Spectroscopy Sample Submission and Data Analysis Information

1) Preparing and submitting samples for ^{1}H-NMR analysis

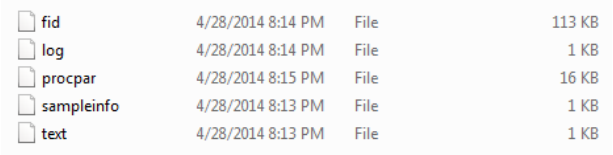
All ^{1}H-NMR analysis in CHEM 344 is performed upon dilute solutions in $CDCl_3$. Undiluted liquids, biphasic solutions, or solutions containing solids give poor quality NMR data. To prepare and submit a sample for ^{1}H-NMR analysis:

a) For liquids or oils, use a clean Pasteur pipette to transfer **~4 drops** of the liquid into a clean sample vial.
b) For solids, add a liberal **spatula-tip full** of compound (40 - 50 mg) into a clean sample vial.
c) With another **clean** Pasteur pipette, add approx. 1.5 mL (~1 pipette load) of $CDCl_3$ to the vial.
d) Mix the two compounds to give a homogeneous solution and then transfer the sample into a clean NMR tube *via* Pasteur pipette. The sample should fill the NMR tube to a volume of ⅓ to ½ full.
e) Once the solution has been transferred, cap the NMR tube and take it to the metal sample rack designated for your laboratory section. Dispose of the glass pipettes in the glass waste bin.
f) Take a spinner from the rack and gently push the NMR tube into the spin collar. Always push the tube into the spin collar from as close to the spin collar as possible. Do not push the tube from the cap. This is unsafe and can cause the tube to snap.
g) Use the depth gauge to ensure that the sample is in the proper position.
h) Once the NMR tube is placed in the spin collar to the correct depth, place the tube in the sample rack.
    i) Always use the next available numbered slot in the rack; do not skip spaces.
    ii) Write your first name and last initials on the NMR sample submission sheet.
    iii) Always include an unknown number or letter when applicable.

2) Obtaining NMR spectral data for analysis.

All ^{1}H-NMR, ^{13}C-NMR, ^{19}F-NMR, and ^{31}P-NMR data will be provided as the raw free-induction-decay (fid) data. You will need to convert the raw data to a useable spectrum to be analyzed and interpreted for each lab report. ***You must submit your own spectral data with your lab report - submitting data as your own that you did not obtain is scientific fraud and academic misconduct. If you fail to obtain data, you will not be penalized, a stock spectrum is available for analysis for each experiment.***

a) Obtain a folder of 5 key files for your NMR data. Detailed instructions are available on the course website. The five files are *fid*, *log*, *procpar*, *sampleinfo*, and text. They have no file extensions.

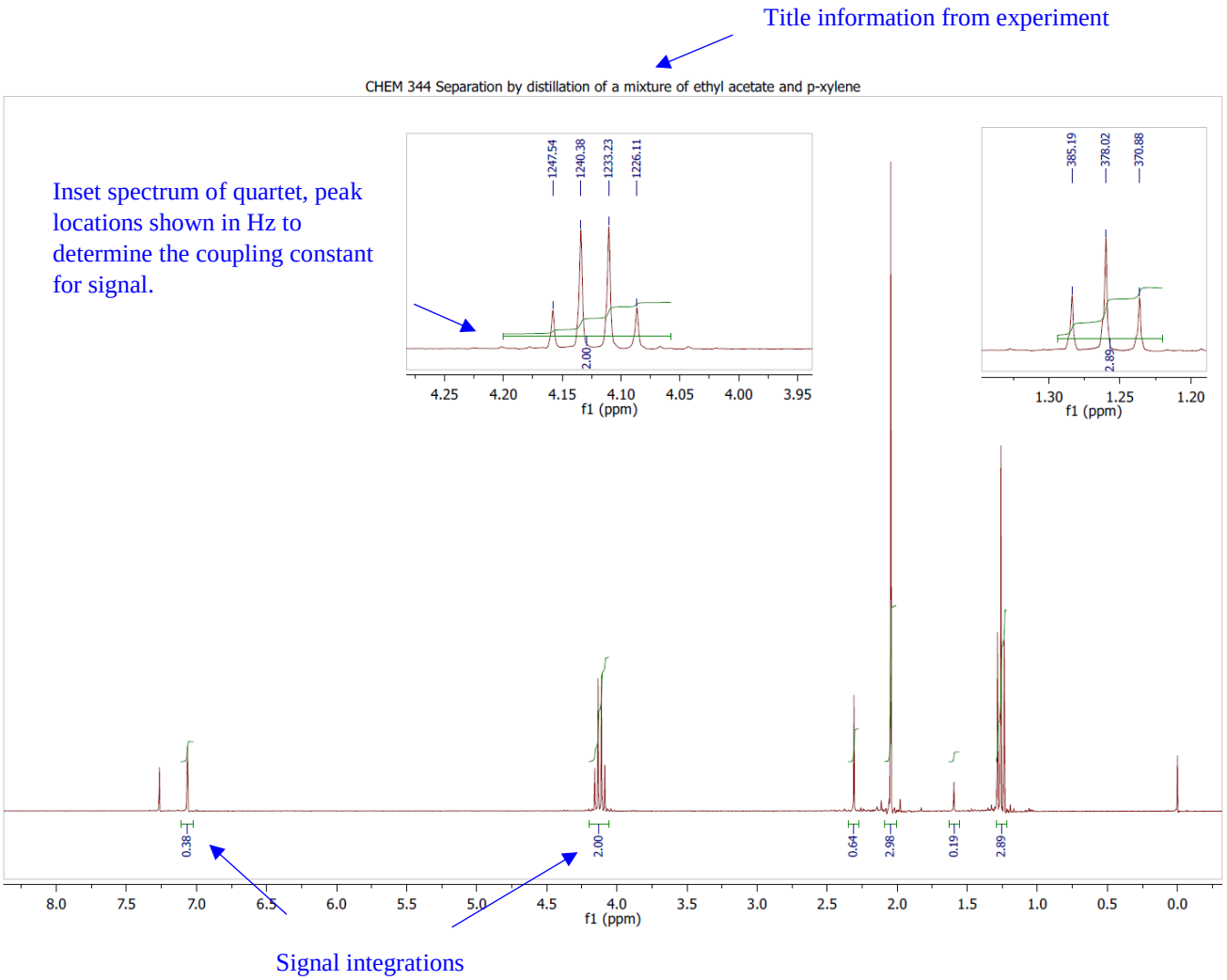


b) Open the fid file in MestReNova. MestReNova will convert the fid from the time-domain (signal intensity vs. time) to the frequency domain (intensity vs. frequency). All NMR spectra in the course are in the frequency-domain, showing intensity vs. chemical shift. Detailed instructions for obtaining MestReNova are on the course website.

c) Work up all spectra by following the directions on the course website for each experiment and in the same manner as the stock spectrum. The directions will change for each experiment, so be sure to consult the example stock spectrum and specific directions each time. A video of how to work up the spectrum will be provided for the early experiments.

i) Make sure the x-axis scale is set to display all important signals are shown in the spectrum.
ii) Make sure that the baseline is relatively flat and correctly phased.
iii) Make sure all signals related to the reagents, products, byproducts, or solvents are integrated (excluding $CDCl_3$ and TMS).
iv) Make sure that all signals that need specific coupling information are peak picked in Hz.

d) Save the MNova spectrum in worked-up format and as a pdf for easy printing. You must include a hard copy of all NMR spectra for each experiment with your laboratory report.



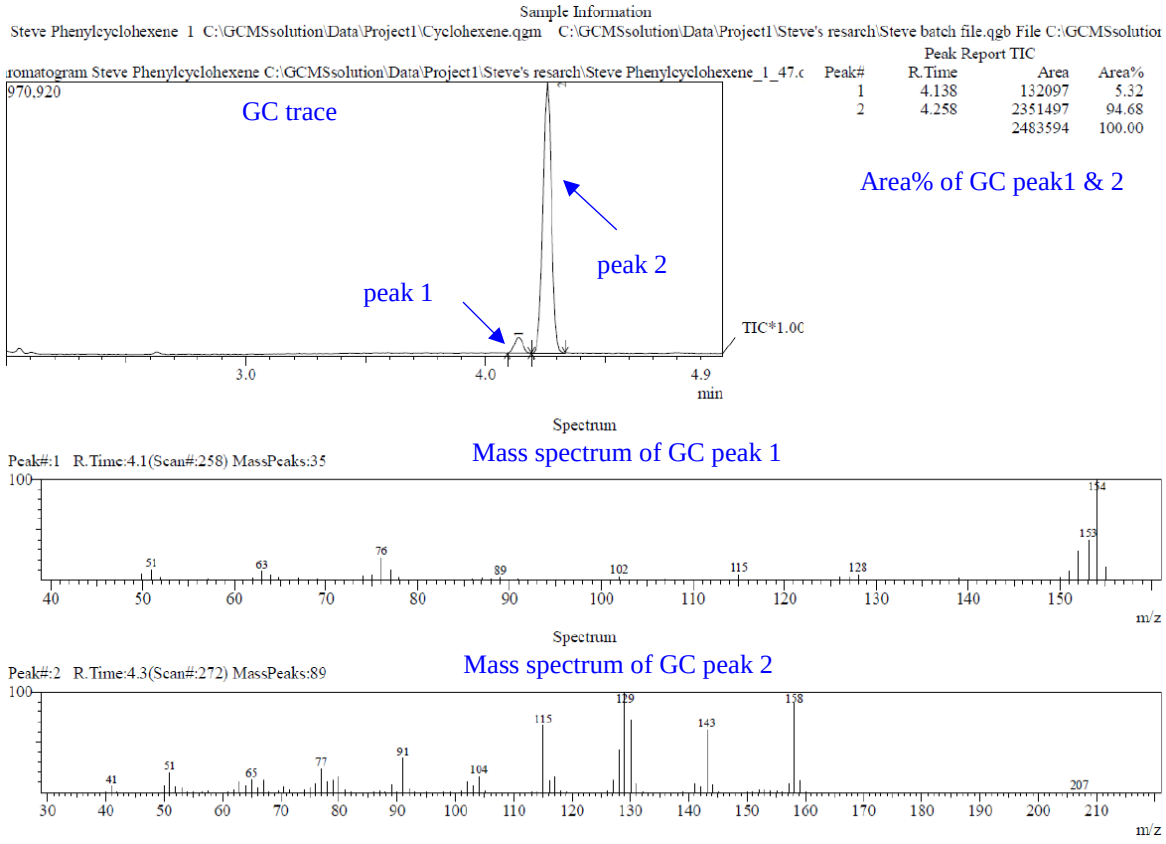
3) Preparing and submitting samples for GC-MS analysis

All GC-MS analysis in CHEM 344 is performed upon dilute solutions **except for the E1 and E2 product samples**. To protect the instrument, it is important that all samples are free of solid particulates. To prepare and submit a sample for GC-MS analysis:

a) For liquids or oils, use a clean Pasteur pipette to transfer **~4 drops** of the liquid into a clean sample vial.
b) For solids, add a liberal **spatula-tip full** of compound (40 - 50 mg) into a clean sample vial.
c) With another **clean** Pasteur pipette, place dichloromethane (CH_2Cl_2 not $CDCl_3$) into the sample vial until it is approx. ½ full.
d) Mix the two compounds to give a homogeneous mixture and then transfer the sample into a clean GC-MS sample vial *via* a **clean** Pasteur pipette.
e) Once the solution has been transferred, attach the screw cap to the GC-MS vial.
f) Place the tube in the sample box.
    i) Always use the next available numbered slot in the row designated for your section; do not skip spaces or put your sample in a different row.
    ii) Write your first name and last initials on the GC-MS sample submission sheet.
    iii) Always include an unknown number or letter when applicable.

4) Obtaining a GC-Mass spectrum for analysis.

Unlike the NMR spectra, the GC-MS data will be provided for you as a combined gas chromatogram and a mass spectrum. A pdf containing the GC-MS data from your sample will be available for download via the course website.



5) Obtaining an Infrared (IR) spectrum for analysis.
The Bruker Alpha Platinum ATR FT-IR spectrometers are available in the laboratory for student use and spectra can be obtained during the laboratory session.

- **Remove your gloves before touching the mouse or computer!**
- **Do not pull down on the lever and press the pressure device without placing a sample on the crystal!**
- **LEAVE EVERYTHING CLEANER THAN YOU FOUND IT!**

Preparation

a) If not already open, open the program **Opus 7**. **Login:** *Student* **Password :** (*none, leave blank*) Press enter. Click ok. It will take the program a few seconds to setup the instrument.

b) Click the **Measure Background** button. It is critical that the crystal is clean at this point and NO SAMPLE has been placed on the platform. Wait for a short time while the spectrometer completes several scans of the region with no sample and averages the signal. This will allow the spectrometer to accurately measure the IR absorptions due your sample by subtracting the background.

c) Place a small amount of your solid or oil sample directly on the crystal window in the center of the metallic disc. The sample should completely cover the crystal.

d) Pull the lever down until the pressure device locks in place.

Data Collection and Analysis

e) Click the Measure Sample button. Enter a descriptive filename in the general format "STUDENT(S)_NAMES TA_NAME EXPERIMENT MOLECULE." This name will appear on the printout of your spectrum

f) Click the **Start Sample Measurement** Button. Wait for a short time while the spectrometer completes several scans of the region and averages the signal. The spectrometer will use the background spectrum collected earlier to produce the spectrum of your sample.

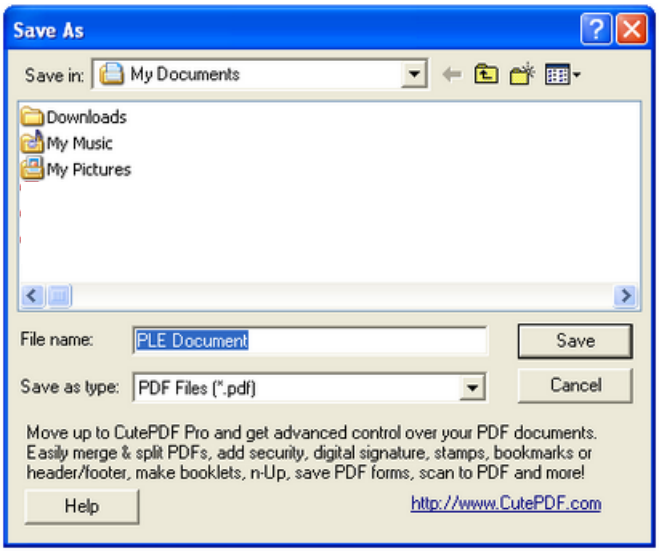
g) Choose **Manipulate > Baseline Correction** from the file menu.

h) Choose **Manipulate > Smooth** from the file menu. Highlight the file name and hit the **Smooth button**. Steps g and h, combined with completing multiple scans, are designed to enhance your spectrum and improve the signal-to-noise ratio of the data.

i) Choose **Evaluate > Peak Picking** from the file menu. Move the target cursor so that all desired absorptions pass below the threshold (horizontal) line. Click the **Store button**. This will place convenient frequency labels next to all picked peaks directly on the spectrum.

Saving Data Via Printing a pdf

j) There is no printer in the lab, but a pdf of the spectrum can be saved by clicking the **Print Report** Button. As before, enter a descriptive filename in the general format "STUDENT(S)_NAMES TA_NAME EXPERIMENT MOLECULE." This will be the name of the pdf file generated for your spectrum. Save the pdf reports in the **My Documents** folder only.



k) Use any of the web browsers on the computer to email this file to yourself and your labmates.

Spectrometer Clean-up

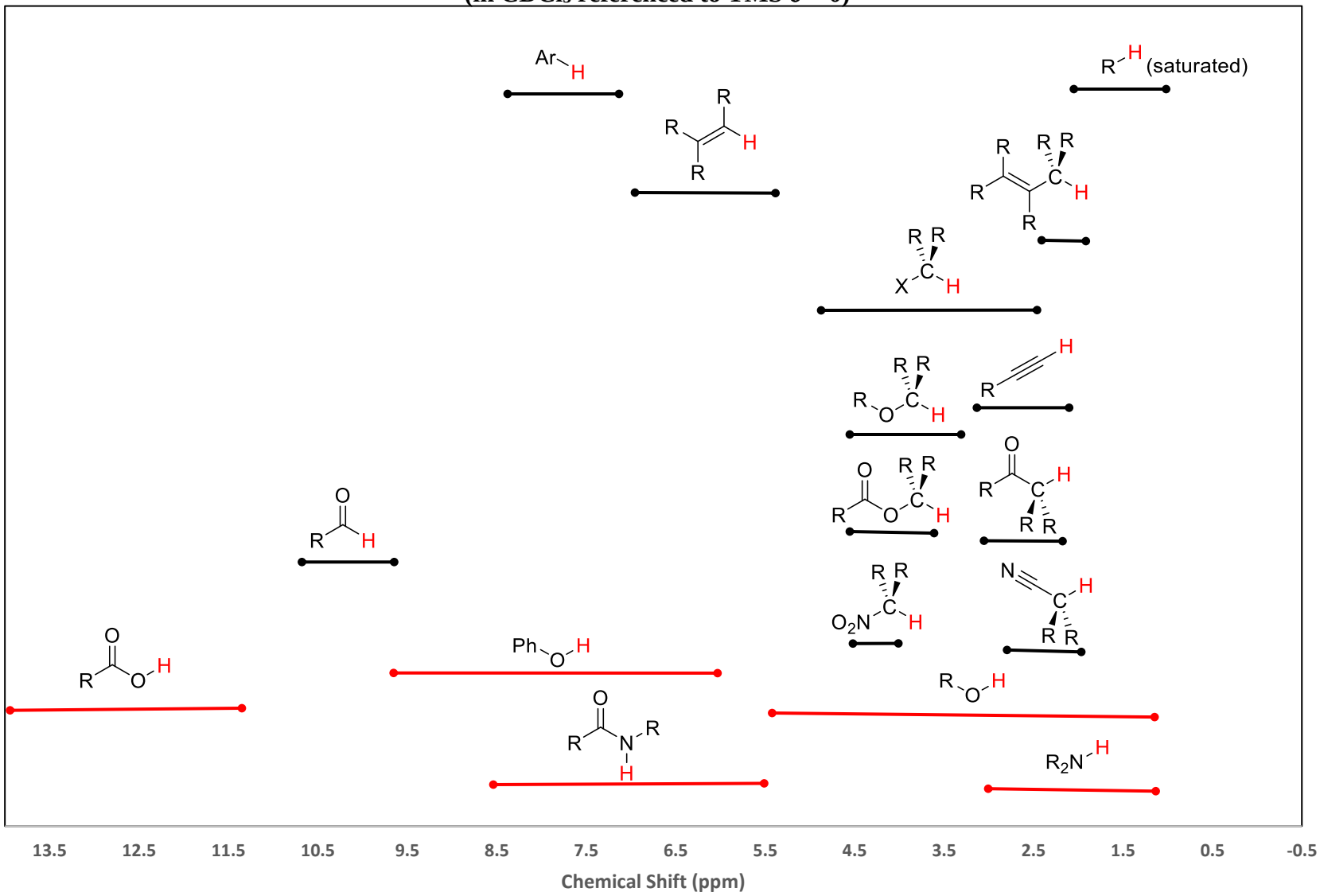
l) Clean the pressure device and crystal with an isopropanol soaked wipe and a clean/dry Kimwipe. **CLEAN UP ALL CHEMICAL SPILLS FROM ON AND AROUND THE INSTRUMENT!!!!** Move the pressure device off center. **Throw away all trash!** Unless someone else is directly following you, close all programs.

Troubleshooting

m) We have noticed that after many samples, the communications between the spectrometer and computer may fail. Simply unplug the spectrometer and restart the computer. When both power back up, the communications should be fine.

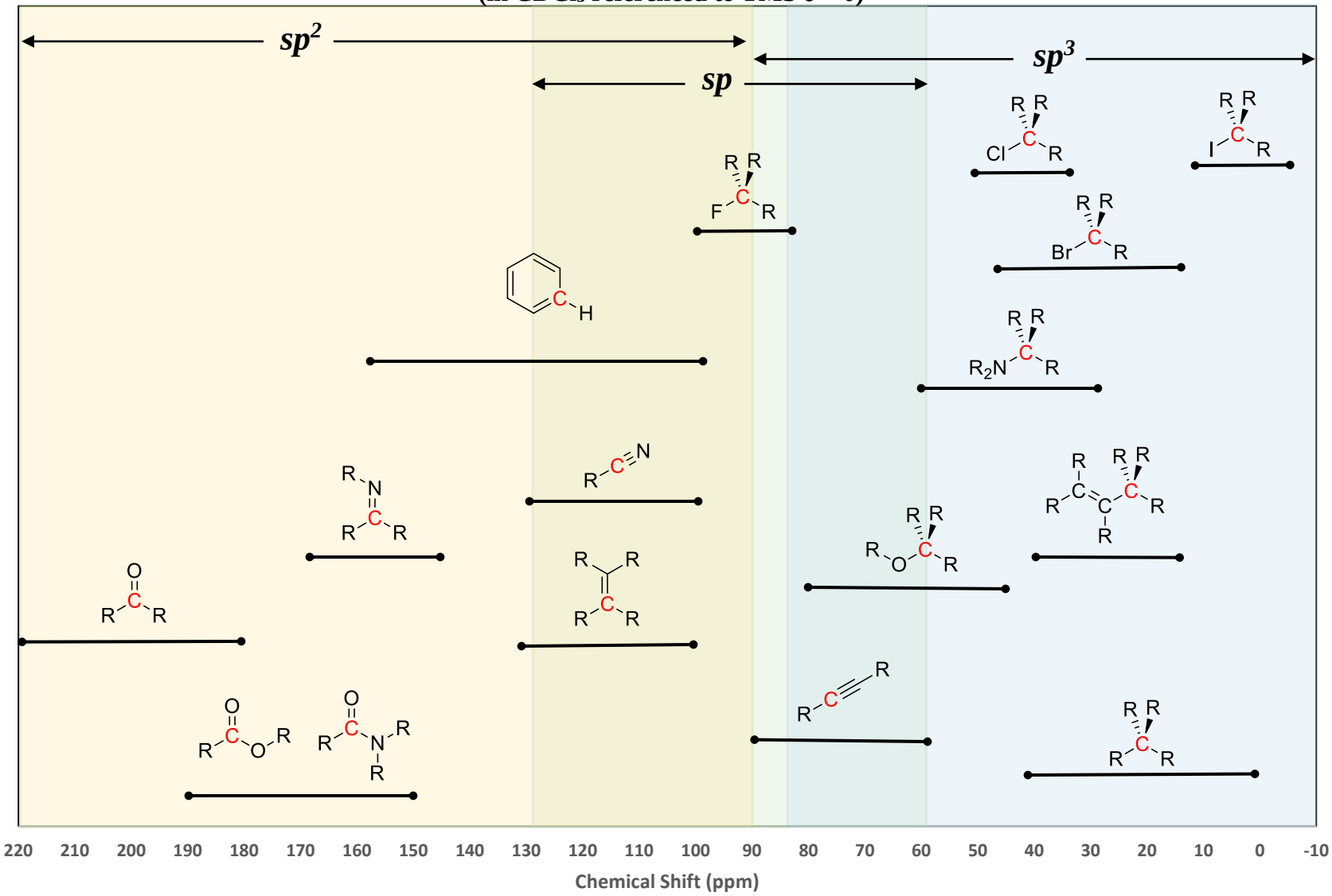
Typical ^{1}H-NMR Chemical Shift Ranges

(in $CDCl_3$ referenced to TMS $\delta = 0$)

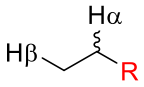


Typical ^{13}C-NMR Chemical Shift Ranges

(in $CDCl_3$ referenced to TMS $\delta = 0$)

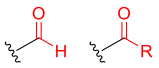
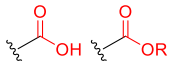
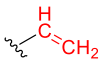
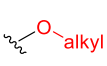
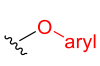


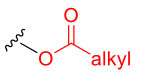
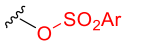
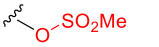
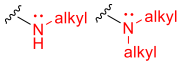
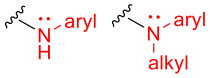
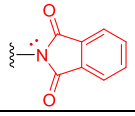
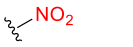
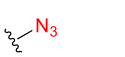
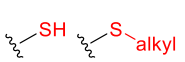
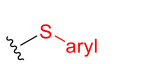
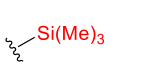
Curphy-Morrison Additivity Constants for Proton NMR

α and β Substituent Effects: 

Standard Shift: Methyl (-CH_3) 0.90 δ, Methylene (-CH_2-) 1.20 δ, Methine (-CH-) 1.55 δ

Shift Estimate: δ_H = Standard Shift + $\Sigma_{\alpha\text{-shifts}}$ + $\Sigma_{\beta\text{-shifts}}$

Substituent (R)		α-shift	β-shift
	-CH_3	2.30	0.60
	-CH_2-	2.30	0.55
	-CH-	2.55	0.15
	-CH_3	1.80	0.80
	-CH_2-	2.15	0.80
	-CH-	2.20	0.25
	-CH_3	1.80	0.80
	-CH_2-	2.15	0.80
	-CH-	2.20	0.25
	-CH_3	1.45	0.35
	-CH_2-	1.45	0.55
	-CH-	1.35	----
	-CH_3	1.25	0.25
	-CH_2-	1.10	0.30
	-CH-	0.95	----
	-CH_3	1.70(6)	0.28(4)
	-CH_2-	1.64(10)	0.50(3)
	-CH-	1.76(2)	0.76(1)
	-CH_3	1.20	0.25
	-CH_2-	1.00	0.30
	-CH-	0.95	----
	-CH_3	1.10	0.45
	-CH_2-	1.10	0.40
	-CH-	0.95	----
	-CH_3	0.90	0.05
	-CH_2-	0.75	0.10
	-CH-	0.65	----
	-CH_3	0.90	0.15
	-CH_2-	0.80	0.05
	-CH-	0.35	----
	-CH_3	2.45	0.40
	-CH_2-	2.30	0.20
	-CH-	2.10	----
	-CH_3	2.45	0.30
	-CH_2-	2.30	0.15
	-CH-	2.10	----
	-CH_3	2.95	0.40
	-CH_2-	2.65(11)	0.45
	-CH-	3.06(2)	----

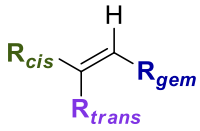
Substituent (R)		α-shift	β-shift
	-CH_3	2.90	0.40
	-CH_2-	2.95	0.45
	-CH-	3.45	----
	-CH_3	2.84	0.39(1)
	-CH_2-	2.66(6)	0.28(5)
	-CH-	3.16(3)	0.32(2)
	-CH_3	3.01	0.47(2)
	-CH_2-	2.90(5)	0.43(2)
	-CH-	2.64(1)	0.61(1)
	-CH_3	1.25	0.20
	-CH_2-	1.40	0.15
	-CH-	1.35	----
	-CH_3	2.08(8)	0.28(10)
	-CH_2-	2.03(12)	0.34(2)
	-CH-	2.33(2)	?
	-CH_3	2.08(8)	0.28(10)
	-CH_2-	2.03(12)	0.34(2)
	-CH-	2.33(2)	?
	-CH_3	3.50	0.65
	-CH_2-	3.15	0.85
	-CH-	3.05	----
	-CH_3	2.08(1)	0.45(1)
	-CH_2-	1.45(3)	0.46(1)
	-CH-	1.46(2)	-0.22(1)
	-CH_3	1.20	0.40
	-CH_2-	1.30	0.30
	-CH-	1.30	----
	-CH_3	1.47(2)	0.35(2)
	-CH_2-	1.45(8)	0.31(2)
	-CH-	1.60(4)	0.01(4)
	-CH_3	-0.90(1)	0.06(2)
	-CH_2-	-0.39(2)	?
	-CH-	-0.83(8)	?

Adapted from: P. L. Fuchs and C. A. Bunnell, "Carbon-13 NMR Based Spectral Problems," John Wiley, New York, 1979. Data with numbers in parentheses were added by H. J. Reich with limited number of examples (number is sample size).

(Adapted from Hans J. Reich, http://www.chem.wisc.edu/areas/reich/nmr/notes-9-hmr-5-curphy-morrison.pdf)

Curphy-Morrison Additivity Constants for Calculating Vinyl Chemical Shifts

Substituent Effects on:



Shift Estimate: $\delta_{H\ (vinyl)} = 5.25 + Z_{gem} + Z_{cis} + Z_{trans}$

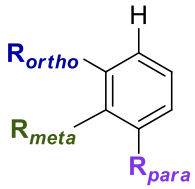
Substituent (R)	Z_{gem}	Z_{cis}	Z_{trans}	Substituent (R)	Z_{gem}	Z_{cis}	Z_{trans}
H	0.00	0.00	0.00	F	1.54	-0.40	-1.02
alkyl	0.45	-0.22	-0.28	Cl	1.08	0.18	0.13
Alkyl (cyclic) [a]	0.69	-0.25	-0.28	Br	1.07	0.45	0.55
CH_2OH	0.64	-0.01	-0.02	I	1.14	0.81	0.88
CH_2SH	0.71	-0.13	-0.22	OR (R = aliphatic)	1.22	-1.07	-1.21
CH_2X (X = F, Cl, Br)	0.71	-0.13	-0.22	OR (R = conjugated)	1.21	-0.60	-1.00
CH_2NR_2	0.58	-0.10	-0.08	O-C(O)R	2.11	-0.35	-0.64
CF_3	0.66	0.61	0.32	NR_2 (R = aliphatic)	0.80	-1.26	-1.21
$C=CR_2$ (isolated)	1.00	-0.09	-0.23	NR_2 (R = conjugated)	1.17	-0.53	-0.99
$C=CR_2$ (conjugated) [b]	1.24	0.02	-0.05	N=N-Ph	2.39	1.11	0.67
C≡C-R	0.47	0.38	0.12	NO_2	1.87	1.30	0.62
C≡N	0.27	0.75	0.55	N-C(O)R	2.08	-0.57	-0.72
COOH (isolated)	0.97	1.41	0.71	N_3	1.21	-0.35	-0.71
COOH (conjugated) [b]	0.80	0.98	0.32	$SiMe_3$	0.77	0.37	0.62
COOR (isolated)	0.80	1.18	0.55				
COOR (conjugated) [b]	0.78	1.01	0.46				
C(O)H (aldehyde)	1.02	0.95	1.17				
$C(O)NR_2$ (amide)	1.37	0.98	0.46				
C(O)Cl (acid chloride)	1.11	1.46	1.01				
C(O)R (ketone)	1.10	1.12	0.87				
C(O)R (conj. ketone) [b]	1.06	0.91	0.74				
CH_2-C(O)R; CH_2-CN	0.69	-0.08	-0.06				
CH_2Ar (benzyl)	1.05	-0.29	-0.32				
Aryl	1.38	0.36	-0.07				
Aryl (*o*-substituted)	1.65	0.19	0.09				

[a] The increment alkyl (cyclic) is to be used when both the substituent and the double bond form part of a ring. (Data for compounds containing 3- and 4-membered rings have not been considered.) [b] The increments 'R conjugated' are to be used instead of 'R isolated' when either the substituent or the double bond is conjugated with further substituents. Numbers in parentheses represent the number of examples used to calculate the parameters.

[1] Pascual, C. *Helv. Chem. Acta* **1966**, *49*, 164.
[2] L'Abbe, G. *Chem. & Ind*. (London) **1971**, 278.

(Adapted from Hans J. Reich, http://www.chem.wisc.edu/areas/reich/nmr/notes-9-hmr-6-vinyl-aryl-shifts.pdf)

Curphy-Morrison Additivity Constants for Calculating Benzene Chemical Shifts



Substituent Effects on:

Shift Estimate: $\delta_{H\ (aryl)} = 7.36 + Z_{ortho} + Z_{meta} + Z_{para}$

Substituent (R)	Z_{ortho}	Z_{meta}	Z_{para}	Substituent (R)	Z_{ortho}	Z_{meta}	Z_{para}
H	0.00	0.00	0.00	OPh	-0.36	-0.04	-0.28
CH_3	-0.18	-0.11	-0.21	O-C(O)CH_3	-0.27	-0.02	-0.13
*t*Bu	0.02	-0.08	-0.21	O-C(O)Ph	-0.14	0.07	-0.09
CH_2Cl	0.02	-0.01	-0.04	O-SO_2CH_3	-0.05	0.07	-0.01
CH_2OH	-0.07	-0.07	-0.07	SH	-0.08	-0.16	-0.22
CF_3	0.32	0.14	0.20	SMe	-0.08	-0.10	-0.24
CCl_3	0.64	0.13	0.10	SPh	0.06	-0.09	-0.15
C=CH_2	0.04	-0.04	-0.12	SO_2Cl	0.76	0.35	0.45
C=CHCOOH	0.19	0.04	0.05	NH_2	-0.71	-0.22	-0.62
C≡C-H	0.15	-0.02	-0.01	NMe_2	-0.66	-0.18	-0.67
C≡C-Ph	0.17	-0.02	-0.03	NEt_2	-0.68	-0.15	-0.73
Ph	0.23	0.07	-0.02	$NMe_3^+ I^-$	0.69	0.36	0.31
COOH	0.77	0.11	0.25	NHC(O)CH_3	0.14	-0.07	-0.27
C(O)OCH_3	0.68	0.08	0.19	NH-NH_2	-0.60	-0.08	-0.55
C(O)OPh	0.85	0.14	0.27	N=N-Ph	0.67	0.20	0.20
C(O)NH_2	0.46	0.09	0.17	N=O	0.58	0.31	0.37
C(O)Cl	0.76	0.16	0.33	NO_2	0.87	0.20	0.35
C(O)CH_3	0.60	0.10	0.20	$SiMe_3$	0.22	-0.02	-0.02
C(O)*t*Bu	0.44	0.05	0.05				
C(O)H	0.53	0.18	0.28				
C(NPh)H	0.60	0.20	0.20				
C(O)Ph	0.45	0.12	0.23				
C(O)C(O)Ph	0.62	0.15	0.30				
CN	0.29	0.12	0.25				
F	-0.29	-0.02	-0.23				
Cl	-0.02	-0.07	-0.13				
Br	0.13	-0.13	-0.08				
I	0.39	-0.21	0.00				
OH	-0.53	-0.14	-0.43				
OCH_3	-0.45	-0.07	-0.41				

Data in dilute $CDCl_3$ by Paul Schatz, UW-Madison. Original data from *J. Am. Chem. Soc*. **1956**, *78*, 3043 at 30 MHz with 50% solutions in cyclohexane.

(Adapted from Hans J. Reich, http://www.chem.wisc.edu/areas/reich/nmr/notes-9-hmr-6-vinyl-aryl-shifts.pdf)

^{1}H- and ^{13}C-NMR Chemical Shifts for Common Solvents in $CDCl_3$

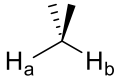
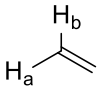
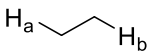
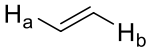
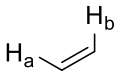
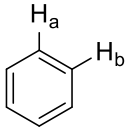
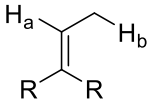
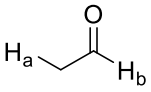
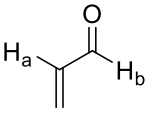
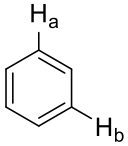
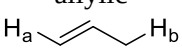
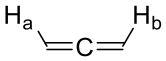
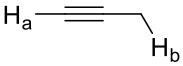
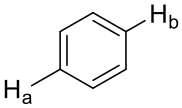
Solvent	ρ (g/cm^3)	^{1}H δ (ppm)	^{1}H Signal Multiplicity	^{13}C δ (ppm)
acetone	0.791	2.17	singlet	207.07 (CO) 30.92 (CH_3)
acetonitrile	0.786	2.10	singlet	116.43 (CN) 1.89 (CH_3)
benzene	0.8765	7.36	singlet	128.57 (Ar)
chloroform	1.489 @ 25 ºC	7.27	singlet	77.58 (CD)* 77.44 (CD)* 77.00 (CD)*
dichloromethane	1.3266 @ 20 ºC	5.30	singlet	53.52 (CH_2)
diethyl ether	0.7134	3.48 1.21	quartet triplet	65.91 (CH_2) 15.20 (CH_3)
ethanol	0.789 @ 25 ºC	3.72 1.25	quartet triplet	58.28 (CH_2) 18.41 (CH_3)
n-hexane	0.6548	1.26 0.88	2nd order multiplet triplet	31.64 (CH_2) 22.70 (CH_2) 14.14 (CH_3)
isopropanol	0.786 @ 20 ºC	4.04 1.73	septet doublet	64.50 (CH) 25.14 (CH_3)
methanol	0.792	3.49 variable	singlet broad singlet	50.41 (CH_3)
n-pentane	0.626	1.27 0.88	2nd order multiplet triplet	34.16 (CH_2) 22.38 (CH_2) 14.08 (CH_3)
tetrahydrofuran	0.8892 @ 20 ºC	3.76 1.85	2nd order multiplet 2nd order multiplet	67.97 (CH_2) 25.62 (CH_2)
toluene	0.87 @ 20 ºC	2.36 (CH_3) 7.1 – 7.3 (Ar)	singlet	137.8 (Ar) 129.0 (Ar) 128.2 (Ar) 125.3 (Ar) 21.46 (CH_3)
water	1.00	1.56	singlet	-

Values obtained from the following:

Gottlieb, H. E.; Kotlyar, V.; Nudelman, A. NMR Chemical Shifts of Common Laboratory Solvents as Trace Impurities. *J. Org. Chem.*, **1997**, *62*, 7512–7515.

Fulmer, G. R.; Miller, A. J. M.; Sherden, N. H.; Gottlieb, H. E.; Nudelman, A.; Stoltz, B. M.; Bercaw, J. E.; Goldberg, K. I. NMR Chemical Shifts of Trace Impurities: Common Laboratory Solvents, Organics, and Gases in Deuterated Solvents Relevant to the Organometallic Chemist. *Organometallics*, **2010**, *29*, 2176–2179.

Typical ^{1}H-NMR Coupling Values*

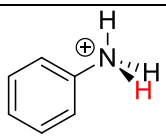
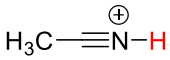
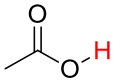
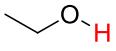
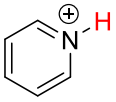
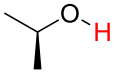
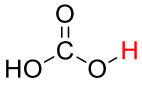
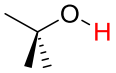
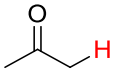
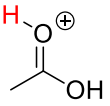
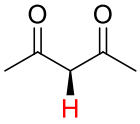
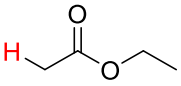
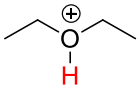
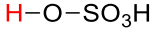
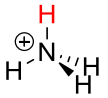
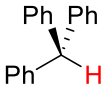
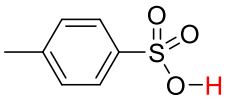
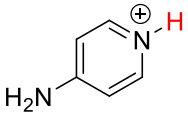
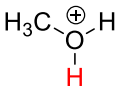
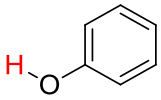
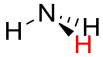
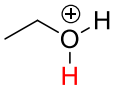
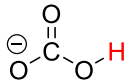
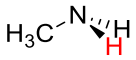
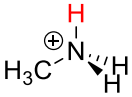
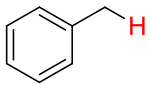
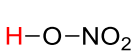
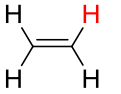
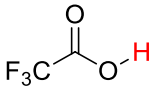
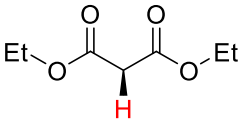
Coupling				
2-bond	*gem* alkyl  $^2J = 2 – 15$ (typical -12 Hz)	*gem* vinyl  $^2J = 1 – 3$		
3-bond	*vicinal* alkyl  $^3J = 2 – 20$ (typical 7 Hz)	*trans* vinyl  $^3J = 12 – 18$	*cis* vinyl  $^3J = 6 – 12$	*ortho* aryl  $^3J = 8 – 12$
	vicinal C(sp^2)-C(sp^3)  $^3J = 3 – 11$ (dihedral dependent)	*vicinal* aldehyde  $^3J = 1 – 3$	*vicinal* conjugated aldehyde  $^3J = 7 – 8$	
4-bond	*meta* aryl  $^4J = 2 – 3$	allylic  $^4J = 0 – 3$	allenic  $^4J = 6 – 7$	propargylic  $^4J = 2 – 4$
5-bond	*para* aryl  $^5J = 0 – 1$			

*J values listed as absolute values of coupling in Hz

Infrared Correlation Chart

	Type of Vibration		Frequency (cm^{-1})	Intensity
C-H	Alkanes	(stretch)	3000-2850	s
	$-CH_3$	(bend)	1450 and 1375	m
	$-CH_2-$	(bend)	1465	m
	Alkenes	(stretch)	3100-3000	m
		(out-of-plane bend)	1000-650	s
	Aromatics	(stretch)	3150-3050	s
		(out-of-plane bend)	900-690	s
	Alkyne	(stretch)	~3300	s
	Aldehyde		2900-2800	w
			2800-2700	w
C-C	Alkane	not interpretatively useful		
C=C	Alkene		1680-1600	m-w
	Aromatic		1600 and 1475	m-w
C≡C	Alkyne		2250-2100	m-w
C=O	Aldehyde		1740-1720	s
	Ketone		1725-1705	s
	Carboxylic Acid		1725-1700	s
	Ester		1750-1730	s
	Amide		1670-1640	s
	Anhydride		1810 and 1760	s
	Acid Chloride		1800	s
C-O	Alcohols, Ethers, Esters, Carboxylic Acids, Anhydrides		1300-1000	s
O-H	Alcohols, Phenols			
		Free	3650-3600	m
		H-bonded	3500-3200	m
	Carboxylic Acids		3400-2400	m
N-H	Primary and Secondary Amines and Amides			
		(stretch)	3500-3100	m
		(bend)	1640-1550	m-s
C-N	Amines		1350-1000	m-s
C=N	Imines and Oximes		1690-1640	w-s
C≡N	Nitriles		2260-2240	m
X=C=Y	Allenes, Ketenes, Isocyanates, Isothiocyanates		2270-1950	m-s
N=O	Nitro ($R-NO_2$)		1550 and 1350	s
S-H	Mercaptans		2550	w
S=O	Sulfoxides		1050	s
	Sulfones, Sulfonyl Chlorides, Sulfates, Sulfonamides		1375-1300	s
C-X	Fluoride		1400-1000	s
	Chloride		800-600	s
	Bromide, Iodide		<667	s

Original Source Unknown. w = weak, m = medium, s= strong

Acid	pK_a	Acid	pK_a	Acid	pK_a
	-10		4.6		15.7
	-10		4.75		16
	-9		5.2		16.5
	-7.5		6.35		18
	-7		7.0		19.2
	-6.2		9.0		24
	-3.8		9.1		25
	-3*		9.2		33
	-2.8		9.2	H–H	35
	-2.5		9.9		38
	-2.4		10.3		38
	-1.74		10.6		41
	-1.4		10.7		44
	0.18		10.7		50
H–F	3.2		15		

*values differ widely depending on source from -9 to -3.

Cyclohexane A-values* (in kcal/mol)

–H	0.0	$–COCH_3$	1.0-1.5
–D	0.006	$–NO_2$	1.1
–CN	0.17	–SH	1.21
–F	0.25-0.42	$–NH_2$	1.23-1.7
–Cl	0.53-0.64	$–CO_2H$	1.4
–Br	0.48-0.67	**$–CH_3$**	**1.74**
–I	0.47-0.61	$–C_2H_5$	1.79
$–OCH_3$	0.55-0.75	$–CH(CH_3)_2$	2.21
–OH	0.60-1.04	$–CF_3$	2.4-2.5
–OPh	0.65	–Ph	2.8
–CHO	0.56-0.8	$– C(CH_3)_3$	4.7-4.9

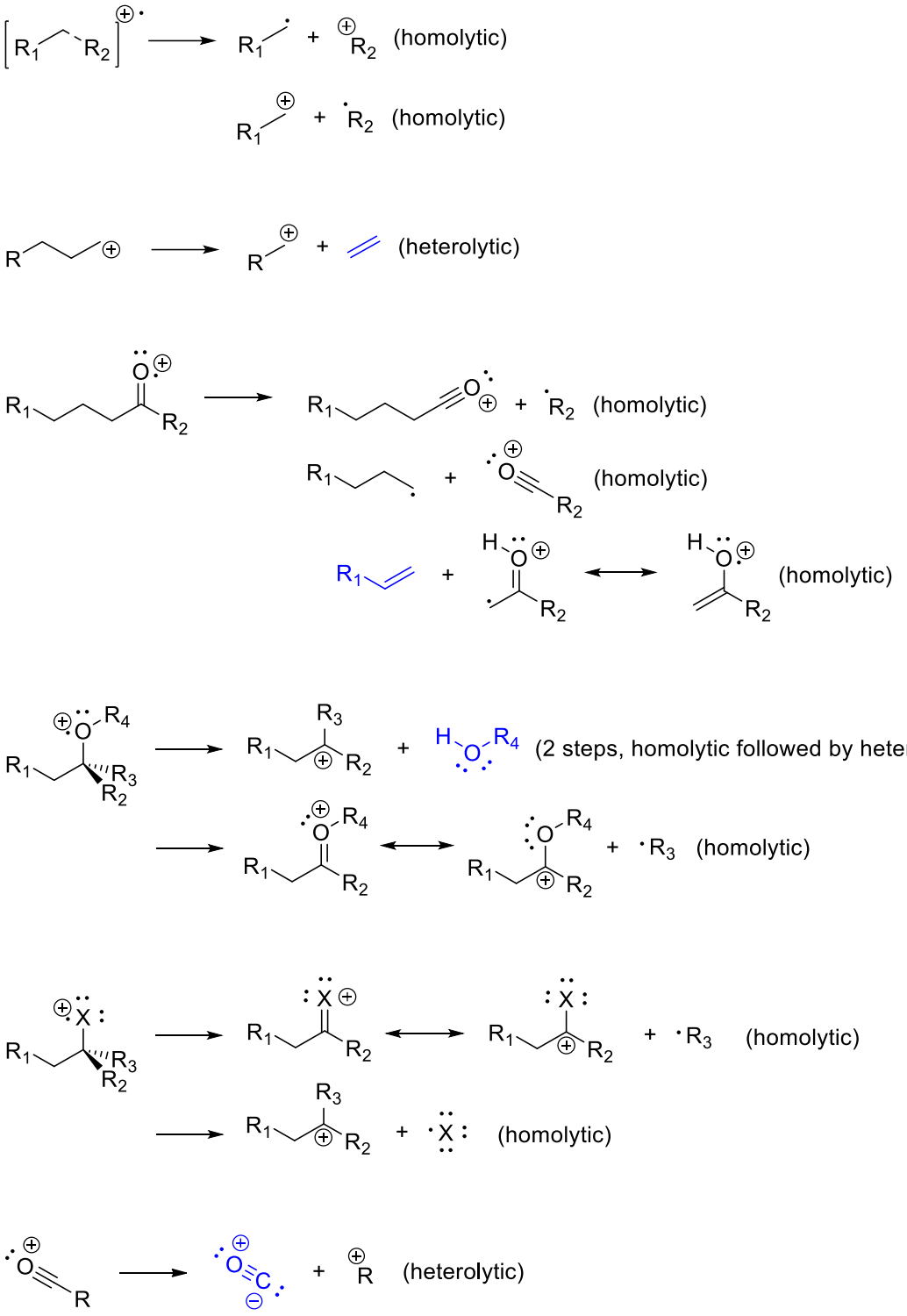
*The energy cost for a substituent to be axial vs. equatorial on a cyclohexane ring.

Adapted from Eliel, E.L.; Wilen, S.H.; Mander, L.N. Stereochemistry of Organic Compounds, Wiley, New York (1994).

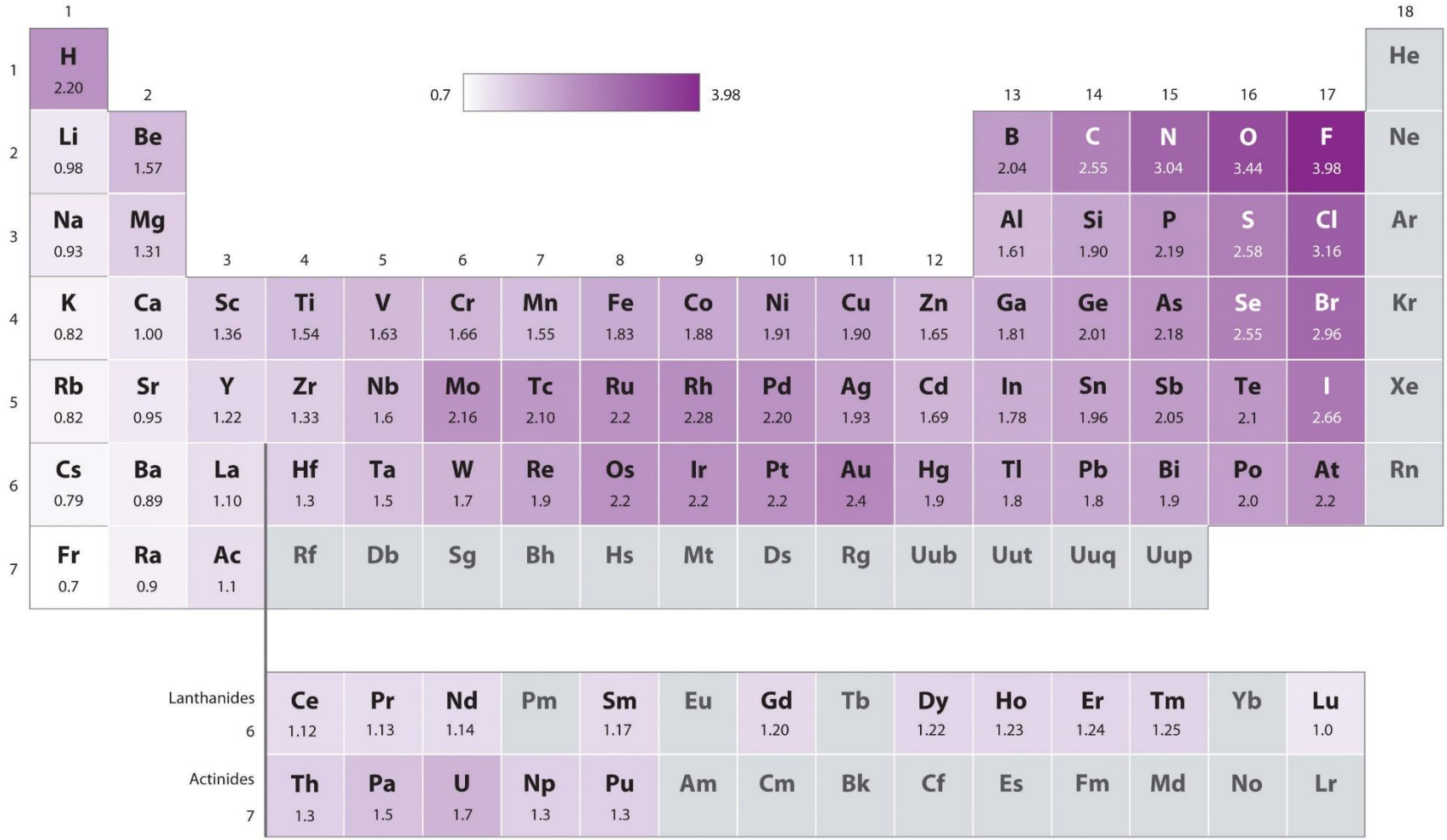
Nuclear Spin, Relative Abundance, and Exact Mass of Several Common Isotopes

Element	Isotope	Nuclear Spin	Exact Mass	Abundance %
Hydrogen	^{1}H	$^{1}/_{2}$	1.007825	99.985
	^{2}H or D	1	2.0140	0.015
Carbon	^{12}C	0	12.0000	98.90
	^{13}C	$^{1}/_{2}$	13.00335	1.10
Nitrogen	^{14}N	1	14.00307	99.63
	^{15}N	$^{1}/_{2}$	15.00011	0.37
Oxygen	^{16}O	0	15.99491	99.759
	^{17}O	$^{5}/_{2}$	16.99913	0.037
	^{18}O	0	17.99916	0.204
Fluorine	^{19}F	$^{1}/_{2}$	18.99840	100.0
Silicon	^{28}Si	0	27.97693	92.21
	^{29}Si	½	28.97649	4.67
	^{30}Si	0	29.97377	3.10
Phosphorus	^{31}P	$^{1}/_{2}$	30.97376	100.0
Sulfur	^{32}S	0	31.97207	95.0
	^{33}S	$^{3}/_{2}$	32.97146	0.75
	^{34}S	0	33.96787	4.22
Chlorine	^{35}Cl	$^{3}/_{2}$	34.96885	75.77
	^{37}Cl	$^{3}/_{2}$	36.96590	24.23
Bromine	^{79}Br	$^{3}/_{2}$	78.91834	50.69
	^{81}Br	$^{3}/_{2}$	80.91629	49.31
Iodine	^{127}I	$^{5}/_{2}$	126.90447	100.0

Common EI-MS Fragmentation Reactions



Periodic Table with Pauling Electronegativities (χ)



Adapted from Averill, B. A.; Eldredge, P. Chemistry: Principles, Patterns, and Applications, Prentice Hall, (2006)