0.0 | -2.6 |
| *i*-$C_3H_7$ | 20.2 | -2.5 | 0.1 | -2.4 |
| *t*-$C_4H_9$ | 22.0 | -3.4 | -0.4 | -3.1 |
| $CH=CH_2$ | 9.5 | -2.0 | 0.2 | -0.5 |
| $C_6H_5$ | 13.1 | -1.1 | 0.4 | -0.2 |
| $CF_3$ | 2.6 | -3.3 | -0.3 | 3.2 |
| OH | 26.9 | -12.7 | 1.4 | -7.3 |
| $OCH_3$ | 31.4 | -14.4 | 1.0 | -7.7 |
| $OC_2H_5$ | 31.0 | -13.7 | 1.1 | -7.9 |
| $SCH_3$ | 10.2 | -1.8 | 0.4 | -3.6 |
| C(O)H | 9.0 | 1.2 | 1.2 | 6.0 |

G. C. Levy, R. L. Lichter, G. L. Nelson: Carbon-13 Nuclear Magnetic Resonance-Spectroscopy. John Wiley & Sons Ltd., New York

| Substituent | Ipso** | Orto | Meta | Para |
|---|---|---|---|---|
| C(O)OH | 2.1 | 1.5 | 0.0 | 5.1 |
| $C(O)CH_3$ | 9.1 | 0.1 | 0.0 | 4.2 |
| CN | -15.4 | 3.6 | 0.6 | 3.9 |
| $NH_2$ | 18.0 | -13.3 | 0.9 | -9.8 |
| $NHC(O)CH_3$ | 11.1 | -9.9 | 0.2 | -5.6 |
| $N(CH_3)_2$ | 22.6 | -15.6 | 1.0 | -11.5 |
| $NO_2$ | 20.0 | -4.8 | 0.9 | 5.8 |
| F | 34.8 | -12.9 | 1.4 | -4.5 |
| Cl | 6.2 | 0.4 | 1.3 | -1.9 |
| Br | -5.5 | 3.4 | 1.7 | -1.6 |

em $CCl_4$ exceto $CH=CH_2$ e $N(CH_3)_2$ (puros)

E. Breitmaier and W. Voelter. Carbon-13 NMR spectroscopy. VCH, Weinheim, 3rd Edition, 1987

**carbono ipso = carbono, do anel aromático, ligado ao substituinte**