

2.1 Introduction to Carbon-13 NMR of Natural Products

Direct observation of carbon atoms in carbon containing functional groups has been available on a practical basis only since the early 1970s. The ^{12}C nucleus is not magnetically active (spin number $I = 0$), but the ^{13}C nucleus like ^1H nucleus, has a spin number of $\frac{1}{2}$. The natural abundance of ^{13}C is only 1.1% that of ^{12}C , its sensitivity is about 1.6% that of ^1H and overall sensitivity of ^{13}C compared with ^1H is about 1/5700. The low natural abundance of ^{13}C (1.1%), relatively small gyromagnetic ratio and relatively long spin-relaxation time present difficulties in recording a ^{13}C -NMR spectrum by continuous-wave (CW) technique. A good spectrum is obtained by the Fourier Transform NMR (FT-NMR). The chemical shifts normally range between δ 0-200 ppm, and therefore, these represent the spread of chemical shifts of about twenty times that of proton. Carbon-13 NMR has emerged as an analytical tool of enormous power. It has been used to detect and study the structure of intermediates in organic reactions including carbocations, free radicals, and carbanions. ^{13}C NMR spectra for a vast variety of compounds from almost all series have been extensively investigated.

This subvolume includes Carbon-13 NMR data of natural products. Chemical shifts δ (in ppm) and coupling constants $^nJ(\text{HX})$ (in Hz) have been organized by arranging the gross formulae according to Hill's system as explained in the introduction (section 1.6). Chemical shifts (in ppm) are expressed relative to the signal of tetramethylsilane (TMS) as an internal standard. The prefix n in nJ indicates the number of bonds over which coupling is occurring.

Abbreviations

D_2O	–	Deuterium oxide	C_6D_6	–	Benzene- d_6
$\text{C}_5\text{D}_5\text{N}$	–	Pyridine- d_5	$\text{DMSO-}d_6$	–	Dimethyl sulfoxide- d_6
CD_3OD	–	Methanol- d_4	CF_3COOD	–	Trifluoroacetic acid- d
n.a.	–	Not assigned	n.d.	–	Not detected
n.m.	–	Not measured	n.o.	–	Not observed due to solvent signal
n.r.	–	Not reported	ax	–	Axial
eq.	–	Equatorial	Ac	–	Acetyl (COCH_3)
Bz	–	Benzoyl	Glc or G	–	Glucose
Nic	–	Nicotinoyl	Rh	–	Rhamnose
iBu	–	Isobutyl	Gem	–	Geminal
Api	–	Apiosyl	Xyl	–	Xylose
Ph(i)	–	Phenyl ipso	Ph(o)	–	Phenyl ortho
Ph(m)	–	Phenyl meta	Ph(p)	–	Phenyl para
Ar or Ph or ϕ	–	Phenyl	Tigl	–	Tiglate
*, **	–	Assignment with same superscript may be interchanged			
R, S	–	Denote configuration (R = Rectus; S = Sinister)			
E, Z	–	Denote configuration (E = Entgegen; Z = Zusammen)			
ff	–	Signal hidden in solvent or overlapped with solvent signal			