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참고 자료집

"화학으로 세계를 연결하기"

49 회 국제화학올림피아드,
나콘파톰, 태국

상수와 공식

아보가드로 수, $N_A = 6.0221\times10^{23}$ mol^{-1}

볼쯔만 상수, $k_B = 1.3807\times10^{-23}$ J K^{-1}

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

빛의 속도, $c = 2.9979\times10^{8}$ m s^{-1}

플랑크 상수, $h = 6.6261\times10^{-34}$ J s

패러데이 상수, $F = 9.64853399\times10^{4}$ C

전자 질량, $m_e = 9.10938215\times10^{-31}$ kg

표준 압력, $P = 1$ bar $= 10^5$ Pa

대기압, $P_{atm} = 1.01325\times10^5$ Pa = 760 mmHg = 760 torr

섭씨 0 도, 273.15 K

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

1 eV = 1.6×10^{-19} J

1 amu = 1.66053904×10^{-27} kg

이상기체 상태방정식: $PV = nRT$

엔탈피: $H = U + PV$

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

$\Delta G^o = -RT\ln K = -nFE^o_{cell}$

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

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

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

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

적분 반응속도식

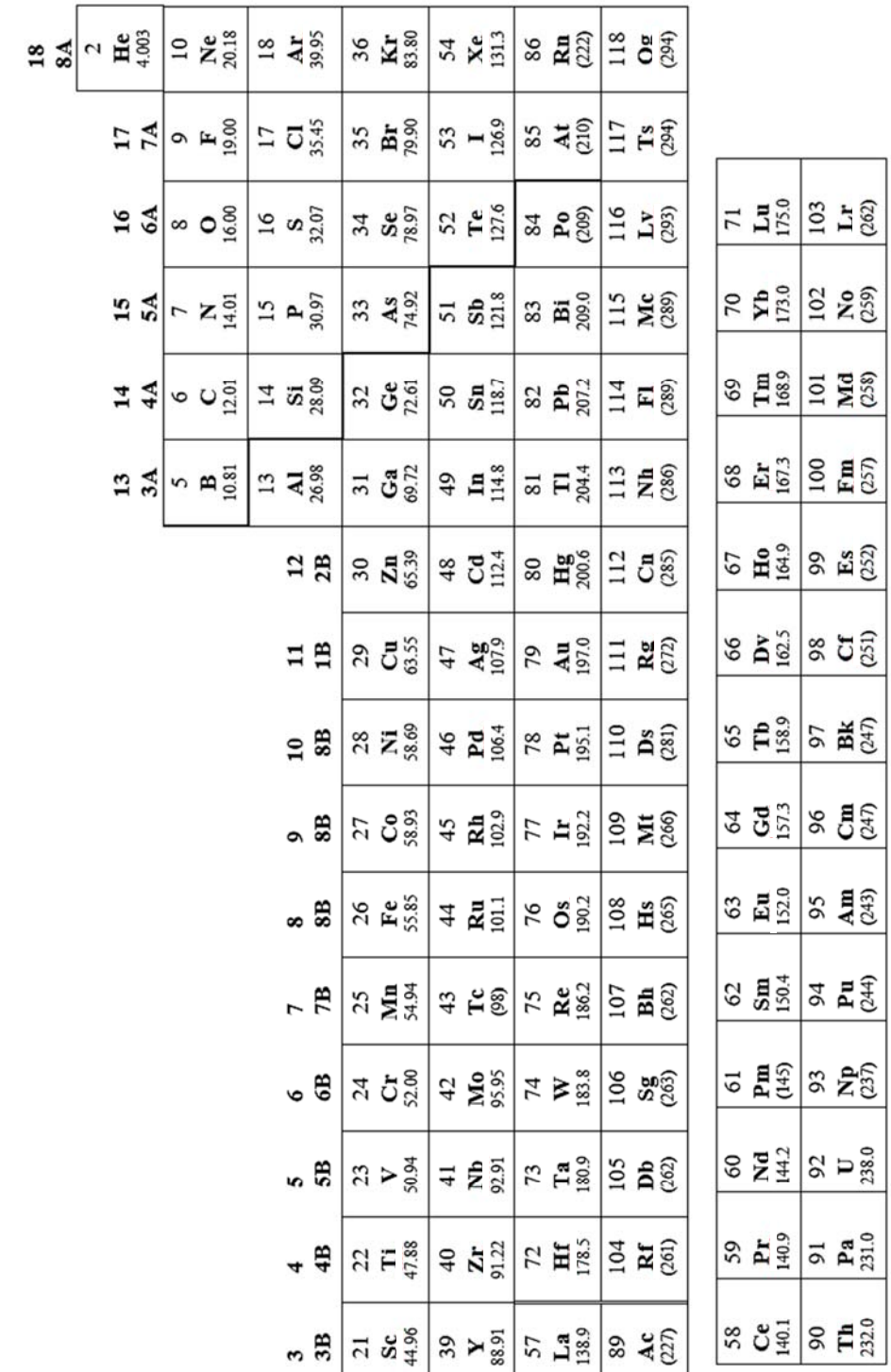
0 차 $[A] = [A]_0 - kt$ 1 차 $\ln[A] = \ln[A]_0 - kt$

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

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

참고자료집(한글번역본), 49th IChO 2017, Thailand

Periodic table of elements



Characteristic ^{1}H NMR Chemical Shifts

Type of Hydrogen (R=Alkyl, Ar=Aryl)	Chemical Shift (ppm)	Type of Hydrogen (R=Alkyl, Ar=Aryl)	Chemical Shift (ppm)
$(CH_3)_4Si$	0 (by definition)		
RCH_3	0.9	RCH=O	9.5-10.1
RCH_2R	1.2-1.4	RCOOH'	10-13
R_3CH	1.4-1.7	$RCOCH_3$	2.1-2.3
RCH_2I	3.2-3.3	$RCOCH_2R$	2.2-2.6
RCH_2Br	3.4-3.5	$RCOOCH_3$	3.7-3.9
RCH_2Cl	3.6-3.8	$RCOOCH_2R$	4.1-4.7
RCH_2F	4.4-4.5	$R_2C=CRCHR_2$	1.6-2.6
RCH_2NH_2	2.3-2.9	$R_2C=CH_2$	4.6-5.0
RCH_2OH	3.4-4.0	$R_2C=CHR$	5.0-5.7
RCH_2OR	3.3-4.0	RC≡CH	2.0-3.0
RCH_2CH_2OR	1.5-1.6	$ArCH_3$	2.2-2.5
R_2NH	0.5-5.0	$ArCH_2R$	2.3-2.8
ROH	0.5-6.0	ArH	6.5-8.5

Characteristic ^{13}C NMR Chemical Shifts

Type of Carbon (R=Alkyl, Ar=Aryl)	Chemical Shift (ppm)	Type of Carbon (R=Alkyl, Ar=Aryl)	Chemical Shift (ppm)
RCH_3	10-25	RC(triplebond)CR	65-85
RCH_2R	20-35	RCH=CHR	120-140
R_3CH	25-35	ArylC	120-140
RCH_2COR	35-50	RCOOR	160-180
RCH_2Br	25-35	$RCONR_2$ (amide)	165-180
RCH_2Cl	40-45	RCOOH	175-185
RCH_2NH_2	30-65	RCHO	190-205
RCH_2OH	60-70	RCOR	200-215
RCH_2OR	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^{-1})**	**Intensity**
Alcohol			
O-H	(stretch, H-bonded)	3200-3600	strong, broad
O-H	(stretch, free)	3500-3700	strong, sharp
C-O	(stretch)	1050-1150	strong
Alkane			
C-H	stretch	2850-3000	strong
-C-H	bending	1350-1480	variable
Alkene			
=C-H	stretch	3010-3100	medium
=C-H	bending	675-1000	strong
C=C	stretch	1620-1680	variable
Alkyl Halide			
C-F	stretch	1000-1400	strong
C-Cl	stretch	600-800	strong
C-Br	stretch	500-600	strong
C-I	stretch	500	strong
Alkyne			
C-H	stretch	3300	strong, sharp
–C≡C–	stretch	2100-2260	variable, not present in symmetrical alkynes
Amine			
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
Aromatic			
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			
Carbonyl			
C=O	stretch	1670-1820	strong
(conjugation moves absorptions to lower wave numbers)			
Ether			
C-O	stretch	1000-1300 (1070-1150)	strong
Nitrile			
CN	Stretch	2210-2260	medium

Nitro			
N-O	stretch	1515-1560 & 1345-1385	strong, two bands

IR Absorption Frequencies of Functional Groups Containing a Carbonyl (C=O)

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

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