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Table 1: Some characteristic absorption frequencies in IR spectroscopy

<u>Bond type</u>	<u>frequency (cm⁻¹)</u>
C-H alkanes	2950 – 2850
C-H alkenes	3080 – 3020
C-H aldehyde	~2900
C-H alkyne	~3300
alkyne triple bond	2250 – 2100 (s)
alkene double bond	1680 - 1620(s)
carbonyl, ketone	1725 – 1700 (s)
carbonyl, aldehyde	1740 – 1720 (s)
carbonyl, ester	1750 – 1730 (s)
carbonyl, acid	1725 – 1700 (s)
carbonyl, amide	1690 – 1650 (s)
O-H, alcohols	3600 – 3200 (s, broad)
O-H, acids	3000 – 2500 (broad)
C-O, alcohols, esters, ethers	1300 - 1000

s = strong absorbance

Table 2: Typical values for $^1\text{H-NMR}$ chemical shifts

<u>Hydrogen type</u>	<u>Chemical shift (ppm)</u>
RCH_3	0.9 - 1.0
RCH_2R	1.2 - 1.7
R_3CH	1.5 - 2.0
$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{CH}_3 \end{array}$	2.0 - 2.3
$\begin{array}{c} \text{R} \quad \text{CH}_3 \\ \diagdown \quad / \\ \text{C}=\text{C} \\ / \quad \diagdown \\ \text{R} \quad \text{R} \end{array}$	1.5 - 1.8
RNH_2	1 - 3
ArCH_3	2.2 - 2.4
$\text{R}-\text{C}\equiv\text{C}-\text{H}$	2.3 - 3.0
$\begin{array}{c} \text{R}-\text{O}-\text{CH}_3 \end{array}$	3.7 - 3.9
$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{O}-\text{CH}_3 \end{array}$	3.7 - 3.9
ROH	1 - 5
$\begin{array}{c} \text{R} \quad \text{H} \\ \diagdown \quad / \\ \text{C}=\text{C} \\ / \quad \diagdown \\ \text{R} \quad \text{R} \end{array}$	3.7 - 6.5
$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{N}-\text{R} \\ \\ \text{H} \end{array}$	5 - 9
ArH	6.0 - 8.7
$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{H} \end{array}$	9.5 - 10.0
$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{OH} \end{array}$	10 - 13

Chemical shift values are in parts per million (ppm) relative to tetramethylsilane.

Table 3: Typical values for ^{13}C -NMR chemical shifts

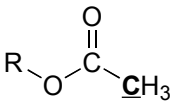
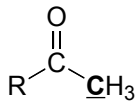
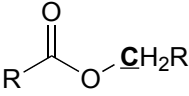
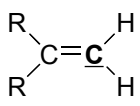
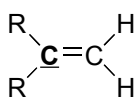
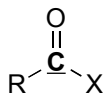
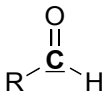
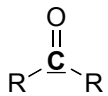
<u>Carbon type</u>	<u>Chemical shift (ppm)</u>
$\text{R}\underline{\text{C}}\text{H}_3$	13 - 16
$\text{R}\underline{\text{C}}\text{H}_2\text{R}$	16 - 25
$\text{R}_3\underline{\text{C}}\text{H}$	25 - 35
	18 - 22
	28 - 32
$\text{R}\underline{\text{C}}\text{H}_2\text{NHR}$	35 - 45
$\text{R}\underline{\text{C}}\text{H}_2\text{OH}$	50 - 65
$\text{R}-\text{C}\equiv\underline{\text{C}}-\text{R}$	65 - 70
$\text{RO}\underline{\text{C}}\text{H}_2\text{R}$	50 - 75
	50 - 75
	115 - 120
	125 - 140
aromatic carbon	125 - 150
 (carboxylic acid derivatives)	165 - 185
	190 - 200
	200 - 220

Table 4: Typical coupling constants in NMR

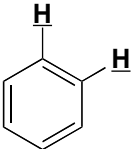
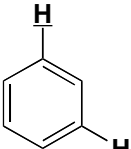
<u>H-H coupling</u>	<u>J (Hz)</u>	<u>C-H coupling</u>	<u>J (Hz)</u>
$\begin{array}{c} \text{R} \quad \text{R} \\ \quad \\ \text{R}-\text{C}-\text{C}-\text{R} \\ \quad \\ \text{H} \quad \text{H} \end{array}$	6 - 8	$\begin{array}{c} \text{R} \\ \\ \text{R}-\text{C}-\text{H} \\ \\ \text{R} \end{array}$	125 - 130
$\begin{array}{c} \text{R} \quad \text{O} \\ \quad \\ \text{R}-\text{C}-\text{C}-\text{H} \\ \\ \text{H} \end{array}$	2 - 3	$\begin{array}{c} \text{R} \quad \text{H} \\ \diagdown \quad / \\ \text{C}=\text{C} \\ / \quad \diagdown \\ \text{R} \quad \text{R} \end{array}$	150 - 170
$\begin{array}{c} \text{H} \quad \text{R} \\ \diagdown \quad / \\ \text{C}=\text{C} \\ / \quad \diagdown \\ \text{R} \quad \text{H} \end{array}$	12 - 18		
$\begin{array}{c} \text{R} \quad \text{R} \\ \diagdown \quad / \\ \text{C}=\text{C} \\ / \quad \diagdown \\ \text{H} \quad \text{H} \end{array}$	6 - 12		
$\begin{array}{c} \text{R} \quad \text{H} \\ \diagdown \quad / \\ \text{C}=\text{C} \\ / \quad \diagdown \\ \text{R} \quad \text{H} \end{array}$	0 - 2		
	6 - 10		
	1 - 3		

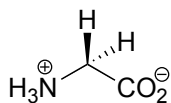
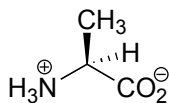
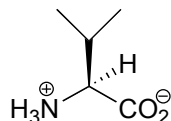
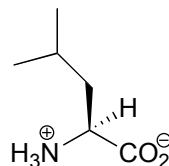
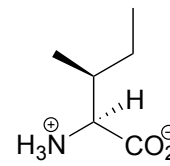
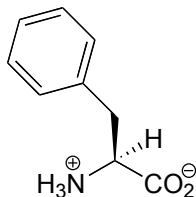
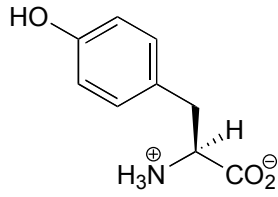
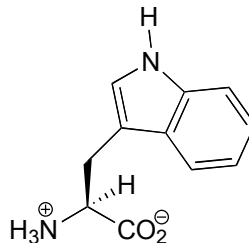
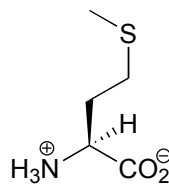
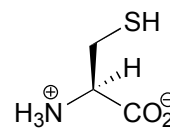
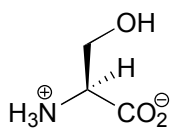
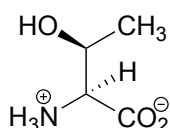
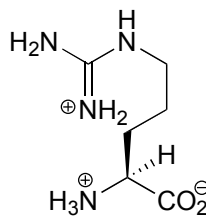
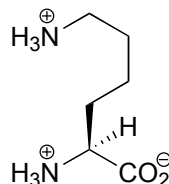
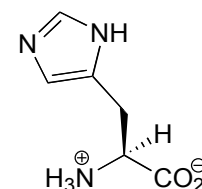
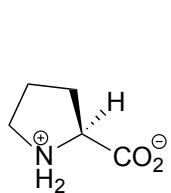
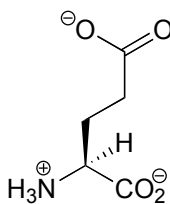
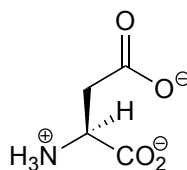
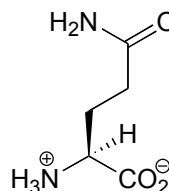
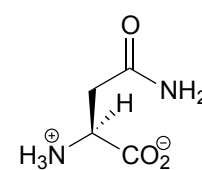
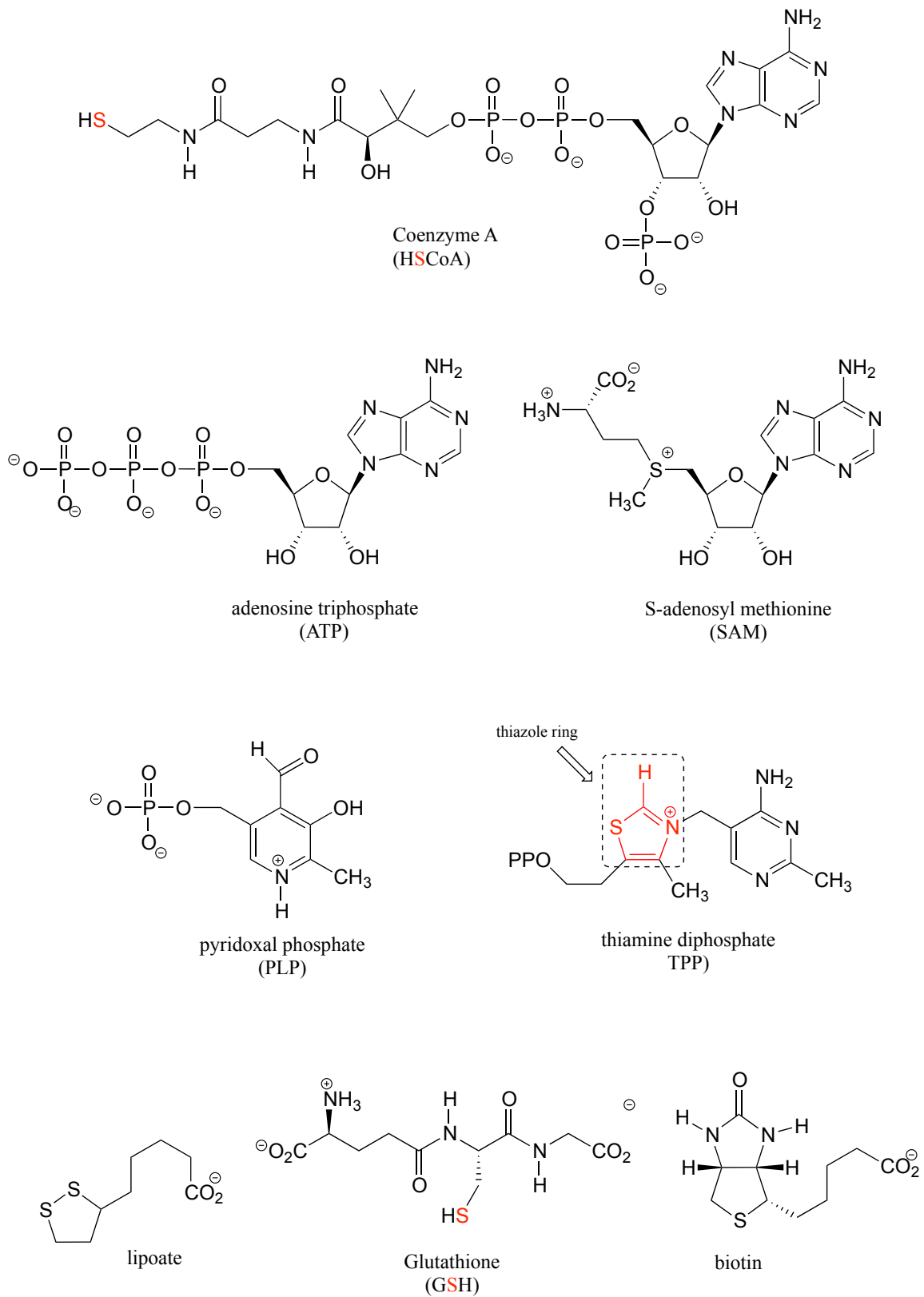
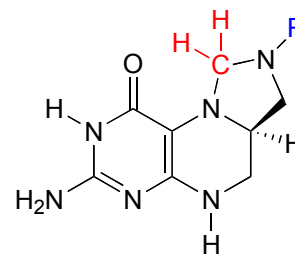
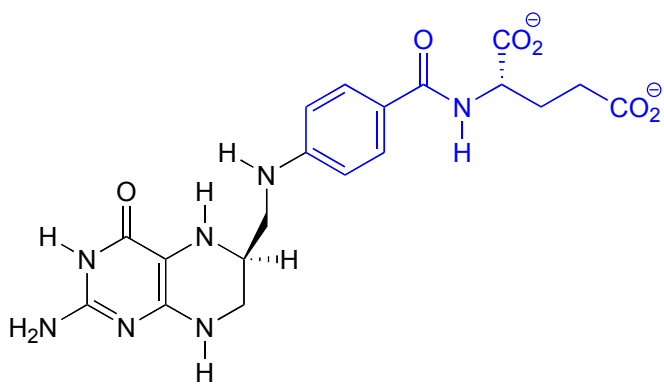
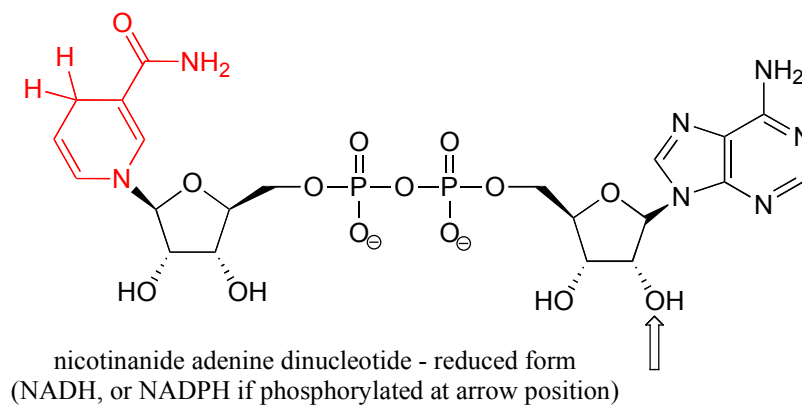
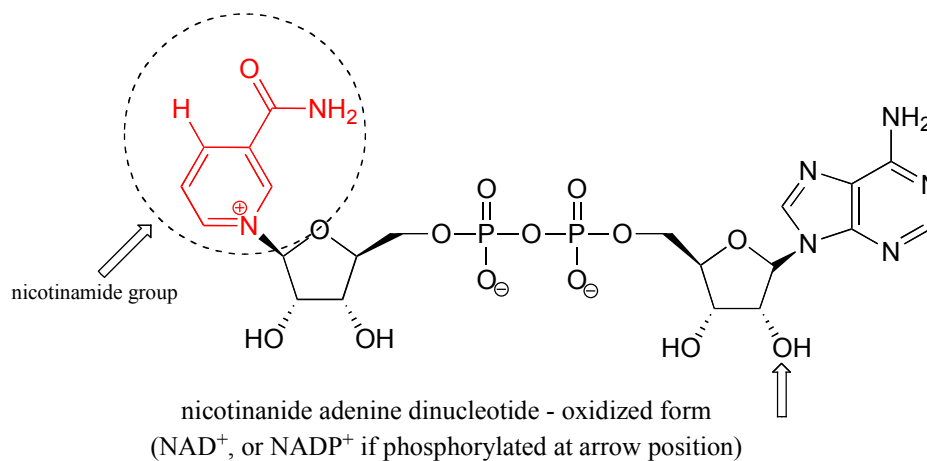
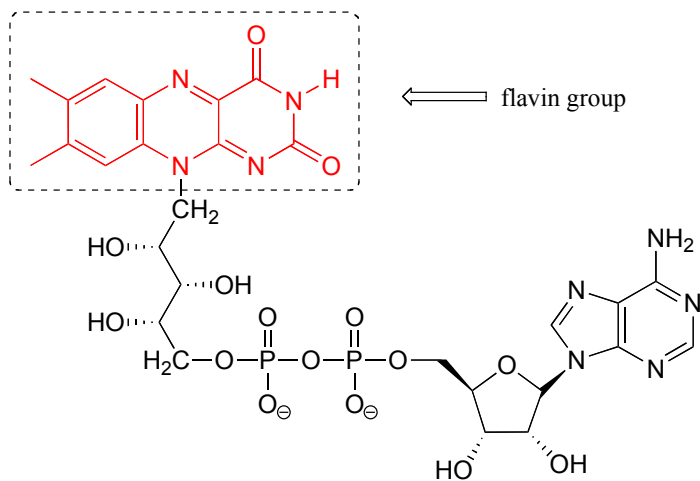
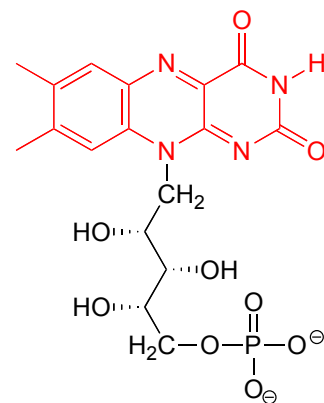
Table 5: The 20 common amino acids**Glycine**
(Gly, G)**Alanine**
(Ala, A)**Valine**
(Val, V)**Leucine**
(Leu, L)**Isoleucine**
(Ile, I)**Phenylalanine**
(Phe, F)**Tyrosine**
(Tyr, Y)**Tryptophan**
(Trp, W)**Methionine**
(Met, M)**Cysteine**
(Cys, C)**Serine**
(Ser, S)**Threonine**
(Thr, T)**Arginine**
(Arg, R)**Lysine**
(Lys, K)**Histidine**
(His, H)**Proline**
(Pro, P)**Glutamate**
(Glu, E)**Aspartate**
(Asp, D)**Glutamine**
(Gln, Q)**Asparagine**
(Asn, N)

Table 6: Structures of common coenzymes

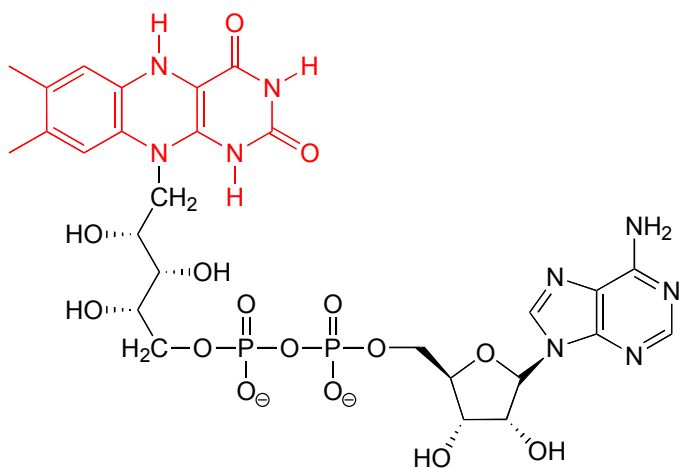




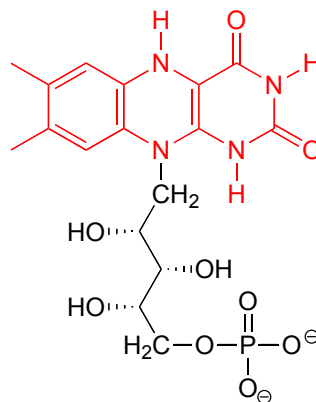
flavin adenine dinucleotide, oxidized form
(FAD)



flavin mononucleotide, oxidized form
(FMN)

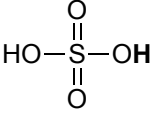
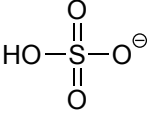
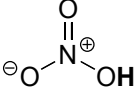
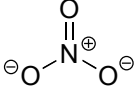
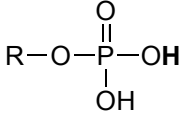
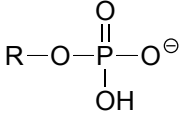
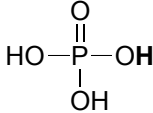
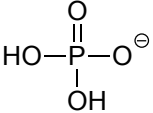
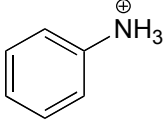
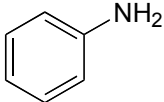
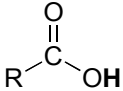
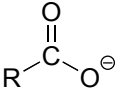
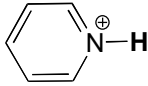
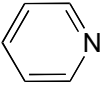


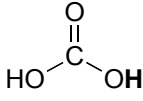
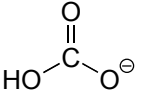
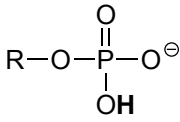
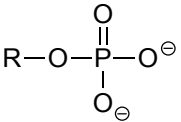
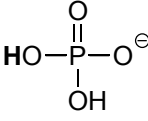
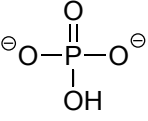
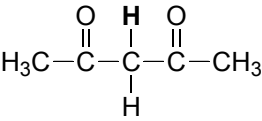
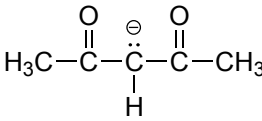

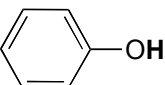
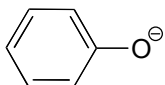
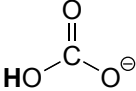
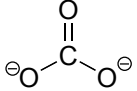
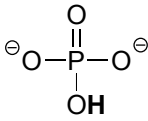
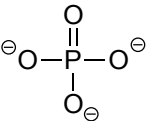
flavin adenine dinucleotide, reduced form
(FADH₂)



flavin mononucleotide, reduced form
(FMNH₂)

Table 7: Representative acid constants.

<u>acid</u>	<u>pK_a</u>	<u>conjugate base</u>
 sulfuric acid	-10	
HCl	-7	Cl ⁻
H ₃ O ⁺	-1.7	H ₂ O
 nitric acid	-1.4	
	1.0 ⁽ⁱ⁾	
 phosphoric acid	2.2 ⁽ⁱⁱ⁾	
HF	3.2	F ⁻
	4.6	
	4-5	
 pyridinium	5.3 ⁽ⁱⁱ⁾	 pyridine

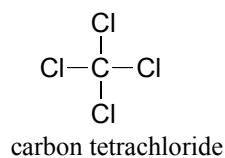
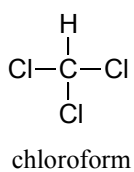
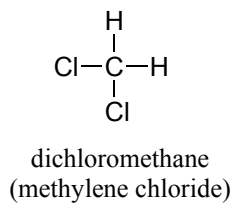
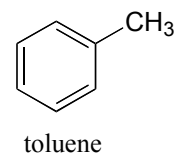
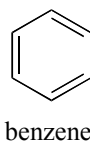
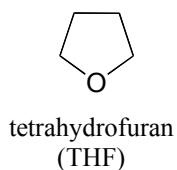
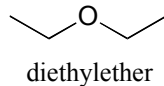
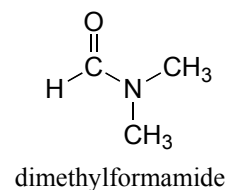
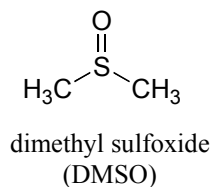
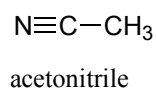
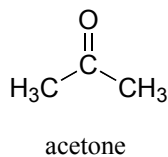
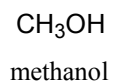
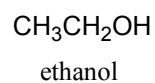
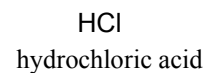
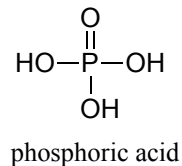
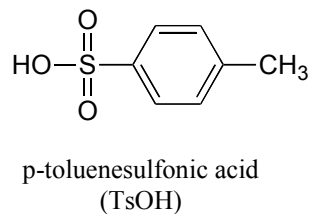
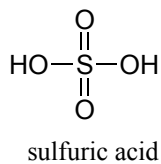
<u>acid</u>	<u>pK_a</u>	<u>conjugate base</u>
 carbonic acid	6.4	 bicarbonate
 	6.5 ⁽ⁱ⁾	
 	7.2 ⁽ⁱⁱ⁾	
 	9.0	
HCN	9.2	CN ⁻
 ammonium	9.2	NH ₃ ammonia
 phenol	9.9 ⁽ⁱⁱ⁾	 phenolate
 bicarbonate	10.3 ⁽ⁱⁱ⁾	 carbonate
RSH	10-11	RS ⁻
RNH ₃ ⁺	10 -11	RNH ₂
 	12.3 ⁽ⁱ⁾	
H ₂ O	15.7	OH ⁻

<u>acid</u>	<u>pK_a</u>	<u>conjugate base</u>
$\begin{array}{c} \text{O} \\ \parallel \\ \text{R}-\text{C}-\text{NH}_2 \end{array}$	17	$\begin{array}{c} \text{O} \\ \parallel \\ \text{R}-\text{C}-\text{NH}^- \end{array}$
RCH ₂ OH	16	RCH ₂ O ⁻
$\begin{array}{c} \text{O} \\ \parallel \\ \text{R}-\text{C}-\text{C}-\text{R} \\ \quad \\ \text{H} \quad \text{H} \end{array}$	19-20	$\begin{array}{c} \text{O} \\ \parallel \\ \text{R}-\text{C}-\text{C}^- -\text{R} \\ \\ \text{H} \end{array}$
RCCH terminal alkyne	25	RCC ⁻
H ₂	35	H ⁻
NH ₃ ammonia	38	NH ₂ ⁻

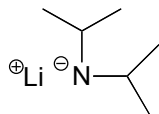
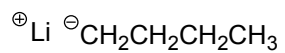
All pK_a values, unless otherwise noted, are taken from March, Jerry, Advanced Organic Chemistry, Fourth Edition, Wiley, New York, 1992.

⁽ⁱ⁾ Silva, J.J.R. Fraústo da, The Biological Chemistry of the Elements: the Inorganic Chemistry of Life, 2nd Edition, Oxford, New York, 2001.

⁽ⁱⁱ⁾ Lide, David R. (ed.) The CRC Handbook of Chemistry and Physics, CRC Press, Boca Raton, FL, 1995.

Table 8: Some common laboratory solvents, acids, and bases**Solvents****Acids**

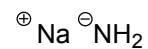
Bases

very strong bases:lithium diisopropylamide
(LDA)

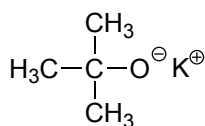
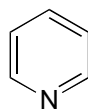
N-butyllithium



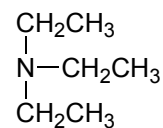
sodium hydride



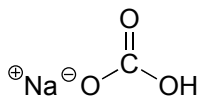
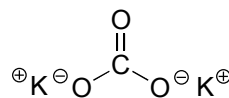
sodium amide

weaker bases:potassium *tert*-butoxide

pyridine

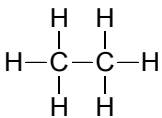
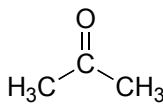
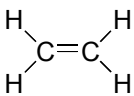
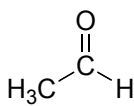
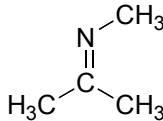

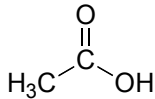
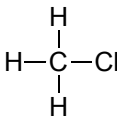
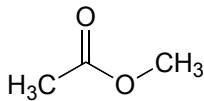
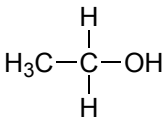
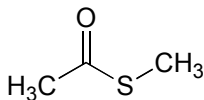
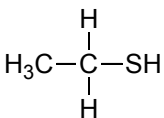
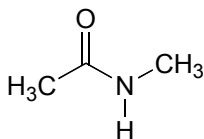
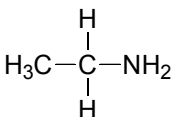
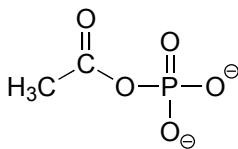
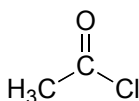
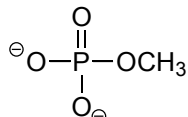
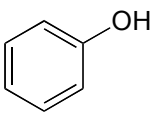


triethylamine

sodium bicarbonate
 NaHCO_3 potassium carbonate
 K_2CO_3 

sodium hydroxide

Table 9: Examples of common functional groups in organic chemistry

alkane		ketone	
alkene		aldehyde	
alkyne	$\text{H}-\text{C}\equiv\text{C}-\text{H}$	imine (Schiff base)	
aromatic hydrocarbon		carboxylic acid	
alkyl halide		ester	
alcohol		thioester	
thiol		amide	
amine		acyl phosphate	
ether	$\text{H}_3\text{C}-\text{O}-\text{CH}_3$	acid chloride	
sulfide	$\text{H}_3\text{C}-\text{S}-\text{CH}_3$	phosphate ester	
phenol		phosphate diester	