

# 참고 자료집

"화학으로 세계를 연결하기"

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## 상수와 공식

아보가드로 수,  $N_A = 6.0221 \times 10^{23} \text{ mol}^{-1}$

볼츠만 상수,  $k_B = 1.3807 \times 10^{-23} \text{ J K}^{-1}$

기체상수,  $R = 8.3145 \text{ J K}^{-1} \text{ mol}^{-1} = 0.08205 \text{ atm L K}^{-1} \text{ mol}^{-1}$

빛의 속도,  $c = 2.9979 \times 10^8 \text{ m s}^{-1}$

플랑크 상수,  $h = 6.6261 \times 10^{-34} \text{ J s}$

패러데이 상수,  $F = 9.64853399 \times 10^4 \text{ C}$

전자 질량,  $m_e = 9.10938215 \times 10^{-31} \text{ kg}$

표준 압력,  $P = 1 \text{ bar} = 10^5 \text{ Pa}$

대기압,  $P_{\text{atm}} = 1.01325 \times 10^5 \text{ Pa} = 760 \text{ mmHg} = 760 \text{ torr}$

섭씨 0 도,  $273.15 \text{ K}$

1 피코미터 (pm) =  $10^{-12} \text{ m}$ ; 1 옴스트롱(Å) =  $10^{-10} \text{ m}$ ; 1 나노미터 (nm) =  $10^{-9} \text{ m}$

1 eV =  $1.6 \times 10^{-19} \text{ J}$

1 amu =  $1.66053904 \times 10^{-27} \text{ kg}$

이상기체 상태방정식:  $PV = nRT$

엔탈피:  $H = U + PV$

깁스자유에너지:  $G = H - TS$   $\Delta G = \Delta G^\circ + RT \ln Q$

$$\Delta G^\circ = -RT \ln K = -nFE_{\text{cell}}^\circ$$

엔트로피 변화:  $\Delta S = \frac{q_{\text{rev}}}{T}$ , ( $q_{\text{rev}}$  는 가역과정의 열)

$$\Delta S = nR \ln \frac{V_2}{V_1} \text{ (이상기체의 등온팽창시)}$$

네른스트(Nernst)식:  $E = E^\circ + \frac{RT}{nF} \ln \frac{C_{\text{ox}}}{C_{\text{red}}} = E^\circ - \frac{RT}{nF} \ln Q$

광자(photon)의 에너지:  $E = \frac{hc}{\lambda}$     램버트-비어(Lambert-Beer)법칙:  $A = \log \frac{I_0}{I} = \epsilon bC$

적분 반응속도식

0 차  $[A] = [A]_0 - kt$                       1 차  $\ln[A] = \ln[A]_0 - kt$

2 차  $\frac{1}{[A]} = \frac{1}{[A]_0} + kt$

아레니우스 식  $k = Ae^{-E_a/RT}$  (A 는 아레니우스 인자)

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Periodic table of elements

		18 8A	
		2 He 4.003	
		10 Ne 20.18	
		18 Ar 39.95	
		36 Kr 83.80	
		54 Xe 131.3	
		86 Rn (222)	
		118 Og (294)	
		117 Ts (294)	
		116 Lv (293)	
		115 Mc (289)	
		114 Fl (289)	
		113 Nh (286)	
		112 Cn (285)	
		111 Rg (272)	
		110 Ds (281)	
		109 Mt (266)	
		108 Hs (265)	
		107 Bh (262)	
		106 Sg (263)	
		105 Db (262)	
		104 Rf (261)	
		103 Lr (262)	
		102 No (259)	
		101 Md (258)	
		100 Fm (257)	
		99 Es (252)	
		98 Cf (251)	
		97 Bk (247)	
		96 Cm (247)	
		95 Am (243)	
		94 Pu (244)	
		93 Np (237)	
		92 U 238.0	
		91 Pa 231.0	
		90 Th 232.0	
		89 Ac (227)	
		88 Ra (226)	
		87 Fr (223)	
		86 Rn (222)	
		85 At (210)	
		84 Po (209)	
		83 Bi 209.0	
		82 Pb 207.2	
		81 Tl 204.4	
		80 Hg 200.6	
		79 Au 197.0	
		78 Pt 195.1	
		77 Ir 192.2	
		76 Os 190.2	
		75 Re 186.2	
		74 W 183.8	
		73 Ta 180.9	
		72 Hf 178.5	
		71 Lu 175.0	
		70 Yb 173.0	
		69 Tm 168.9	
		68 Er 167.3	
		67 Ho 164.9	
		66 Dy 162.5	
		65 Tb 158.9	
		64 Gd 157.3	
		63 Eu 152.0	
		62 Sm 150.4	
		61 Pm (145)	
		60 Nd 144.2	
		59 Pr 140.9	
		58 Ce 140.1	
		57 La 138.9	
		56 Ba 137.3	
		55 Cs 132.9	
		54 Xe 131.3	
		53 I 126.9	
		52 Te 127.6	
		51 Sb 121.8	
		50 Sn 118.7	
		49 In 114.8	
		48 Cd 112.4	
		47 Ag 107.9	
		46 Pd 106.4	
		45 Rh 102.9	
		44 Ru 101.1	
		43 Tc (98)	
		42 Mo 95.95	
		41 Nb 92.91	
		40 Zr 91.22	
		39 Y 88.91	
		38 Sr 87.62	
		37 Rb 85.47	
		36 Kr 83.80	
		35 Br 79.90	
		34 Se 78.97	
		33 As 74.92	
		32 Ge 72.61	
		31 Ga 69.72	
		30 Zn 65.39	
		29 Cu 63.55	
		28 Ni 58.69	
		27 Co 58.93	
		26 Fe 55.85	
		25 Mn 54.94	
		24 Cr 52.00	
		23 V 50.94	
		22 Ti 47.88	
		21 Sc 44.96	
		20 Ca 40.08	
		19 K 39.10	
		18 Ar 39.95	
		17 Cl 35.45	
		16 S 32.07	
		15 P 30.97	
		14 Si 28.09	
		13 Al 26.98	
		12 Mg 24.31	
		11 Na 22.99	
		10 Ne 20.18	
		9 F 19.00	
		8 O 16.00	
		7 N 14.01	
		6 C 12.01	
		5 B 10.81	
		4 Be 9.012	
		3 Li 6.941	
		2 He 4.003	
		1 H 1.008	

### Characteristic $^1\text{H}$ NMR Chemical Shifts

Type of Hydrogen (R=Alkyl, Ar=Aryl)	Chemical Shift (ppm)	Type of Hydrogen (R=Alkyl, Ar=Aryl)	Chemical Shift (ppm)
$(\text{CH}_3)_4\text{Si}$	0 (by definition)		
$\text{RCH}_3$	0.9	$\text{RCH}=\text{O}$	9.5-10.1
$\text{RCH}_2\text{R}$	1.2-1.4	$\text{RCOOH}'$	10-13
$\text{R}_3\text{CH}$	1.4-1.7	$\text{RCOCH}_3$	2.1-2.3
$\text{RCH}_2\text{I}$	3.2-3.3	$\text{RCOCH}_2\text{R}$	2.2-2.6
$\text{RCH}_2\text{Br}$	3.4-3.5	$\text{RCOOCH}_3$	3.7-3.9
$\text{RCH}_2\text{Cl}$	3.6-3.8	$\text{RCOOCH}_2\text{R}$	4.1-4.7
$\text{RCH}_2\text{F}$	4.4-4.5	$\text{R}_2\text{C}=\text{CRCHR}_2$	1.6-2.6
$\text{RCH}_2\text{NH}_2$	2.3-2.9	$\text{R}_2\text{C}=\text{CH}_2$	4.6-5.0
$\text{RCH}_2\text{OH}$	3.4-4.0	$\text{R}_2\text{C}=\text{CHR}$	5.0-5.7
$\text{RCH}_2\text{OR}$	3.3-4.0	$\text{RC}\equiv\text{CH}$	2.0-3.0
$\text{RCH}_2\text{CH}_2\text{OR}$	1.5-1.6	$\text{ArCH}_3$	2.2-2.5
$\text{R}_2\text{NH}$	0.5-5.0	$\text{ArCH}_2\text{R}$	2.3-2.8
$\text{ROH}$	0.5-6.0	$\text{ArH}$	6.5-8.5

### Characteristic $^{13}\text{C}$ NMR Chemical Shifts

Type of Carbon (R=Alkyl, Ar=Aryl)	Chemical Shift (ppm)	Type of Carbon (R=Alkyl, Ar=Aryl)	Chemical Shift (ppm)
$\text{RCH}_3$	10-25	$\text{RC}(\text{triplebond})\text{CR}$	65-85
$\text{RCH}_2\text{R}$	20-35	$\text{RCH}=\text{CHR}$	120-140
$\text{R}_3\text{CH}$	25-35	$\text{ArylC}$	120-140
$\text{RCH}_2\text{COR}$	35-50	$\text{RCOOR}$	160-180
$\text{RCH}_2\text{Br}$	25-35	$\text{RCONR}_2$ (amide)	165-180
$\text{RCH}_2\text{Cl}$	40-45	$\text{RCOOH}$	175-185
$\text{RCH}_2\text{NH}_2$	30-65	$\text{RCHO}$	190-205
$\text{RCH}_2\text{OH}$	60-70	$\text{RCOR}$	200-215
$\text{RCH}_2\text{OR}$	65-70		

*Adapted from RSC E-learning website.*

## IR Absorption Frequencies Table

Characteristic IR Absorption Frequencies of Organic Functional Groups			
Functional Group	Type of Vibration	Characteristic Absorptions (cm <sup>-1</sup> )	Intensity
<b>Alcohol</b>			
O-H	(stretch, H-bonded)	3200-3600	strong, broad
O-H	(stretch, free)	3500-3700	strong, sharp
C-O	(stretch)	1050-1150	strong
<b>Alkane</b>			
C-H	stretch	2850-3000	strong
-C-H	bending	1350-1480	variable
<b>Alkene</b>			
=C-H	stretch	3010-3100	medium
=C-H	bending	675-1000	strong
C=C	stretch	1620-1680	variable
<b>Alkyl Halide</b>			
C-F	stretch	1000-1400	strong
C-Cl	stretch	600-800	strong
C-Br	stretch	500-600	strong
C-I	stretch	500	strong
<b>Alkyne</b>			
C-H	stretch	3300	strong, sharp
-C≡C-	stretch	2100-2260	variable, not present in symmetrical alkynes
<b>Amine</b>			
N-H	stretch	3300-3500	medium (primary amines have two bands; secondary have one band, often very weak)
C-N	stretch	1080-1360	medium-weak
N-H	bending	1600	medium
<b>Aromatic</b>			
C-H	stretch	3000-3100	medium
C=C	stretch	1400-1600	medium-weak, multiple bands
Analysis of C-H out-of-plane bending can often distinguish substitution patterns			
<b>Carbonyl</b>			
C=O	stretch	1670-1820	strong
(conjugation moves absorptions to lower wave numbers)			
<b>Ether</b>			
C-O	stretch	1000-1300 (1070-1150)	strong
<b>Nitrile</b>			
CN	Stretch	2210-2260	medium

<b>Nitro</b>			
N-O	stretch	1515-1560 & 1345-1385	strong, two bands

<b>IR Absorption Frequencies of Functional Groups Containing a Carbonyl (C=O)</b>			
<b>Functional Group</b>	<b>Type of Vibration</b>	<b>Characteristic Absorptions (cm<sup>-1</sup>)</b>	<b>Intensity</b>
<b>Carbonyl</b>			
C=O	stretch	1670-1820	strong
(conjugation moves absorptions to lower wave numbers)			
<b>Acid</b>			
C=O	stretch	1700-1725	strong
O-H	stretch	2500-3300	strong, very broad
C-O	stretch	1210-1320	strong
<b>Aldehyde</b>			
C=O	stretch	1740-1720	strong
=C-H	stretch	2820-2850 & 2720-2750	medium, two peaks
<b>Amide</b>			
C=O	stretch	1640-1690	strong
N-H	stretch	3100-3500	unsubstituted have two bands
N-H	bending	1550-1640	
<b>Anhydride</b>			
C=O	stretch	1800-1830 & 1740-1775	two bands
<b>Ester</b>			
C=O	stretch	1735-1750	strong
C-O	stretch	1000-1300	two bands or more
<b>Ketone</b>			
acyclic	stretch	1705-1725	strong
cyclic	stretch	3-membered - 1850 4-membered - 1780 5-membered - 1745 6-membered - 1715 7-membered - 1705	strong
$\alpha,\beta$ -unsaturated	stretch	1665-1685	strong
aryl ketone	stretch	1680-1700	strong

Data from <http://www2.ups.edu/faculty/hanson/Spectroscopy/IR/IRfrequencies.html>