Information Booklet

"Bonding the World with Chemistry"

49th INTERNATIONAL CHEMISTRY OLYMPIAD

Nakhon Pathom, THAILAND

Constants and Formulae

Avogadro's constant, $N_A = 6.0221\times10^{23}$ mol^{-1}

Boltzmann constant, $k_B = 1.3807\times10^{-23}$ J K^{-1}

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

Speed of light, $c = 2.9979\times10^{8}$ m s^{-1}

Planck's constant, $h = 6.6261\times10^{-34}$ J s

Faraday constant, $F = 9.64853399\times10^{4}$ C

Mass of electron, $m_e = 9.10938215\times10^{-31}$ kg

Standard pressure, $P = 1$ bar $= 10^5$ Pa

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

Zero of the Celsius scale, 273.15 K

1 picometer (pm) = 10^{-12} m; 1 Å = 10^{-10} m; nanometer (nm) = 10^{-9} m

1 eV = 1.6×10^{-19} J

1 amu = 1.66053904×10^{-27} kg

Ideal gas equation: $PV = nRT$

Enthalpy: $H = U + PV$

Gibbs free energy: $G = H - TS$ $\qquad \Delta G = \Delta G^o + RT\ln Q$

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

Entropy change: $\Delta S = \frac{q_{rev}}{T}$, where q_{rev} is heat for the reversible process

$$\Delta S = nR\ln\frac{V_2}{V_1}$$ (for isothermal expansion of an ideal gas)

Nernst equation: $E = E^o - \frac{RT}{nF}\ln Q$

$$E = E^o + \frac{RT}{nF}\ln\frac{C_{ox}}{C_{red}}$$

Energy of a photon: $E = \frac{hc}{\lambda}$ $\qquad$ Lambert-Beer law: $A = \log\frac{I_0}{I} = \varepsilon bC$

Integrated rate law

Zero order $[\mathrm{A}] = [\mathrm{A}]_0 - kt$ $\qquad$ First order $\ln[\mathrm{A}] = \ln[\mathrm{A}]_0 - kt$

Second order $\frac{1}{[\mathrm{A}]} = \frac{1}{[\mathrm{A}]_0} + kt$

Arrhenius equation

$k = Ae^{-E_a/RT}$ (A is Arrhenius factor)

Periodic table of elements

1 1A													13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
1 **H** 1.008	2 2A																	2 **He** 4.003
3 **Li** 6.941	4 **Be** 9.012												5 **B** 10.81	6 **C** 12.01	7 **N** 14.01	8 **O** 16.00	9 **F** 19.00	10 **Ne** 20.18
11 **Na** 22.99	12 **Mg** 24.31	3 3B	4 4B	5 5B	6 6B	7 7B	8 8B	9 8B	10 8B	11 1B	12 2B		13 **Al** 26.98	14 **Si** 28.09	15 **P** 30.97	16 **S** 32.07	17 **Cl** 35.45	18 **Ar** 39.95
19 **K** 39.10	20 **Ca** 40.08	21 **Sc** 44.96	22 **Ti** 47.88	23 **V** 50.94	24 **Cr** 52.00	25 **Mn** 54.94	26 **Fe** 55.85	27 **Co** 58.93	28 **Ni** 58.69	29 **Cu** 63.55	30 **Zn** 65.39	31 **Ga** 69.72	32 **Ge** 72.61	33 **As** 74.92	34 **Se** 78.97	35 **Br** 79.90	36 **Kr** 83.80
37 **Rb** 85.47	38 **Sr** 87.62	39 **Y** 88.91	40 **Zr** 91.22	41 **Nb** 92.91	42 **Mo** 95.95	43 **Tc** (98)	44 **Ru** 101.1	45 **Rh** 102.9	46 **Pd** 106.4	47 **Ag** 107.9	48 **Cd** 112.4	49 **In** 114.8	50 **Sn** 118.7	51 **Sb** 121.8	52 **Te** 127.6	53 **I** 126.9	54 **Xe** 131.3
55 **Cs** 132.9	56 **Ba** 137.3	57 **La** 138.9	72 **Hf** 178.5	73 **Ta** 180.9	74 **W** 183.8	75 **Re** 186.2	76 **Os** 190.2	77 **Ir** 192.2	78 **Pt** 195.1	79 **Au** 197.0	80 **Hg** 200.6	81 **Tl** 204.4	82 **Pb** 207.2	83 **Bi** 209.0	84 **Po** (209)	85 **At** (210)	86 **Rn** (222)
87 **Fr** (223)	88 **Ra** (226)	89 **Ac** (227)	104 **Rf** (261)	105 **Db** (262)	106 **Sg** (263)	107 **Bh** (262)	108 **Hs** (265)	109 **Mt** (266)	110 **Ds** (281)	111 **Rg** (272)	112 **Cn** (285)	113 **Nh** (286)	114 **Fl** (289)	115 **Mc** (289)	116 **Lv** (293)	117 **Ts** (294)	118 **Og** (294)

58 **Ce** 140.1	59 **Pr** 140.9	60 **Nd** 144.2	61 **Pm** (145)	62 **Sm** 150.4	63 **Eu** 152.0	64 **Gd** 157.3	65 **Tb** 158.9	66 **Dy** 162.5	67 **Ho** 164.9	68 **Er** 167.3	69 **Tm** 168.9	70 **Yb** 173.0	71 **Lu** 175.0
90 **Th** 232.0	91 **Pa** 231.0	92 **U** 238.0	93 **Np** (237)	94 **Pu** (244)	95 **Am** (243)	96 **Cm** (247)	97 **Bk** (247)	98 **Cf** (251)	99 **Es** (252)	100 **Fm** (257)	101 **Md** (258)	102 **No** (259)	103 **Lr** (262)

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)		
RC**H**$_3$	0.9	RC**H**=O	9.5-10.1
RC**H**$_2$R	1.2-1.4	RCOO**H'**	10-13
R$_3$C**H**	1.4-1.7	RCOC**H**$_3$	2.1-2.3
RC**H**$_2$I	3.2-3.3	RCOC**H**$_2$R	2.2-2.6
RC**H**$_2$Br	3.4-3.5	RCOOC**H**$_3$	3.7-3.9
RC**H**$_2$Cl	3.6-3.8	RCOOC**H**$_2$R	4.1-4.7
RC**H**$_2$F	4.4-4.5	R$_2$C=CRC**H**R$_2$	1.6-2.6
RC**H**$_2$NH$_2$	2.3-2.9	R$_2$C=C**H**$_2$	4.6-5.0
RC**H**$_2$OH	3.4-4.0	R$_2$C=C**H**R	5.0-5.7
RC**H**$_2$OR	3.3-4.0	RC≡C**H**	2.0-3.0
RC**H**$_2$CH$_2$OR	1.5-1.6	ArC**H**$_3$	2.2-2.5
R$_2$N**H**	0.5-5.0	ArC**H**$_2$R	2.3-2.8
RO**H**	0.5-6.0	Ar**H**	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)
R**C**H$_3$	10-25	R**C**(triplebond)CR	65-85
R**C**H$_2$R	20-35	RCH=**C**HR	120-140
R$_3$**C**H	25-35	Aryl**C**	120-140
R**C**H$_2$COR	35-50	R**C**OOR	160-180
R**C**H$_2$Br	25-35	R**C**ONR$_2$ (amide)	165-180
R**C**H$_2$Cl	40-45	R**C**OOH	175-185
R**C**H$_2$NH$_2$	30-65	R**C**HO	190-205
R**C**H$_2$OH	60-70	R**C**OR	200-215
R**C**H$_2$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^{-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