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Analogous to the importance of ^{13}C isotropic shieldings for chemical analysis of liquids with nuclear magnetic resonance spectroscopy, ^{13}C chemical shielding anisotropies are proving to be valuable in the characterization of solids. Specifically, molecular geometry is revealed by the full shielding anisotropy and molecular motion may be characterized by changes in the powder pattern. In particular, the principal components of the shielding reveal differences in bonding geometry which may not be correlated to monotonic changes in the isotropic shift. This report is a comprehensive, critical compilation of ^{13}C chemical shieldings in solids, organized by carbon functionality. From these data, representative shieldings of common carbon functionalities are calculated.

Key words: ^{13}C chemical shielding; chemical shift anisotropy; critical review; nuclear magnetic resonance; solid state.

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1. Introduction

The chemical shielding at a nucleus in a diamagnetic material is the magnetic field caused by electronic currents induced by an applied magnetic field.[1,2] The applied field causes two effects: (1) induced precession of electron orbits, quenched by electrostatic charges of the molecule (diamagnetic contribution) and (2) mixing of the electronic ground state with excited states, which polarizes the electron distribution and thus alters the current path (paramagnetic contribution). The diamagnetic effect decreases the net magnetic field at a nucleus, whereas the paramagnetic effect increases the field. Both effects, and therefore the net chemical shielding, are proportional to the applied magnetic field. Consequently, chemical shieldings are reported as fractional shifts of the applied magnetic field, relative to the shift of an arbitrary liquid standard. For ^{13}C, chemical shifts are generally ~0.001%–0.02% (10–200 ppm) of the applied field and the standard shift reference is tetramethylsilane (TMS).

The orientational anisotropy of the chemical shielding may be represented by a second-rank, dimensionless Cartesian tensor, $\boldsymbol{\sigma}$.[3–5] Each chemically and crystallographically distinct site has a distinct chemical shielding tensor. The trace of $\boldsymbol{\sigma}$ yields the isotropic shift, σ_{iso}, which is the observed shift of molecular sites undergoing rapid isotropic reorientation, such as liquids. The chemical shift of a fixed

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site in a given orientation, σ_{obsd}, is given by Eq. (1), where H_0 is the applied field vector, I is the spin vector, and all quantities are expressed in laboratory frame coordinates:

$$\sigma_{\text{obsd}} = \frac{H_0 \cdot \sigma_{\text{lab}} \cdot I}{|H_0|} . \qquad (1)$$

There exists a unique coordinate frame in which σ is diagonal; this frame is termed the principal axis system of the chemical shielding. The shielding tensor in the principal axis frame, σ_{pas}, is related to the tensor in the laboratory frame by a rotational transformation as given in Eq. (2), where $R(\theta,\phi)$ is the rotation matrix about polar angles θ and ϕ, the orientation of H_0 in the principal axis system,

$$\sigma_{\text{pas}} = R(\theta,\phi)\sigma_{\text{lab}} R^{-1}(\theta,\phi) . \qquad (2)$$

Equations (1) and (2) yield Eq. (3), a useful expression for the observed shielding in terms of the principal shielding components ($\sigma_{xx}, \sigma_{yy}, \sigma_{zz}$), and the orientation of H_0 relative to the principal axis frame.

$$\sigma_{\text{obsd}} = \sigma_{xx} \sin^2\theta \cos^2\phi + \sigma_{yy} \sin^2\theta \sin^2\phi + \sigma_{zz} \cos^2\phi . \qquad (3)$$

The spectrum of a powder, in which all orientations are present, is a broad pattern spanning the range σ_{xx} to σ_{zz}. The lineshape of the powder pattern $I(\sigma)$, which may be obtained by integration of Eq. (3), is given in Eq. (4), where $K(\theta)$ is the complete elliptic integral of the first kind,[3,5]

$$I(\sigma) = \begin{cases} \dfrac{1}{\pi\Delta_1} K\left[\arcsin\left(\dfrac{\Delta_2}{\Delta_1}\right)^{1/2}\right], & \text{for } \sigma_{yy} \leqslant \sigma \leqslant \sigma_{zz} \\ \dfrac{1}{\pi\Delta_2} K\left[\arcsin\left(\dfrac{\Delta_1}{\Delta_2}\right)^{1/2}\right], & \text{for } \sigma_{xx} \leqslant \sigma \leqslant \sigma_{yy}, \end{cases} \qquad (4)$$

such that

$$\Delta_1 = [(\sigma_{zz} - \sigma_{yy})(\sigma - \sigma_{xx})]^{1/2}$$
$$\Delta_2 = [(\sigma_{zz} - \sigma)(\sigma_{yy} - \sigma_{xx})]^{1/2} .$$

Equation (4) holds for $\sigma_{xx} \leqslant \sigma_{yy} \leqslant \sigma_{zz}$; analogous expressions are readily obtained for permutations of the shielding assignments.

The principal components of the chemical shielding may be determined experimentally using nuclear magnetic resonance (NMR) spectroscopy, detailed below. There are two primary obstacles to ^{13}C measurements: (1) poor spectral intensity due to low natural abundance, usually overcome by isotopic enrichment and/or cross-polarization techniques, and (2) spectral broadening caused by adjacent nuclear dipoles (especially ^{1}H and ^{19}F), which may be suppressed routinely by various rf irradiation schemes.[3,4] The orientation of the chemical shielding principal axis system relative to the molecular axis frame is not always obtained with the principal shielding components. Determination of the orientational parameters requires a known relation between the observed chemical shift and coordinates of the molecule. Single crystals fulfill this requirement and have provided most of the orientational parameters to date, but single crystals are not always available. Nuclear dipoles adjacent to the nuclear site of interest (e.g., ^{1}H, ^{13}C, ^{14}N, and ^{19}F) can serve as reference points on the molecule and can furnish orientational parameters via more complex two-dimensional chemical shift–dipolar coupling experiments.[6–9] Finally, for nuclear sites with threefold or higher rotational symmetry, the orientational parameters may be assigned; two shielding components are degenerate ($\sigma_{xx} = \sigma_{yy}$ or $\sigma_{yy} = \sigma_{zz}$) and this shielding corresponds to shielding perpendicular to the symmetry axis. Because the orientation of the chemical shielding principal axes is reported for only about 10% of the molecules studied, this information is not included in these compilation.

2. Criteria for Selection of Data

The principal shielding components of a nuclear site may be derived from the results of any of at least four NMR experiments: (1) the angular dependence of the chemical shielding of single crystals, (2) the observed shift of molecules oriented in a liquid crystal, (3) the line shape of a powder, and (4) reconstruction from sideband intensities observed with magic-angle spinning. Each technique has inherent advantages and caveats, as discussed in detail elsewhere.[5] Parameters derived from rotation patterns of single crystals yield the most reliable results, owing to unambiguous spectral assignments and good spectral resolution. Liquid crystal studies are effective only for molecules composed of a few atoms (four or less) and are essentially equivalent to a single crystal study at one orientation. Also, any asymmetry in the shielding of the guest molecule about the azimuthal angle is generally averaged out and thus liquid crystal studies assume the chemical shielding is axially symmetric, which is valid only for threefold or higher rotational symmetry at the carbon site. Liquid crystal studies should be examined carefully; these studies are identified in Tables 1–10 by the notation "(lc)" in the temperature column. Studies of powder patterns are reliable if the principal components are obtained by a fit of the data to the expression for the powder pattern, Eq. (4). Shielding parameters obtained by visual estimation of the discontinuities in the line shape are less accurate; studies with spectra that do not resemble powder patterns (cf. Figs. 1–3) are not included here. This report does not contain chemical shieldings obtained with spin-rotation methods in which the spin-rotation tensor is measured in the gas phase (preferably using a molecular beam) and the magnetic shielding tensor is calculated with theoretical relationships. Chemical shielding anisotropies obtained by spin-rotation studies are not included because they are generally found to be inaccurate, as revealed by a lack of agreement with subsequent results obtained by one of the four aforementioned techniques.

3. Description of Tables

3.1. Data Tables

This report is a compilation of the ^{13}C NMR spectra of over 350 distinct carbon sites in the solid state, obtained from literature reports of experimental studies of over 200 compounds. The data are presented in Tables 1–10 organized into ten functional groups: paraffinic, olefinic, acetylenic, alcohols and ethers, aldehydes and ketones, carboxylic acids and esters, carbon–nitrogen species, aromatics, carbon

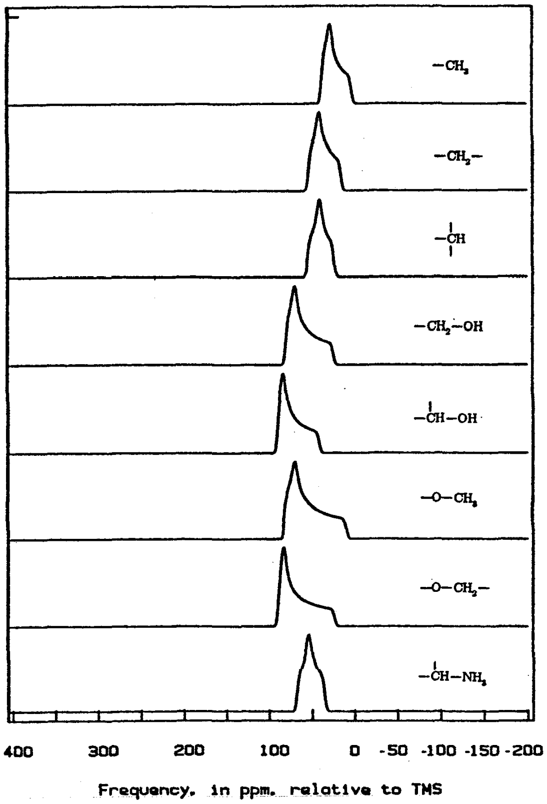

FIG. 1. Typical ^{13}C chemical shielding powder patterns of sp^3-hybridized carbon functionalities, calculated from the data in Tables 1–10. All spectra are convoluted with Lorentzian broadening of halfwidth 2 ppm. A dangling bond in the chemical structures implies a bond to a carbon atom.

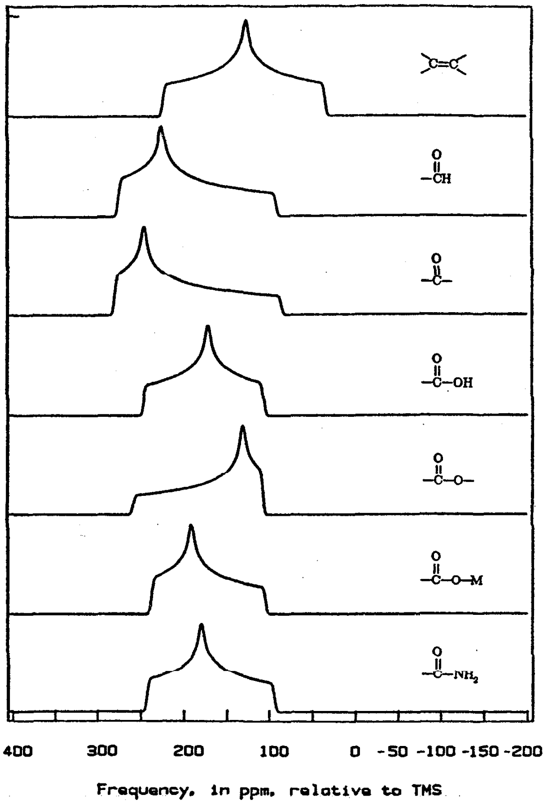

FIG. 2. Typical ^{13}C chemical shielding powder patterns of sp^2-hybridized carbon functionalities, calculated from the data in Tables 1–10. All spectra are convoluted with Lorentzian broadening of halfwidth 2 ppm. A dangling bond in the chemical structures implies a bond to a carbon atom.

monoxide and inorganic carbonyls, and miscellaneous. Each entry contains the compound name (proper and common), the structural chemical formula, the temperature of the measurement, the three chemical shielding principal components, the isotropic shift, and the literature reference. All studies meeting the above criteria were included, thus some species have multiple entries. The shieldings are reported relative to TMS, on the δ scale, such that downfield shifts are positive. Studies with frequency references other than TMS were converted using the isotropic shifts given in Stothers's monograph.[10] The most common alternate references are benzene (128.7 ppm relative to TMS on the δ scale) and CS_2 (192.8 ppm). When no shift reference is given, the isotropic shift of the solid is taken as that of the liquid, given in Stothers's monograph; these entries are indicated by a footnote in the tables. The convention for the relative assignment of the Cartesian components σ_{xx}, σ_{yy}, and σ_{zz} varies with investigator. The principal components are tabulated here as σ_{11}, σ_{22}, and σ_{33}, such that $\sigma_{11} \leqslant \sigma_{22} \leqslant \sigma_{33}$, with no inference to the Cartesian axes. In some cases the principal components were calculated from reports of the anisotropy and asymmetry, definitions of which also vary. Some define the anisotropy as the total width of the powder pattern ($\sigma_{11} - \sigma_{33}$), whereas others define it as the difference between the isotropic shift and the extreme shielding component ($\sigma_{11} - \sigma_{\rm iso}$, or $\sigma_{\rm iso} - \sigma_{33}$). However, in each of these cases the principal components were obtained without ambiguity.

The quality of the experimental data vary and confidence limits (when reported) range from ± 20 to ± 0.2 ppm; confidence limits are not tabulated here. The tabulated data are not corrected for second-order dipolar perturbations, which are typically $\leqslant 1$ ppm upfield.[11] It is important to note the temperature at which each spectrum was obtained because some species (especially methyl and aromatic groups) may possess some residual motion and the spectrum will not reflect the full anisotropy. Residual motional averaging is often indicated by the degeneracy of two principal shielding components for a site that does not have C_{3v} (or higher) symmetry. In summary, readers are advised to consult the original references to assess individual spectra.

3.2. Summary Table

Table 11 contains the typical shielding components for 23 carbon functionalities, obtained from averages of the data in Tables 1–10. Only the spectra of compounds free of conformational restraints were used in the averages (e.g., no data from cyclic compounds with other than six atoms). In some cases, these typical spectra are based on small data bases and are expected to change as more spectra are reported and as accuracy improves. Powder patterns of the 23

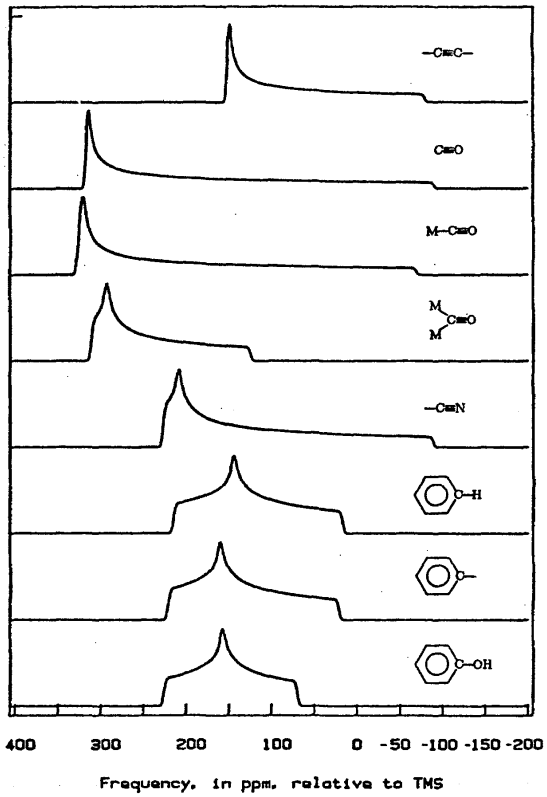

FIG. 3. Typical ^{13}C chemical shielding powder patterns of *sp*-hybridized carbon functionalities and aromatic carbon, calculated from the data in Tables 1–10. All spectra are convoluted with Lorentzian broadening of halfwidth 2 ppm. A dangling bond in the chemical structures implies a bond to a carbon atom.

functionalities, generated with Eq. (4) and the data in Table 11, are shown graphically in Figs. 1–3.

The standard deviations of the average components in Table 11 suggest the degree of variation within a carbon functionality. Several studies of homologous series of compounds offer discussions for trends within a group. Such studies include alkenes and cycloalkenes,[12] methylene carbons,[13] methylidyne carbons,[14] polyalkylbenzenes,[15] halobenzenes,[16] metallocenes,[17] pyridine and diazines,[18] metal acetates,[19] metal carbonyls,[20] and linear and pseudolinear molecules.[21] Finally, insightful discussions of general trends are offered in recent reviews.[4,5,22]

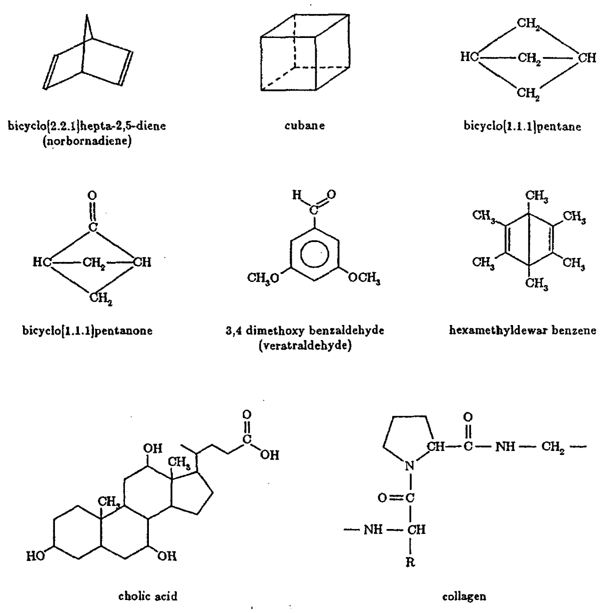

FIG. 4. Structural formulas of selected compounds.

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TABLE 1. Paraffinic carbons

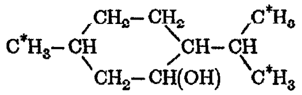
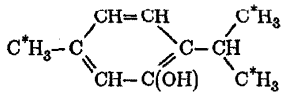
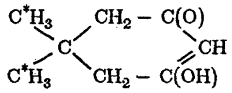
Compound	Formula	T (K)	Chemical shielding parameters[(a)]				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
Methyl carbons							
n-eicosane	$C^*H_3CH_2(CH_2)_{16}CH_2C^*H_3$	RT	26	22	3	17	VanderHart (1976)
ethanol	$C^*H_3CH_2OH$	103	25	16	1	14	Pines *et al.* (1972)
trans-2-butene	$C^*H_3CH_2{=}\ CH_2C^*H_3$	30	27	27	5	20	Zilm *et al.* (1980)
cis-2-butene	$C^*H_3CH_2{=}\ CH_2C^*H_3$	30	28	6	6	13	Zilm *et al.* (1980)
dimethyl acetylene (2-butyne)	$C^*H_3C\equiv CC^*H_3$	87	16	16	2	11	Pines *et al.* (1972)
diethyl ether	$(C^*H_3CH_2)_2O$	133	29	19	5	18	Pines *et al.* (1972)
methyl benzene (toluene)	$C_6H_5C^*H_3$	87	33	22	5	20	Pines *et al.* (1972)
1,4 dimethyl benzene (*p*-xylene)	$C_6H_4(C^*H_3)_2$	100	34	23	2	18	Van Dongen Torman and Veeman (1978)
1,2,4,5 tetramethyl benzene (durene)	$C_6H_2(C^*H_3)_4$	RT	31 30	24 24	2 3	20 19	Pausak *et al.* (1973)
hexamethyl benzene	$C_6(C^*H_3)_6$	87 RT	25 18	25 17	25 16	25 17	Pines *et al.* (1972) Pausak *et al.* (1974)
hexamethyl dewar benzene	$(CC^*H_3)_4(CC^*H_3)_2$ (see Fig. 4)	87	11	11	11	11	Pines *et al.* (1972)
hexaethyl benzene	$C_6(CH_2C^*H_3)_6$	RT	27	16	6	16	Pausak *et al.* (1974)
2-isopropyl, 5-methyl-cyclohexanol (1-menthol)[(b)]		RT	36	25	2	21	Maciel *et al.* (1985)
2-isopropyl, 5-methyl-phenol (thymol)[(b)]		RT	34	24	0	19	Maciel *et al.* (1985)
dimedone		RT	51 47	42 33	3 -1	32 26	Takegoshi *et al.* (1985)
acetaldehyde	C^*H_3CHO	87 15	55 53	43 40	3 -1	34 33	Pines *et al.* (1972) Zilm and Grant (1981)
dimethyl ketone (acetone)	$C^*H_3C(O)C^*H_3$	87	48	48	-2	31	Pines *et al.* (1972)

TABLE 1. Paraffinic carbons—Continued

Compound	Formula	T (K)	Chemical shielding parameters[(a)]				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
Methyl carbons, continued							
methylphenyl ketone (acetophenone)	$(C_6H_5)C(O)C^*H_3$	100	42	31	0	24	Van Dongen Torman *et al.* (1978)
1,1,2,2-tetra-acetylethane	$C^*H_3C(OH){=}CC(O)CH_3$	RT	35	32	3	23	Takegoshi and McDowell (1986)
	$CH_3C(OH){=}CC(O)C^*H_3$	RT	40	39	6	28	
thioacetic acid	C^*H_3COSH	87	56	49	0	35	Waugh *et al.* (1973)
acetic acid	C^*H_3COOH	87	46	46	11	34	Pines *et al.* (1972)
		90	40	27	6	24	Van Dongen Torman *et al.* (1974)
L-alanine	$NH_3CH(C^*H_3)COOH$	RT	31	22	8	20	Naito *et al.* (1981)
L-threonine	$C^*H_3CH(OH)CH(NH_3)COOH$	RT	32	23	1	19	Janes *et al.* (1983)
acetic anhydride	$(C^*H_3CO)_2O$	91	39	36	1	25	Pines *et al.* (1972)
methyl acetate	$C^*H_3COOCH_3$	133	43	40	22	35	Pines *et al.* (1972)
ammonium acetate	$NH_4(C^*H_3COO)$	RT	46	27	-4	23	Ganapathy *et al.* (1984b)
lithium acetate	$Li(C^*H_3COO)$	RT	41	33	3	24	Ganapathy *et al.* (1984b)
potassium acetate	$K(C^*H_3COO)$	RT	50	28	7	26	Ganapathy *et al.* (1984b)
magnesium acetate	$Mg(C^*H_3COO)_2$	RT	42	25	-4	23	Ganapathy *et al.* (1984b)
strontium acetate	$Sr(C^*H_3COO)_2$	RT	50	30	5	25	Ganapathy *et al.* (1984b)
lanthanum acetate	$La(C^*H_3COO)_2$	RT	41	31	1	24	Ganapathy *et al.* (1984b)
silver acetate	$Ag(C^*H_3COO)$	87	35	29	-7	19	Pines *et al.* (1972)
zinc acetate	$Zn(C^*H_3COO)_2$	RT	36	25	-3	20	Ganapathy *et al.* (1984b)
cadmium (II) acetate dihydrate	$Cd(C^*H_3COO)_2$	RT	42	30	0	24	Ganapathy *et al.* (1984a)
			41	29	-1	23	
dimethyl dimethoxy silane	$Si(C^*H_3)_2(CH_3O)_2$	87	-3	-3	-3	-3	Pines *et al.* (1974)
octamethyl cyclotetra-siloxane	$(-Si(CH_3)_2O-)_4$	87	1	1	1	1	Waugh *et al.* (1973)
hexamethyl disiloxane	$(C^*H_3)_3Si-O-Si(C^*H_3)_3$	87	5	5	5	5	Waugh *et al.* (1973)

TABLE 1. Paraffinic carbons—Continued

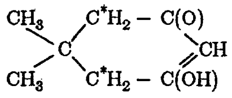
Compound	Formula	T (K)	Chemical shielding parameters[a]				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
Methyl carbons, continued							
trimethyl phosphine	$P(CH_3)_3$	(lc)	16	16	16	16	Albrand *et al.* (1977)
trimethyl phosphorus oxide	$O{=}P(CH_3)_3$	(lc)	25	25	-9	14	Albrand *et al.* (1977)
trimethyl phosphorus sulfide	$S{=}P(CH_3)_3$	(lc)	24	24	16	21	Albrand *et al.* (1977)
trimethyl phosphorus selenide	$Se{=}P(CH_3)_3$	(lc)	27	27	9	21	Albrand *et al.* (1977)
methyl fluoride	CH_3F	15	105	105	15	75	Zilm and Grant (1981)
		(lc)	104	104	17	75	Jokisaari *et al.* (1986)
methyl iodide	CH_3I	(lc)	32	32	-1	21	Yannoni and Whipple (1967)
Methylene carbons							
n-eicosane	$CH_3C^*H_2(CH_2)_{16}C^*H_2CH_3$	RT	37	30	15	27	VanderHart (1976)
	$CH_3CH_2(C^*H_2)_{16}CH_2CH_3$	RT	50	38	17	35	
polyethylene	$(-CH_2-)_x$	RT	52	39	14	35	Opella and Waugh (1977)
		RT	50	37	13	33	Urbina and Waugh (1974)
polymethyl-methacrylate	$(-C^*H_2C(CH_3)(C(O)(OCH_3))-)_n$	RT	79	48	29	52	Edzes (1983)
poly(vinylidene fluoride)	$(-C^*H_2CF_2-)_n$	297	56	49	30	45	Fleming *et al.* (1980)
L-asparagine monohydrate	$NH_2C(O)C^*H_2CH(NH_3)COOH$	RT	49	43	16	36	Naito and McDowell (1984)
malonic acid	$HOOCC^*H_2COOH$	RT	62	50	18	43	Tegenfeldt *et al.* (1980)
ammonium hydrogen malonate	$(OOCC^*H_2COO)(H)(NH_4)$	RT	63	52	19	45	Chang *et al.* (1975)
dihydro muconic acid	$HOOCC^*H_2CH{=}CHC^*H_2COOH$	RT	40	38	7	28	Wolff *et al.* (1977)
hexaethyl benzene	$C_6(C^*H_2CH_3)_6$	RT	27	25	7	20	Pausak *et al.* (1974)
malononitrile	$N{\equiv}CC^*H_2C{\equiv}N$	20	30	11	-11	10	Facelli *et al.* (1985)
dimedone		RT	57	48	28	44	Takegoshi *et al.* (1985)
			61	55	33	49	

TABLE 1. Paraffinic carbons—Continued

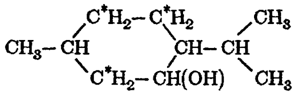
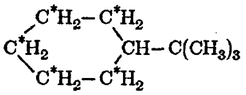
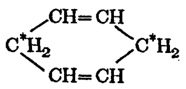
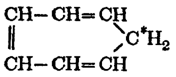
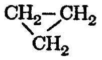
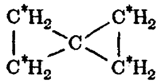
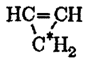
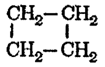
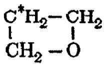
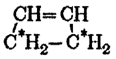
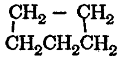
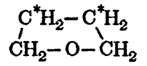
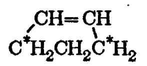
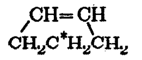
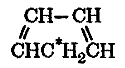
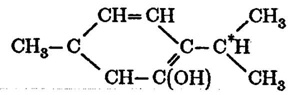
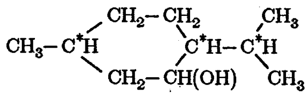
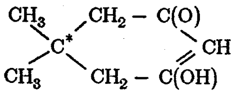
Compound	Formula	T (K)	Chemical shielding parameters(a)				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
Methylene carbons, continued							
2-isopropyl, 5-methyl-cyclohexanol (1-menthol)(b)		RT	33 48 72	27 38 52	21 30 24	27 39 50	Maciel *et al.* (1985)
tert-butyl-cyclohexane		20	57	25	9	30	Facelli *et al.* (1985)
1,4-cyclohexadiene		20	44	21	10	25	Facelli *et al.* (1985)
1,3,5-cyclo-heptatriene (tropilidene)		20	55	25	16	32	Facelli *et al.* (1985)
cyclopropane		20	22	2	-36	-4	Zilm *et al.* (1981)
spiropentane (bowtie-ane)		20	37	16	-23	10	Facelli *et al.* (1985)
bicyclo[2.2.1]hepta-2,5-diene (norbornadiene)	C_7H_8 (see Fig. 4)	20	97	69	63	76	Facelli *et al.* (1985)
bicyclo[1.1.1]pentane	C_5H_8 (see Fig. 4)	20	56	54	38	49	Facelli *et al.* (1985)
bicyclo[1.1.1]pentanone	C_5H_6O (see Fig. 4)	20	87	47	1	45	Facelli *et al.* (1985)
cyclopropene		20	40	29	-59	3	Zilm *et al.* (1980)
cyclobutane		20	39	23	14	25	Facelli *et al.* (1985)
trimethylene oxide (oxetane)		20	41	22	4	22	Facelli *et al.* (1985)
cyclobutene		30	43	33	23	33	Zilm *et al.* (1980)

TABLE 1. Paraffinic carbons—Continued

Compound	Formula	T (K)	Chemical shielding parameters[a]				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
Methylene carbons, continued							
cyclopentane		20	49	21	12	27	Facelli *et al.* (1985)
1,4-epoxybutane (tetrahydrofuran)		20	52	17	17	29	Facelli *et al.* (1985)
cyclopentene		30	52	30	12	31	Zilm *et al.* (1980)
		30	39	22	7	23	Zilm *et al.* (1980)
1,3-cyclopentadiene		20	51	39	33	41	Facelli *et al.* (1985)
Methylidyne carbons							
2-methyl propane (isobutane)	$CH_3C^*H(CH_3)CH_3$	20	26	26	22	25	Facelli *et al.* (1986)
2-isopropyl, 5-methyl phenol (thymol)[b]		RT	30	24	21	25	Maciel *et al.* (1985)
2-isopropyl, 5-methyl cyclohexanol (1-menthol)[b]		RT	36 42 64	26 36 48	21 30 44	28 36 52	Maciel *et al.* (1985)
bicyclo[2.2.1]hepta-2,5-diene (norbornadiene)	C_7H_8 (see Fig. 4)	20	58	56	32	49	Facelli *et al.* (1986)
bicyclo[1.1.1]pentane	C_5H_8 (see Fig. 4)	20	42	42	17	34	Facelli *et al.* (1986)
bicyclo[1.1.1]pentanone	C_5H_6O (see Fig. 4)	20	101	47	21	56	Facelli *et al.* (1986)
cubane	$(CH)_8$ (see Fig. 4)	6 20	71 62	35 35	35 35	47 44	Facelli *et al.* (1986)
Quaternary carbons							
polymethyl-methacrylate	$(-CH_2C^*(CH_3)(C(O)(OCH_3))-)_n$	RT	53	43	37	44	Edzes (1983)
hexamethyl dewar benzene	$(CCH_3)_4(C^*CH_3)_2$ (see Fig. 4)	87	72	57	43	57	Pines *et al.* (1972)
dimedone		RT	38	34	30	34	Takegoshi *et al.* (1985)
diamond	C_n	RT RT	33 36	33 36	33 36	33 36	Duijvestijn *et al.* (1983) Retcofsky and Friedel (1973)

(a) relative to TMS (tetramethylsilane), on the δ scale, such that $C_6H_{6(l)}$ = 128.7 ppm and CS_2 = 192.8 ppm (*i.e.*, upfield is negative).
(b) peak assignments not given in original reference; assignments proposed here are based on isotropic shifts given in Stothers (1972).
(lc) oriented in a liquid crystal, only anisotropy given; principal components calculated by assuming isotropic shift is that of neat liquid given in Stothers (1972).

TABLE 2. Olefinic carbons

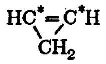
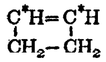
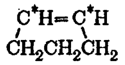
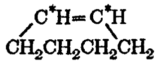
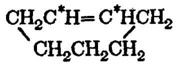
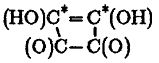
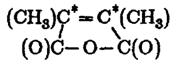
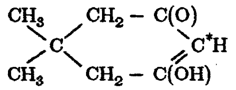
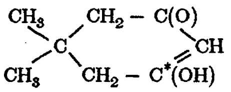
Compound	Formula	T (K)	Chemical shielding parameters$^{(a)}$				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
ethylene	$C^*H_2{=}C^*H_2$	30	234	120	24	126	Zilm *et al.* (1980)
trans-2-butene	$CH_3C^*H_2{=}C^*H_2CH_3$	30	232	113	37	127	Zilm *et al.* (1980)
cis-2-butene	$CH_3C^*H_2{=}C^*H_2CH_3$	30	232	119	22	124	Zilm *et al.* (1980)
cis-1,4-polybutadiene	$(-CH_2C^*H{=}C^*HCH_2-)_n$	123	236	115	35	129	Fleming *et al.* (1980)
dihydro muconic acid	$HOOCCH_2C^*H{=}C^*HCH_2COOH$	RT	211	106	30	115	Wolff *et al.* (1977)
trans-polyacetylene	$({=}CH{=})_n$	RT	220	142	51	137	Resing *et al.* (1982)
		RT	218	138	22	126	Terao *et al.* (1984a)
		RT	217	143	45	135	Manenschijn *et al.* (1984)
cis-polyacetylene	$({=}CH{=})_n$	RT	221	137	20	126	Resing *et al.* (1982)
		RT	219	144	47	137	Terao *et al.* (1984a)
propenoic acid, amide (acrylamide)	$C^*H_2{=}CHC(O)NH_2$	RT	223	136	25	128	Igner and Fiat (1982)
	$CH_2{=}C^*HC(O)NH_2$		220	123	50	131	
1,1,2,2-tetra-acetylethane	$CH_3C^*(OH){=}CC(O)CH_3$	RT	267	216	86	190	Takegoshi and McDowell (1986)
	$CH_3C(OH){=}C^*C(O)CH_3$	RT	209	87	35	110	
allene	$C^*H_2{=}C{=}C^*H_2$	20	158	54	23	78	Beeler *et al.* (1984)
	$CH_2{=}C^*{=}CH_2$	20	233	233	175	214	
ketene	$CH_2{=}C^*{=}O$	20	265	239	77	194	Beeler *et al.* (1984)
	$C^*H_2{=}C{=}O$	20	39	4	-27	3	
1,3 dioxo propadiene (dioxoallene)	$O{=}C^*{=}C{=}C^*{=}O$	20	235	235	-90	127	Beeler *et al.* (1984)
	$O{=}C{=}C^*{=}C{=}O$	20	24	24	-90	-14	
cyclopropene	 $HC^*{=}C^*H$ CH_2	20	239	79	5	108	Zilm *et al.* (1980)
cyclobutene	 $C^*H{=}C^*H$ CH_2-CH_2	30	244	138	30	137	Zilm *et al.* (1980)
cyclopentene	 $C^*H{=}C^*H$ $CH_2CH_2CH_2$	30	235	118	39	131	Zilm *et al.* (1980)
cyclohexene	 $C^*H{=}C^*H$ $CH_2CH_2CH_2CH_2$	30	236	123	23	127	Zilm *et al.* (1980)
cycloheptene	 $CH_2C^*H{=}C^*HCH_2$ $CH_2CH_2CH_2$	30	245	126	27	133	Zilm *et al.* (1980)

TABLE 2. Olefinic carbons—Continued

Compound	Formula	T (K)	Chemical shielding parameters(a)				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
cis-cyclooctene	C_8H_{14}	30	240	123	28	130	Zilm *et al.* (1980)
trans-cyclooctene	C_8H_{14}	30	238	127	37	134	Zilm *et al.* (1980)
squaric acid (3,4-dihydroxy-3-cyclobutene 1,2dione)	 $(HO)C^*{=}C^*(OH)$ $(O)C{-}C(O)$	RT	264	209	102	192	Mehring and Becker (1981)
			265	208	102	192	
hexamethyl dewar benzene	$(C^*CH_3)_4(CCH_3)_2$ (see Fig. 4)	87	244	149	55	149	Pines *et al.* (1972)
dimethyl maleic anhydride	 $(CH_3)C^*{=}C^*(CH_3)$ $(O)C{-}O{-}C(O)$	RT	252	129	45	142	Igner and Fiat (1982)
			249	126	44	140	
dimedone		RT	158	108	43	103	Takegoshi *et al.* (1985)
		RT	298	188	76	187	Takegoshi *et al.* (1985)

(a) relative to TMS (tetramethylsilane), on the δ scale, such that $C_6H_{6(l)}$ = 128.7 ppm and CS_2 = 192.8 ppm (*i.e.*, upfield is negative).

TABLE 3. Acetylenic carbons

Compound	Formula	T (K)	Chemical shielding parameters(a)				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
acetylene	$HC{\equiv}CH$	30	150	150	-90	70	Zilm *et al.* (1978)
		(b)	154	154	-99	70	Englert (1972)
diacetylene	$HC{\equiv}C{-}C{\equiv}CH$	163	138	138	-80	66	Cross and Waugh (1977)
1-propyne	$CH_3C{\equiv}C^*H$	20	140	140	-74	69	Beeler *et al.* (1984)
	$CH_3C^*{\equiv}CH$	20	166	166	-93	80	
dimethyl acetylene (2-butyne)	$CH_3C^*{\equiv}C^*CH_3$	87	158	158	-44	91	Pines *et al.* (1972)
		(lc)	149	149	-77	74	Diehl and Moia (1983)
		20	152	152	-75	76	Beeler *et al.* (1984)
lithium acetylide	Li_2C_2	RT	308	308	33	216	Duncan (1986)
sodium acetylide	Na_2C_2	RT	292	292	-72	171	Duncan (1986)
calcium acetylide	CaC_2	RT	313	313	-37	196	Duncan (1986)
strontium acetylide	SrC_2	RT	322	322	-3	214	Duncan (1986)
barium acetylide	BaC_2	RT	320	320	45	228	Duncan (1986)

(a) relative to TMS (tetramethylsilane), on the δ scale, such that $C_6H_{6(l)}$ = 128.7 ppm and CS_2 = 192.8 ppm (*i.e.*, upfield is negative).
(lc) oriented in a liquid crystal, only anisotropy given; principal components calculated by assuming isotropic shift is that of neat liquid given in Stothers (1972).

TABLE 4. Alcohols and ethers

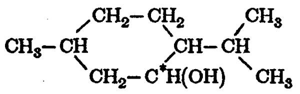
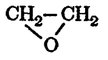
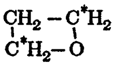
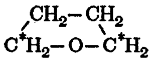
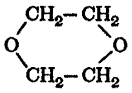
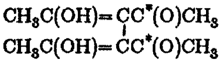
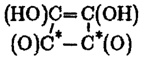
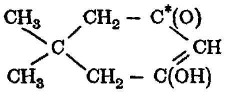
Compound	Formula	T (K)	Chemical shielding parameters(a)				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
Alcohols							
methanol	CH_3OH	87	74	74	11	53	Pines *et al.* (1972)
		4.2	84	76	10	56	Strub *et al.* (1982)
ethanol	$CH_3C^*H_2OH$	103	73	73	16	54	Pines *et al.* (1972)
L-serine monohydrate	$NH_3CH(C^*H_2OH)COOH$	RT	86	66	34	62	Naito *et al.* (1983)
2-isopropyl, 5-methyl cyclohexanol (1-menthol)(b)		RT	94	84	42	73	Maciel *et al.* (1985)
ammonium *d*-tartrate	$(-C^*H(OH)COONH_4)_2$	RT	87	81	55	74	Pines *et al.* (1974)
L-threonine	$CH_3C^*H(OH)CH(NH_3)COOH$	RT	83	74	39	65	Janes *et al.* (1983)
cholic acid(b)	$C_{24}H_{40}O_5$ (see Fig. 4)	RT	94	83	35	71	Maciel *et al.* (1985)
			93	88	36	72	
			91	87	46	75	
Ethers							
methyl formate	$HCOOC^*H_3$	87	76	64	8	49	Pines *et al.* (1972)
methyl acetate	$CH_3COOC^*H_3$	133	92	76	8	59	Pines *et al.* (1972)
polymethyl-methacrylate	$(-CH_2C(CH_3)(C(O)(OC^*H_3))-)_n$	RT	80	63	10	51	Edzes (1983)
dimethoxy methane	$CH_2(OC^*H_3)_2$	25	98	70	9	58	Alderman *et al.* (1986)
	$C^*H_2(OCH_3)_2$		129	93	80	100	
1,4-dimethoxy benzene	$C^*H_3O-C_6H_4-OC^*H_3$	RT	80	72	16	56	Maricq and Waugh (1979)
		RT	78	74	15	56	Bax *et al.* (1983)
3,4-dimethoxy-benzaldehyde (veratraldehyde)	$HC(O)-C_6H_3-(OC^*H_3)_2$ (see Fig. 4)	RT	82	74	13	57	Terao *et al.* (1984b)
p-azoxydianisole	$C^*H_3O-C_6H_4-N{=}N(O)-C_6H_4-OC^*H_3$	(lc)	80	74	15	56	Pines and Chang (1974)
dimethyl carbonate	$(C^*H_3O)_2CO$	87	79	73	8	53	Pines *et al.* (1972)
dimethyl oxalate	$(C^*H_3OCO)_2$	87	85	70	14	56	Pines and Abramson (1974)
polyethylene oxide	$(-C^*H_2C^*H_2O-)_n$	133	91	83	33	69	Fleming *et al.* (1980)
polyethylene-terephthalate	$(-OC(O)C_6H_4C(O)OC^*H_2C^*H_2-)_n$	RT	80	80	28	63	Murphy *et al.* (1982)
diethyl ether	$(CH_3C^*H_2)_2O$	133	98	86	19	68	Pines *et al.* (1972)

TABLE 4. Alcohols and ethers—Continued

Compound	Formula	T (K)	Chemical shielding parameters(a)				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
Ethers, cont'd							
polyoxymethylene	$(-OCH_2-)_n$	RT	114	87	64	88	Veeman (1984)
1,2-epoxy ethane (ethylene oxide)		20	93	19	19	44	Facelli *et al.* (1985)
trimethylene oxide (oxetane)		20	104	93	15	71	Facelli *et al.* (1985)
1,4-epoxybutane (tetrahydrofuran)		20	110	75	21	68	Facelli *et al.* (1985)
1,4-dioxane		20	86	81	37	68	Facelli *et al.* (1985)
trimethoxymethane	$C^*H(OCH_3)_3$	20	123	116	99	113	Facelli *et al.* (1986)
dimethyl dimethoxy silane	$Si(CH_3)_2(OC^*H_3)_2$	87	74	69	-3	47	Waugh *et al.* (1973)
tetramethoxy silane	$Si(OCH_3)_4$	87	72	66	2	47	Waugh *et al.* (1973)

(a) relative to TMS (tetramethylsilane), on the δ scale, such that $C_6H_{6(l)}$ = 128.7 ppm and CS_2 = 192.8 ppm (*i.e.*, upfield is negative).
(b) peak assignments not given in original reference; assignments proposed here are based on isotropic shifts given in Stothers (1972).
(lc) oriented in a liquid crystal, only anisotropy given; principal components calculated by assuming isotropic shift is that of neat liquid given in Stothers (1972).

TABLE 5. Aldehydes and ketones

Compound	Formula	T (K)	Chemical shielding parameters$^{(a)}$				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
Aldehydes							
acetaldehyde	CH_3C^*HO	87	276	234	87	199	Pines *et al.* (1972)
		15	285	231	84	200	Zilm and Grant (1981)
1,1,2,2-tetra-acetylethane	 $CH_3C(OH){=}CC^*(O)CH_3$ $CH_3C(OH){=}CC^*(O)CH_3$	RT RT	278	240	85	201	Takegoshi and McDowell (1986)
3,4-dimethoxy-benzaldehyde (veratraldehyde)	$HC^*(O)-C_6H_3-(OCH_3)_2$ (see Fig. 4)	RT	264	211	101	192	Terao *et al.* (1984b)
Ketones							
dimethyl ketone (acetone)	$CH_3C^*(O)CH_3$	87	279	265	79	208	Pines *et al.* (1972)
methylphenyl ketone (acetophenone)	$(C_6H_5)C^*(O)CH_3$	100	279	231	84	198	Van Dongen Torman *et al.* (1978)
diphenyl ketone (benzophenone)	$C_6H_5C^*(O)C_6H_5$	RT	272	229	99	200	Kempf *et al.* (1972)
squaric acid (3,4-dihydroxy-3-cyclobutene-1,2-dione)	 $(HO)C{=}C(OH)$ $(O)C^*-C^*(O)$	RT	241 236	230 235	84 84	185 182	Mehring and Becker (1981)
dimedone		RT	284	255	79	206	Takegoshi *et al.* (1985)

(a) relative to TMS (tetramethylsilane), on the δ scale, such that $C_6H_{6(l)} = 128.7$ ppm and $CS_2 = 192.8$ ppm (*i.e.*, upfield is negative).

TABLE 6. Carboxylic acids and esters

Compound	Formula	T (K)	Chemical shielding parameters[(a)]				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
Carboxylic acids							
formic acid	HCOOH	125	251	162	92	168	Duncan and Vaughan (1981)
acetic acid	CH_3C^*OOH	87	269	184	110	188	Pines *et al.* (1972)
		93	265	181	105	184	Van Dongen Torman *et al.* (1977)
benzoic acid	$(C_6H_5)C^*OOH$	RT	227	186	107	173	Nagaoka *et al.* (1981)
		55	238	180	103	174	
benzoic acid-*d*6	$(C_6D_5)C^*OOD$	RT	231	188	103	174	Kempf *et al.* (1974)
		RT	231	188	103	174	Nagaoka *et al.* (1981)
1,2,4,5-benzene-tetracarboxylic acid (pyromellitic acid)	$(C_6H_4)(C^*OOH)_4$	RT	247	163	107	172	Tegenfeldt *et al.* (1980)
			263	169	105	179	
oxalic acid, anhydrous	$HOOC^*C^*OOH$	RT	251	123	112	162	Griffin *et al.* (1975a)
oxalic acid, dihydrate	$HOOC^*C^*OOH \cdot 2H_2O$	RT	249	132	109	163	Griffin *et al.* (1975a)
oxalic acid, diammonium monohydrate	$NH_4OOC^*C^*OONH_4 \cdot H_2O$	RT	245	159	109	171	Griffin *et al.* (1975a)
oxalic acid, ammonium hydrogen hemihydrate	$NH_4OOC^*C^*OOH \cdot ½H_2O$	RT	253	135	111	166	Griffin and Ruben (1975b)
malonic acid	$HOOC^*CH_2COOH$	RT	244	179	108	177	Tegenfeldt *et al.* (1980)
	$HOOCCH_2C^*OOH$	RT	248	174	111	178	
dihydro muconic acid	$HOOC^*CH_2CH{=}CHCH_2C^*OOH$	RT	245	180	97	174	Wolff *et al.* (1977)
glycine	$N^+H_3CH_2C^*OO^-$	RT	247	182	103	177	Haberkorn *et al.* (1981)
			248	177	106	177	
		RT	251	183	107	180	Griffin *et al.* (1975c)
glutamic acid	$NH_2C(O)CH_2CH_2C(N^+H_3)HC^*OO^-$	RT	267	162	111	180	Jelinski and Torchia (1980)
L-alanine	$NH_3CH(CH_3)C^*OOH$	RT	243	184	107	178	Naito *et al.* (1981)
L-serine monohydrate	$NH_3CH(CH_2OH)C^*OOH$	RT	239	181	107	176	Naito *et al.* (1983)
L-threonine	$CH_3CH(OH)CH(NH_3)C^*OOH$	RT	240	165	105	170	Janes *et al.* (1983)
L-asparagine monohydrate	$NH_2C(O)CH_2CH(NH_3)C^*OOH$	RT	240	180	109	176	Naito and McDowell (1984)

TABLE 6. Carboxylic acids and esters—Continued

Compound	Formula	T (K)	Chemical shielding parameters[a]				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
Esters							
methyl formate	$HC^{*}OOCH_3$	87	253	136	107	165	Pines *et al.* (1972)
			255	136	103	165	Linder *et al.* (1980)
methyl acetate	$CH_3C^{*}OOCH_3$	133	267	160	120	182	Pines *et al.* (1972)
acetic anhydride	$(CH_3C^{*}O)_2O$	91	281	116	116	171	Pines *et al.* (1972)
trifluoro acetic anhydride	$(CF_3C^{*}O)_2O$	109	260	106	90	152	Waugh *et al.* (1973)
dimethyl oxalate	$(CH_3OC^{*}O)_2$	87	253	116	112	160	Pines and Abramson (1974)
benzoic acid anhydride	$((C_6H_5)C^{*}O)_2O$	RT	236	144	80	153	Kempf *et al.* (1974)
polyethylene-terephthalate	$(-OC^{*}(O)C_6H_4C^{*}(O)OCH_2CH_2-)_n$	RT	250	122	122	165	Murphy *et al.* (1982)
polymethyl-methacrylate	$(-CH_2C(CH_3)(C^{*}(O)(OCH_3))-)_n$	RT	268	150	112	177	Edzes (1983)
ammonium formate	$(NH_4)HC^{*}O_2$	185	225	168	99	164	Duncan and Vaughan (1981)
calcium formate	$Ca(HC^{*}O_2)_2$	RT	235	190	105	177	Ackerman *et al.* (1974)
			240	186	105	177	
		125	235	186	96	172	Duncan and Vaughan (1981)
lead formate	$Pb(HC^{*}O_2)_2$	RT	220	183	97	167	Linder *et al.* (1980)
ammonium acetate	$NH_4(CH_3C^{*}OO)$	RT	231	201	108	180	Ganapathy *et al.* (1984b)
lithium acetate	$Li(CH_3C^{*}OO)$	RT	226	208	118	184	Ganapathy *et al.* (1984b)
potassium acetate	$K(CH_3C^{*}OO)$	RT	217	193	113	177	Ganapathy *et al.* (1984b)
magnesium acetate	$Mg(CH_3C^{*}OO)_2$	RT	230	203	103	183	Ganapathy *et al.* (1984b)
strontium acetate	$Sr(CH_3C^{*}OO)_2$	RT	241	200	104	183	Ganapathy *et al.* (1984b)
lanthanum acetate	$La(CH_3C^{*}OO)_2$	RT	226	213	113	184	Ganapathy *et al.* (1984b)
silver acetate	$Ag(CH_3C^{*}OO)$	87	239	202	90	177	Pines *et al.* (1972)
zinc acetate	$Zn(CH_3C^{*}OO)_2$	RT	227	219	106	184	Ganapathy *et al.* (1984b)
cadmium (II) acetate dihydrate	$Cd(CH_3C^{*}OO)_2$	RT	229	214	103	182	Ganapathy *et al.* (1984a)
			230	208	102	180	

TABLE 6. Carboxylic acids and esters—Continued

Compound	Formula	T (K)	Chemical shielding parameters$^{(a)}$				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
Esters, cont'd							
silver trifluoroacetate	CF_3C^*OOAg	296	245	129	129	168	Waugh *et al.* (1973)
silver benzoate	$(C_6H_5)C^*OOAg$	RT	247	176	93	172	Kempf *et al.* (1974)
ammonium hydrogen malonate	$(OOC^*CH_2C^*OO)(H)(NH_4)$	RT	242	175	102	173	Chang *et al.* (1975)
potassium hydrogen malonate	$(OOC^*CH_2C^*OO)(H)(K)$	RT	253	173	97	174	Schroter *et al.* (1983)
potassium hydrogen succinate	$(OOC^*CH_2CH_2C^*OO)(H)(K)$	RT	263$^{(b)}$	179$^{(b)}$	105$^{(b)}$	182	Schroter *et al.* (1983)
ammonium *d*-tartrate	$(-CH(OH)C^*OONH_4)_2$	RT	239	190	107	179	Pines *et al.* (1974)
ammonium hydrogen maleate (*cis*-butenedioic acid)	$(OOC^*CH{=}CHC^*OO)(H)(NH_4)$	RT	240$^{(c)}$	172$^{(c)}$	104$^{(c)}$	172	Schroter *et al.* (1983)
ammonium hydrogen fumarate (*trans*-butenedioic acid)	$(OOC^*CH{=}CHC^*OO)(H)(NH_4)$	RT	249$^{(b)}$	172$^{(b)}$	101$^{(b)}$	174	Schroter *et al.* (1983)
ammonium hydrogen glutarate (pentanedioic acid)	$(OOC^*CH{=}CHC^*OO)(H)(NH_4)$	RT	251$^{(c)}$	179$^{(c)}$	110$^{(c)}$	180	Schroter *et al.* (1983)
dimethyl maleic anhydride	$(CH_3)C{=}C(CH_3)$ $(O)C^*{-}O{-}C^*(O)$	RT	258 263	126 128	120 122	168 171	Igner and Fiat (1982)

(a) relative to TMS (tetramethylsilane), on the δ scale, such that $C_6H_{6(l)}$ = 128.7 ppm and CS_2 = 192.8 ppm (*i.e.*, upfield is negative).
(b) determined from spinning sidebands of a rotating sample.
(c) determined from narrowed powder pattern obtained spinning 7° off magic angle.

TABLE 7. Carbon–nitrogen compounds

Compound	Formula	T (K)	Chemical shielding parameters$^{(a)}$				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
Amines							
glycine	$NH_3C^*H_2COOH$	RT	66 67	46 45	27 27	46 46	Haberkorn *et al.* (1981)
L-alanine	$NH_3C^*H(CH_3)COOH$	RT	65	57	32	51	Naito *et al.* (1981)
L-serine monohydrate	$NH_3C^*H(CH_2OH)COOH$	RT	70	61	44	58	Naito *et al.* (1983)
L-threonine	$CH_3CH(OH)C^*H(NH_3)COOH$	RT	69	59	53	60	Janes *et al.* (1983)
L-asparagine monohydrate	$NH_2C(O)CH_2C^*H(NH_3)COOH$	RT	71	54	30	52	Naito and McDowell (1984)
Amides							
propenoic acid, amide (acrylamide)	$CH_2{=}CHC^*(O)NH_2$	RT	259	185	80	174	Igner and Fiat (1982)
glycyl glycine	$H_2NCH_2C^*(O)NH-$ $-CH_2COOH{\cdot}H_2O{\cdot}HCl$	RT	244	177	88	170	Stark *et al.* (1983)
L-asparagine monohydrate	$NH_2C^*(O)CH_2CH(NH_3)COOH$	RT	246	197	89	177	Naito and McDowell (1984)
poly(glycine)	$(NHCH_2C^*(O))_n$	RT	237	175	93	168	Jelinski and Torchia (1979)
β-poly(glycine)	$(NHCH_2C^*(O))_n$	RT	243	174	88	168	Ando *et al.* (1985)
3_1-poly(glycine)		RT	243	179	94	172	Ando *et al.* (1985)
penta glycine		RT	242	179	93	171	Ando *et al.* (1985)
collagen, [1-^{13}C]glycine-labeled	(see Fig. 4)	RT	224	173	121	173	Jelinski and Torchia (1979)
copoly(L-alanine,glycine)$^{(b)}$	$\ldots-CH_2C^*(O)-NH-\ldots$	RT	244	178	94	172	Ando *et al.* (1985)
copoly(L-leucine,glycine)$^{(b)}$	$\ldots-CH_2C^*(O)-NH-\ldots$	RT	242	179	94	172	Ando *et al.* (1985)
copoly(γ-benzyl glutamate, glycine)$^{(b)}$	$\ldots-CH_2C^*(O)-NH-\ldots$	RT	243	178	95	172	Ando *et al.* (1985)
copoly(β-benzyl aspartate, glycine)$^{(b)}$	$\ldots-CH_2C^*(O)-NH-\ldots$	RT	243 243	178 178	95 93	172 171	Ando *et al.* (1985)
copoly(L-valine,glycine)$^{(b)}$	$\ldots-CH_2C^*(O)-NH-\ldots$	RT	242	171	93	169	Ando *et al.* (1985)
Nitriles							
acetonitrile	$CH_3C^*{\equiv}N$	83 (lc) (lc)	191 216 224	191 216 224	-7 -78 -96	125 117 117	Kaplan *et al.* (1974) Ripmeester *et al.* (1982) Diehl *et al.* (1982)
benzonitrile	$C_6H_5C^*{\equiv}N$	(lc)	231	213	-88	119	Fung (1983)
potassium tetracyanoplatinate(II)	$K_2Pt(CN)_4Br_{0.3}{\cdot}3H_2O$	RT	225	187	-84	109	Stoll *et al.* (1974)

(a) relative to TMS (tetramethylsilane), on the δ scale, such that $C_6H_{6(l)} = 128.7$ ppm and $CS_2 = 192.8$ ppm (*i.e.*, upfield is negative).
(b) carbonyl carbon on glycine residue ($<8\%$) incorporated into the polypeptide.
(lc) oriented in a liquid crystal, only anisotropy given; principal components calculated by assuming isotropic shift is that of neat liquid given in Stothers (1972).

TABLE 8. Aromatic carbons

Compound	Formula	T (K)	Chemical shielding parameters$^{(a)}$				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
benzene	C_6H_6	14	217	141	1	120	Linder *et al.* (1979)
		20	234	146	9	130	Strub *et al.* (1983)
		223	192	192	12	132	Pines *et al.* (1972)
methyl benzene (toluene)	$C_6^*H_5(CH_3)$	87	222	135	-3	118	Pines *et al.* (1972)
1,4-dimethyl benzene (*p*-xylene)	$C_6^*H_4(CH_3)_2$	100	233	162	7	134	Van Dongen Torman and Veeman (1979)
			227	138	20	128$^{(c)}$	
			227	134	23	128$^{(c)}$	
1,2,4,5-tetramethyl benzene (durene)	$C_6^*H_2(CH_3)_4$	RT	231	147	18	134.5	Pausak *et al.* (1973)
			226	156	3	133	
			223	123	46	131$^{(c)}$	
pentamethyl benzene	$C_6^*H(CH_3)_5$	RT	215	163	20	133	Pausak *et al.* (1974)
			218	163	20	134	
			216	160	24	133	
			218	163	21	134	
			216	161	21	132	
			215	130	48	131$^{(c)}$	
hexamethyl benzene (mellitene)	$C_6^*(CH_3)_6$	87	232	154	25	137	Pines *et al.* (1972)
		87	227	154	19	133	Pausak *et al.* (1974)
		RT	188	187	21	132	
hexaethyl benzene	$C_6^*(C_2H_5)_6$	RT	221	164	22	135	Pausak *et al.* (1974)
1,4-dihydroxy benzene (hydroquinone)	$(C_6^*H_4)(OH)_2$	77	235	146	63	148	Matsui *et al.* (1982)
			196	131	19	115$^{(c)}$	
			200	134	20	118$^{(c)}$	
	$(C_6^*H_4)(OH)_2$	RT	235	145	67	149	Burgar (1984)
			198	132	25	118$^{(c)}$	
			194	132	22	116$^{(c)}$	
methylphenyl ketone (acetophenone)	$(C_6^*H_5)C(O)(CH_3)$	100	224	158	30	134	Van Dongen Torman *et al.* (1978)
			228	157	-2	128$^{(c)}$	
			230	145	8	128$^{(c)}$	
			241	156	4	134$^{(c)}$	
			235	146	7	129$^{(c)}$	
			223	158	8	130$^{(c)}$	
1,2,4,5-benzene-tetracarboxylic acid (pyromellitic acid)	$(C_6^*H_2)(COOH)_4$	RT	222	156	31	136	Tegenfeldt *et al.* (1980)
			233	163	30	142	
			217	171	12	133$^{(c)}$	
benzonitrile	$C_6^*H_5C\equiv N$	(lc)	211	104	23	113	Fung (1983)
			202	180	14	133$^{(c)}$	
			195	178	14	129$^{(c)}$	
			232	158	9	133$^{(c)}$	

TABLE 8. Aromatic carbons—Continued

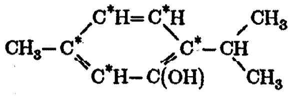
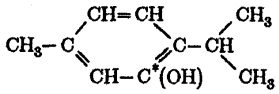
Compound	Formula	T (K)	Chemical shielding parameters(a)				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
1,4-dimethoxy benzene	$CH_3O-C_6^*H_4-OCH_3$	RT	230	162	74	155	Maricq and Waugh (1979)
			198	136	23	119(c)	
			193	134	12	113(c)	
		RT	234	159	73	155	Bax *et al.* (1983)
			201	132	24	119(c)	
			195	137	9	113(c)	
3,4-dimethoxy-benzaldehyde (veratraldehyde)	$HC(O)-C_6^*H_3-(OCH_3)_2$ (see Fig. 4)	RT	204	163	26	131	Terao *et al.* (1984b)
			184	135	4	108	
			212	166	74	151	
			220	175	74	156	
			190	136	12	113	
			223	154	13	130	
2-isopropyl, 5-methyl phenol (thymol)(b)		RT	191	119	39	116	Maciel *et al.* (1985)
			218	127	25	123	
			222	145	10	126	
			193	180	24	132	
			232	169	14	138	
		RT	228	152	72	151(c)	Maciel *et al.* (1985)
polyethylene-terephthalate	$(-OC(O)C_6^*H_4C(O)OCH_2CH_2-)_n$	RT	226	153	15	131	Murphy *et al.* (1982)
fluorobenzene	C_6H_5F	(lc)	238	157	94	163	Fung and Kong (1984)
			175	157	14	115(c)	
			203	179	7	130(c)	
			216	155	0	124(c)	
hexafluoro benzene	C_6F_6	233	171	171	131	158	Pines *et al.* (1972)
chlorobenzene	C_6H_5Cl	(lc)	237	111	54	134	Fung and Kong (1984)
			184	171	29	128(c)	
			192	182	15	130(c)	
			239	130	10	126(c)	
bromobenzene	C_6H_5Br	(lc)	233	82	52	122	Fung and Kong (1984)
			183	170	40	131(c)	
			182	180	28	130(c)	
			240	116	24	127(c)	
iodobenzene	C_6H_5I	(lc)	230	41	12	94	Fung and Kong (1984)
			188	173	51	137(c)	
			178	179	33	130(c)	
			242	113	26	127(c)	

TABLE 8. Aromatic carbons—Continued

Compound	Formula	T (K)	Chemical shielding parameters(a)				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
Heterocyclic aromatics							
azine (pyridine)	C_5H_5N	(lc)	241	173	36	150	Parhami and Fung (1985)
			205	158	8	124	
			233	170	4	136	
1,2-diazine (pyridazine)	$C_4H_4N_2$	(lc)	293	130	31	152	Parhami and Fung (1985)
			190	186	3	126	
1,3-diazine (pyrimidine)	$C_4H_4N_2$	(lc)	246	176	55	159	Parhami and Fung (1985)
			239	201	30	157	
			221	138	4	121	
1,4-diazine (pyrazine)	$C_4H_4N_2$	(lc)	223	173	39	145	Parhami and Fung (1985)
Miscellaneous							
cyclopentadienide anion	$C_5H_5^-$	20	182	114	21	106	Strub *et al.* (1983)
tropylium cation	$C_7H_7^+$	20	280	168	22	167	Strub *et al.* (1983)

(a) relative to TMS (tetramethylsilane), on the δ scale, such that $C_6H_{6(l)}$ = 128.7 ppm and CS_2 = 192.8 ppm (*i.e.*, upfield is negative).
(b) peak assignments not given in original reference; assignments proposed here are based on isotropic shifts given in Stothers (1972).
(c) non-substituted ring carbon.

TABLE 9. Carbon monoxide and inorganic carbonyls

Compound	Formula	T (K)	Type$^{(b)}$	Chemical shielding parameters$^{(a)}$				Reference
				σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
carbon monoxide	CO	46	–	293	293	-42	181	Gibson *et al.* (1977)
		4.2	–	303	303	-62	181	
		(c)	–	316	316	-90	181	
		20	–	305	305	-48	187	Beeler *et al.* (1984)
chromium hexacarbonyl	$Cr(CO)_6$	RT	t	353	353	-70	212	Gleeson and Vaughan (1983)
		RT	t	369$^{(d)}$	335$^{(d)}$	-69$^{(d)}$	212	Oldfield *et al.* (1985)
iron pentacarbonyl	$Fe(CO)_5$	RT	t	355	355	-70	213	Spiess *et al.* (1974)
nickel tetracarbonyl	$Ni(CO)_4$	RT	t	326	326	-69	194	Spiess *et al.* (1974)
molybdenum hexacarbonyl	$Mo(CO)_6$	RT	t	343	343	-75	204	Gleeson and Vaughan (1983)
		RT	t	338$^{(d)}$	332$^{(d)}$	-65$^{(d)}$	202	Oldfield *et al.* (1985)
tungsten hexacarbonyl	$W(CO)_6$	RT	t	324	324	-71	192	Gleeson and Vaughan (1983)
		RT	t	326$^{(d)}$	319$^{(d)}$	-70$^{(d)}$	192	Oldfield *et al.* (1985)
ruthenium carbonyl	$Ru_3(CO)_{12}$	RT	t	348	319	-63	201	Gleeson and Vaughan (1983)
osmium carbonyl	$Os_3(CO)_{12}$	RT	t	292	292	-55	176	Gleeson and Vaughan (1983)
iridium carbonyl	$Ir_3(CO)_{12}$	RT	t	277	277	-53	167	Gleeson and Vaughan (1983)
rhodium carbonyl	$Rh_6(CO)_{16}$	RT	t	315	305	-80	181	Gleeson and Vaughan (1983)
			br	296	296	102	231	
iron carbonyl	$Fe_3(CO)_{12}$	RT	t	325	316	-6	212	Gleeson and Vaughan (1983)
iron cyclopentadienyl dicarbonyl dimer	$(\eta^5-C_5H_5)_2-Fe_2(C^*O)_4$	RT	t	354	354	-85	211	Gleeson and Vaughan (1983)
			br	328	309	179	272	
rhodium dicarbonyl chloride	$Rh_2(CO)_4Cl_2$	RT	t	306	299	-99	186	Duncan *et al.* (1980)
Rh-CO on alumina	–	RT	t	315	305	-80	180	Duncan *et al.* (1980)
Rh-CO on silica	–	RT	t	312	290	-54	184	Duncan and Root (1986)
		RT	br	296	266	116	226	
Ru-CO on silica	–	RT	t	327	327	-73	194	Gay (1984)
	–	RT	t	317	317	30	221	Duncan *et al.* (1985)
	–	RT	t	331	324	-86	180	Duncan and Root (1986)
	–	RT	br	323	295	103	240	
Ru-CO on Y-zeolite	–	RT	t	320$^{(d)}$	310$^{(d)}$	-89$^{(d)}$	180	Shoemaker and Apple (1985)

(a) relative to TMS (tetramethylsilane), on the δ scale, such that $C_6H_{6(l)} = 128.7$ ppm and $CS_2 = 192.8$ ppm (*i.e.*, upfield is negative).
(b) terminal (t) or bridging (br).
(c) estimated anisotropy in the absence of librational motion; principal components calculated from the reported anisotropy and the isotropic shift of CO (Stothers (1972)).
(d) determined from spinning sidebands of a rotating sample.

TABLE 10. Miscellaneous compounds

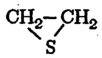
Compound	Formula	T (K)	Chemical shielding parameters(a)				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
Carbon-oxygen							
carbon dioxide	CO_2	20	245	245	-90	133	Beeler *et al.* (1984)
carbonyl sulfide	SCO	20	275	275	-90	154	Beeler *et al.* (1984)
calcium carbonate	$CaCO_3$	RT	194	194	119	169	Lauterbur (1958)
		RT	195	195	119	169	Pines *et al.* (1971)
dimethyl carbonate	$(CH_3O)_2C^*O$	87	231	110	110	150	Pines *et al.* (1972)
Carbon-sulfur							
carbon disulfide	CS_2	73	333	333	-92	193	Pines *et al.* (1971)
		20	332	332	-90	191	Zilm *et al.* (1978)
thioacetic acid	CH_3C^*OSH	87	264	230	101	202	Waugh *et al.* (1973)
dimethyl sulfoxide	$(C^*H_3)_2SO$	226	66	44	18	43	Pines *et al.* (1972)
dimethyl sulfone	$(C^*H_3)_2SO_2$	295	63	63	7	44	Solum *et al.* (1983)
dimethyl disulfide	$C^*H_3S-SC^*H_3$	87	48	18	6	24	Pines *et al.* (1972)
ethylene sulfide		20	54	11	7	24	Facelli *et al.* (1985)
Carbon-fluorine							
trifluoro silver acetate	C^*F_3COOAg	296	129	129	110	123	Waugh *et al.* (1973)
trifluoro acetic anhydride	$(C^*F_3CO)_2)O$	109	119	119	102	113	Waugh *et al.* (1973)
poly(vinylidene fluoride)	$(-CH_2C^*F_2-)_n$	297	131	120	111	121	Fleming *et al.* (1980)
Inorganic carbides							
boron carbide	$B_{12}(CC^*C)$	RT	190	170	-105	85	Duncan (1984)
tungsten carbide	WC	RT	348	286	286	307	Duncan (1986)
molybdenum carbide	Mo_2C	RT	307	274	244	275	Duncan (1986)
—	$CsZr_6I_{14}C$	RT	54	54	15	41	Fry *et al.* (1986)

TABLE 10. Miscellaneous compounds—Continued

Compound	Formula	T (K)	Chemical shielding parameters[(a)]				Reference
			σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
Metal-sandwich compounds							
ferrocene	$(C_5H_5)_2Fe$	–	95	95	19	70	Wemmer and Pines (1981)
bis(cyclopentadienyl) ruthenium	$(C_5H_5)_2Ru$	–	100	100	21	74	Wemmer and Pines (1981)
bis(cyclopentadienyl) magnesium	$(C_5H_5)_2Mg$	–	153	153	21	109	Wemmer and Pines (1981)
bis(cyclopentadienyl) titanium dichloride	$(C_5^*H_5)_2TiCl_2$	–	168	168	13	116	Wemmer and Pines (1981)
permethyl ferrocene	$(C_5^*(CH_3)_5)_2Fe$	–	128	87	24	45	Wemmer and Pines (1981)
			102	102	35	62	
		88	128	116	24	89	Wemmer *et al.* (1981)
bis(pentamethyl cyclopentadienyl) cobalt chloride	$(C_5^*(CH_3)_5)_2CoCl$	–	180	124	39	114	Wemmer and Pines (1981)
			172	111	39	107	
bis(benzene) chromium	$(C_6H_6)_2Cr$	–	115	115	1	77	Wemmer and Pines (1981)
Others							
graphite	C_n	RT	178	178	0	119	Resing *et al.* (1982)
		RT	251	20	20	97	Duncan *et al.* (1985)

(a) relative to TMS (tetramethylsilane), on the δ scale, such that $C_6H_{6(l)} = 128.7$ ppm and $CS_2 = 192.8$ ppm (*i.e.*, upfield is negative).

TABLE 11. Typical chemical shieldings of carbon functionalities

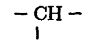
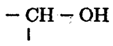
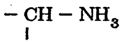
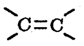
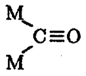
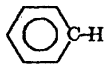
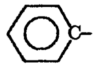
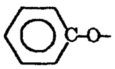
Compound	Formula[(a)]	Chemical shielding parameters[(b)]								Number of Reference Spectra
		σ_{11}		σ_{22}		σ_{33}		σ_{iso}		
methyl	$-CH_3$	38	(10)	29	(10)	3	(5)	23	(6)	38
methylene	$-CH_2-$	54	(13)	41	(10)	16	(6)	37	(8)	9
methylidyne	 $-\underset{\mid}{C}H-$	40	(15)	32	(10)	28	(10)	33	(11)	5
alcohol	$-CH_2OH$	80		70		25		58		2
	 $-\underset{\mid}{C}H-OH$	90	(4)	83	(5)	42	(8)	72	(4)	6
ether	$-O-CH_3$	83	(7)	71	(4)	12	(3)	55	(3)	10
	$-O-CH_2-$	90	(9)	83	(3)	27	(7)	67	(3)	3
amine	 $-\underset{\mid}{C}H-NH_3$	68	(2)	54	(7)	36	(11)	52	(6)	6
olefinic		223	(8)	127	(14)	34	(11)	128	(6)	9
aldehyde	$-C(O)H$	276	(9)	229	(13)	90	(8)	198	(4)	4
ketone	$-C(O)-$	279	(5)	245	(18)	85	(10)	203	(5)	4
acid	$-C(O)OH$	247	(10)	171	(18)	106	(4)	175	(6)	24
ester	$-C(O)-O-$	258	(13)	132	(18)	107	(14)	166	(10)	9
salt	$-C(O)-O-M$	239	(13)	188	(19)	105	(8)	176	(6)	24
amide	$-C(O)-NH_2$	243	(7)	179	(6)	94	(9)	172	(3)	14
acetylenic	$-C\equiv C-$	151	(9)	151	(9)	-79	(17)	75	(8)	8
CO	$C\equiv O$	316		316		-90		181		1
carbonyl (t)	$M-C\equiv O$	327	(22)	320	(21)	-64	(28)	195	(15)	21
carbonyl (br)		311	(18)	292	(18)	125	(37)	242	(21)	4
nitrile	$-C\equiv N$	227	(4)	208	(19)	-89	(6)	115	(5)	3

TABLE 11. Typical chemical shieldings of carbon functionalities—Continued

Compound	Formula$^{(a)}$	Chemical shielding parameters$^{(b)}$				Number of Reference Spectra
		σ_{11}	σ_{22}	σ_{33}	σ_{iso}	
aromatic		215 (16)	145 (17)	17 (13)	126 (7)	24
		221 (11)	160 (9)	21 (9)	134 (5)	18
		227 (10)	158 (13)	71 (5)	152 (3)	5

(a) a dangling bond implies a bond to a carbon atom

(b) relative to TMS (tetramethylsilane), on the δ scale, such that $C_6H_{6(l)}$ = 128.7 ppm and CS_2 = 192.8 ppm (*i.e.*, upfield is negative). The number in parenthesis is the standard deviation of the data compiled to date.

5. Table References

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