# Water

## 1. Problem involving multiplication factor:

$$\text{Multiplication factor} = \frac{\text{equivalent mass of CaCO3}}{\text{Equivalent mass of hardness causing impurity}}$$

Equivalent hardness of CaCO3 = mass of hardness causing impurity x multiplication factor

$$= \text{mass of impurity} \times \frac{\text{equivalent mass of CaCO3}}{\text{equivalent mass if impurity}}$$

1 PPM = 1 mg/L = 0.1 French = 0.07 Clarke

**ex.1** Calculate the hardness of water containing 9.5 mg of MgCl2 in 500 ml solution.

Soln: 9.5 mg of MgCl2 is present in 500 ml solution
Therefore, 9.5 x2 mg of MgCl2 will be present in 1 litre soln

Harness of MgCl2 = 19 ppm

$$\text{Equivalent harness Of CaCO3} = 19 \times \frac{100}{95} = 20 \text{ ppm}$$

## 2. Problem involving Temporary, permanent and Total hardness

Calculate the temporary, permant and total hardenss of water having following composition

; Mg(HCO3)2 = 14.6 ppm, CaCO3=5 ppm, Ca(HCO3)2= 8.1 ppm, Mg(NO3)2= 7.4 ppm, CaSO4= 6.8ppm, CO2=22 ppm, HCl= 3.65 ppm, Ca(NO3)2 = 4.1 ppm, SiO2 = 10 ppm, KNO3= 15 ppm, $MgCl_2$= 3.8 ppm, MgCl2= 3.8 ppm, $Al_2(SO_4)_3$ = 11.4 ppm, $NaHCO_3$ = 10 ppm

| Name of impurity | Amount present in ppm | Multiplication factor | Equivalent hardness of CaCO3 | Hardness Type |
|---|---|---|---|---|
| $Mg(HCO_3)_2$ | 14.6 | 100/146 | 10 | T |
| $CaCO_3$ | 5 | 1 | 5 | T |
| , $Ca(HCO_3)_2$ | 8.1 | 100/162 | 5 | T |
| $Mg(NO_3)_2$ | 7.4 | 100/148 | 5 | P |
| $CaSO_4$ | 6.8 | 100/136 | 5 | P |
| $CO_2$ | 22 | - | - | N.H |
| HCl | 3.65 | - | - | N.H |
| $Ca(NO_3)_2$ | 4.1 | 100/164 | 2.5 | P |
| $SiO_2$ | 10 | - | - | N.H |
| $KNO_3$ | 15 | - | - | N.H |
| $MgCl_2$ | 3.8 ppm | 100/95 | 4 | P |
| $NaHCO_3$ | 10 ppm | - | - | N.H |
| $Al_2(SO_4)_3$ | 11.4 ppm | 100/114 | 10 | P |

Temporary Hardness = 10 + 5 + 5 =20 ppm

Permanent hardness = 5 +5+ 2.5+ 4 + 10 =26.5 ppm

Total hardness = 20 + 26.5 = 46.5 ppm

Problem Based On EDTA Method:

Calculate the total , permanent and temporary hardness of water sample if

i) 50ml of SHW (containing 1g $CaCo_3$ per liter) consumed 20 ml of EDTA solution
ii) 50 ml of water sample consumed 30 ml of EDTA solution and 100 ml of boiled water sample consumed 28 ml of same EDTA solution.

Solution:

1 liter of SHW contains = 1 gram of $CaCO_3$

Therefore, 1 ml of SHW = 1 mg of $CaCO_3$

[ from concentration of SHW]

Given,

50 ml of SHW required= 20 ml of EDTA

Therefore,

50 mg of $CaCO_3$ = 20 ml of EDTA

Therefore,

1 ml of EDTA solution = 5/2 mg of $CaCO_3$.

[ titration of EDTA with SHW]

50 ml of water sample required = 30 ml of EDTA solution

= 30 x ( 5/2 mg of $CaCO_3$)

= 75 mg of $CaCO_3$ Therefore,

Total hardness = 75 x(1000/50 ) = 1500 mg $CaCO_3$ /liter

= 1500 ppm

Also,

100 ml of boiled water sample required = 28 ml of EDTA

= 28 x2.5 mg of $CaCO_3$

Permanent Hardness= 70 x(1000/100) = 700 ppm

**3. Problem involving lime soda calculation**

| **Name of Impurities** | **Reaction with Lime** | **Reaction With Soda** | **L & S Requirement** |
|---|---|---|---|
| | | | |
| **1.Temp** i)Temp Ca | $Ca(OH)_2$ + $Ca(HCO_3)_2$ -------->2**$CaCO_3$** + 2 $H_20$ | No Reaction | L |
| | | | |
| ii)Temp Mg | $Mg(HCO_3)_2$ + 2 $Ca(OH)_2$ --------> **Mg(OH)2** + 2**CaCO3** + 2 H20 | No Reaction | 2L |
| | | | |
| **2 Perm** i)Mg | Ca(OH)2 +MgSO4 -------->CaSO4+ **Mg(OH)2** | CaSO4 +Na2CO3 -------->CaCO3+ Na2SO4 | L+ S |
| | | | |
| ii)Perm Al | 3Ca(OH)2 +Al2(SO4)3 --------> **2Al(OH)3**+ **3** CaSO4 | CaSO4 +Na2CO3 -------->CaCO3+ Na2SO4 | L + S |
| | | | |
| iii)Perm Fe | Ca(OH)2 +FeCl2 -------->**Fe(OH)2**+ CaCl2 | CaCl2 +Na2CO3 -------->CaCO3+ 2Nacl | L + S |
| | | | |
| iv).Perm Ca | | CaSO4/CaCl2 +Na2CO3 -------->CaCO3+ Na2SO4/2 NaCl | S |
| | | | |
| **3. CO2** | CO2 + Ca(OH)2 --------> 2 **CaCO3** + 2H2O | No Reaction | L |
| | | | |
| **4. NaHCO3** | 2NaHCO3 + Ca(OH)2 --------> **CaCO3** + **Na2CO3** +2H20 | No Reaction | L - S |
| | | | |

| | | | |
|---|---|---|---|
| **5. $NaAlO_2$** | $NaAlO_2 + H_2O$ --------> $Al(OH)_3$ + $NaOH$ | | **(-L)**eq to $Ca(OH)_2$ |
| | | | |
| **6. Acid**<br>-i) HCl | $2HCl + Ca(OH)_2$ ------> $2H_2O + CaCl_2$ | $CaCl_2 + Na_2CO_3$--->$2NaCl + CaCO_3$ | L + S |
| | | | |
| ii) $H_2SO_4$ | $H_2SO_4 + Ca(OH)_2$ ----> $2H_2O + CaSO_4$ | $CaSO_4 + Na_2CO_3$ -------->$CaCO_3$+ $Na_2SO_4$ | L +S |
| | | | |
| | | | |

Lime required = 74/100 [( temp Ca + 2x temp Mg) + Perm (Mg, Al, Fe…)

+ Acid ( HCl, $H_2SO_4$,..) + $CO_2$

+ $NaHCO_3$ – $NaAlO_2$] all in terms of $CaCO_3$ hardness

X (vol of water / $10^{6)}$ x (100 / % purity)

Soda required = 106/100 [ Perm (Ca, Mg, Al, Fe…)

+ Acid ( HCl, $H_2SO_4$,..) - $NaHCO_3$ ] all in terms of $CaCO_3$hardness

X (vol of water / $10^{6)}$ x (100 / % purity)

1. Calculate the amt of lime (80% pure) and soda (70% pure) for the removal of one million liter of hard water containing following impurities:

$Ca(HCO_3)_2$ = 8.1 ppm $Mg(HCO_3)_2$ = 3.9 ppm, $CO_2$ = 11 ppm HCl = 7.3 ppm

$NaHCO_3$ = 2.2 ppm, $NaAlO_2$ =3.24 ppm. $CaSO_4$ = 6.8 ppm

| Name of impurity | Amt present | M.F | Equivalence of $CaCO_3$ hardness | Hardness type | Lime required | Soda required |
|---|---|---|---|---|---|---|
| | | | | | | |
| $Ca(HCO_3)_2$ | 8.1 ppm | 100/162 | 5 | T | 5 | - |
| $Mg(HCO_3)_2$ | 3.9 ppm | 100/146 | 2.67 | T | 2 x 2.67 | - |
| $CO_2$ | 11 ppm | 100/44 | 25 | N.H | 25 | |
| HCl | 7.3 ppm | 100/36.5 x2 | 10 | N.H | 10 | 10 |
| $NaHCO_3$ | 2.2 ppm | 100/84x 2 | 1.31 | N.H | 1.31 | -1.31 |
| $NaAlO_2$ | 3.24 ppm | 100/82 x2 | 1.97 | N.H | -1.97 | |
| $CaSO_4$ | 6.8 ppm | 100/136 | 5 | P | - | 5 |

Lime= 44.68 soda= 13.69

Lime reqd = $74/100 \times [44.68] \times 10^6/10^6 \times 100/80$

= 41.33 kg

= $74/100\ [\ ] \times 10^6/10^6 \times 100/80$

Soda required = $106/100\ [13.69] \times 10^6/10^6 \times 100/70$

2. Calculate the lime (85%) and soda (90%) pure for the treatment of 75000 litre of hard water containing following impurities;

   $Mg(HCO_3)_2$ = 10.22 mg/L   $CaSO_4$ = 22.67 mg /L   $Al_2(SO_4)_3$ = 17.1 mg/L

   $CO_2$ =5.5 ppm   $NaHCO_3$ = 2.1 ppm   Ca $(NO_3)_2$ = 16.4 ppm

   $FeSO_4.7H_2O$ = 2.78 ppm  HCl= 3.65 ppm  $SiO_2$ = 22 ppm

| Impurity | Amt present in mg/L | M.F | Equivalence of $CaCO_3$ hardness | Lime | Soda |
|---|---|---|---|---|---|
| $Mg(HCO_3)_2$ | 10.22 | 100/146 | 7 | 2 x7 (2 x L) | - |
| $CaSO_4$ | 22.67 | 100/136 | 16.67 | - | 16.67(S) |
| $Al_2(SO_4)_3$ | 17.1 | (100/2)/(342/6) =100/114 | 15 | 15 | 15 |
| $CO_2$ | 5.5 | 100/44 | 12.5 | 12.5 | |
| $NaHCO_3$ | 2.1 | 100/84 x 2 | 1.25 | 1.25 | -1.25 |
| Ca $(NO_3)_2$ | 16.4 | 100 /164 | 10 | - | 10 |
| $FeSO_4.7H_2O$ | 2.78 | 100/278 | 1 | 1 | 1 |
| HCl | 3.65 | 100/36.5 x 2 | 5 | 5 | 5 |
| $SiO_2$ | 22 | -- | | 48.75 | 46.52 |

**4. Problem on Zeolite Calculation:**

An exhausted zeolite column required 75 litre of brine solution containing 125 g Nacl /l. Calculate the hardness of water if 32000 litre of hard water has passed through the column before getting exhausted.

Let X ppm of 3200o litre hardwater has passed before the exhaustion of column.

Therefore ,

Hardness of 32000 lit Of X ppm hardwater = volume of brine solution required for regeneration

= 75 litre of brine soln containing 125 g /l NaCl
= 75 x 125 g of NaCl
= 75 x 125 x 1000 mg of NaCl
= 75 x 125 x 1000 x (50/58.5) mg of $CaCO_3$

Therefore,

Hardness X ppm $= \frac{75 \times 125 \times 1000 \times 50}{58.5 \times 32000}$

X = 250.4 ppm

**Problem based on Ion Exchange:**

After treating 20,000 liter of hard water by ion exchanger the exhausted ion exchanger required 200 liter of 0.1 N HCl solution and 200 liter of 0.1 N NaOH solutions for regeneration. Find the hardness of water.

Soln:

Hardness of50,000 liter of hard water = 200 liter of 0.1 N HCl solution

= 200 lit of 0.1 N $CaCO_3$ solutions.
= 20 lit of 1 N $CaCO_3$ solution

= 20 x 50 g of $CaCO_3$
= 1000 x 1000 mg of $CaCO_3$

Therefore hardness = 1000000/20000
= 50 ppm

**5. Problem on Chemical Oxygen Demand**

20 ml of sample of water was refluxed with 15 ml of $K_2Cr_2O_7$ solution and the unreacted dichromate solution required 22 ml of 0.25 N ferrous ammonium sulphate (FAS) solution for the oxidation reaction. Under similar condition 20 ml distilled water was refluxed with 15 ml of dichromate solution and then it required 48 ml of 0.25 N FAS solution for reaction. Calculate COD of water sample.

$$\text{COD} = \frac{(V_{blank} - V_{sample}) \times N_{FAS} \times 8000}{\text{Volume of water sample}}$$

$$= \frac{(48 - 22) \times 0.25 \times 8000}{20}$$

= 2600 ppm

**6. Problem on Biological Oxygen Demand**

A 2 % solution of sewage sample is kept in incubation for 5 days at 20 Celsius.If dissolved oxygen of day 1 and day 5 are 8.5 mg/lit and 5.5 mg/lit respectively. Calculate BOD
Soln:

Formula:

BOD = (DO1 -DO5) x dilution factor
= ( 8.5 - 5.5 ) x Vf/Vi
= 3 x 100/2
= 150 mg /lit

ENERGY

1 K cal= 2.2 C.H.U= 3.968 B.T.U

**1. Problem on Dulong-Petit's formula:**

Calculate the GCV and NCV of coal sample containing C= 74 % , H= 10%, S = 6%, O= 5% and ash=5%.
Soln:

GCV = 1/100 [ 8080 x %C + 34500 (H-O/8) +2240 xS]
= 1/100[ 8080 x 74 + 34500 ( 10-5/8) + 2240 x 6]
= 9347.97 Kcal /Kg

NCV = GCV - 9/100x % H x 587
= 9347.97 - 0.09 x 10 x 587
= 8819.67 Kcal/Kg

**2. _Proximate analysis**

i)1.5 gram of coal was subjected for proximate analysis. The weight of coal after heating at 100 $^{o}$ C for 60 minutes was found to be 1.28 g. This was further heated in muffle furnace at 925 $^{o}$ C for 7 minutes, the weight after heating was found 1.08 g. Finally, the coal is heated further at 750 $^{o}$ C for 30 minutes the weight of residue was found as 0.35 g. Calculate % Moisture, % volatile matter, % ash and % fixed carbon.

Soln: Weight of coal taken for analysis = W1 = 1.5 g
Weight of coal after heating 100 ° C fr 60 minutes = W2 = 1.28 g
Weight of coal after heating in furnace at 925 ° C for 7 minute=W3= 1.08 g
Wight of coal after heatng in furnace at 750 ° C for 30 min= W4= 0.35 g

Formula:

$$\% \text{ Moisture} = \frac{W1-W2}{W1} \times 100$$

$$= \frac{1.5 - 1.28}{1.5} \times 100$$

$$= 14.66$$

$$\% \text{ V.M} = \frac{W2 - W3}{W1} \times 100$$

$$= \frac{1.28 - 1.08}{1.5} \times 100$$

$$= 13.33\%$$

$$\% \text{ Ash} = \frac{W4}{W1} xx100$$

$$= \frac{0.35}{1.5} \times 100$$

$$= 23.33\%$$

**3. Problem on Ultimate analysis**

**i)Determination of % Carbon and % Hydrogen**:

1.8 gram of coal was analyzed for % C and % H in combustion tube experiment. The vapour released during combustion was absorbed in dry CaCl2 tube and KOH bulb. The increase in mass of CaCl2 tube and KOH bulb was found to be 0.35 g and 0.68 g respectively. Calculate % C and % H.

Soln:
Mass of coal = 1.8 g

Increase in mass of CaCl2 tube = 0.35 g
Increase in mass of KOH bulb = 0.68 g

$$\% \text{ Carbon} = \frac{\text{increase in mass of KOH bulb}}{\text{Mass of coal}} \times \frac{12}{44} \times 100$$

$$= \frac{0.35 \times 12 \times 100}{1.8 \times 44}$$

$$= 5.3$$

$$\% \text{ Hydrogen} = \frac{\text{increase in mass of CaCl2 tube}}{\text{Mass of coal}} \times \frac{2}{18} \times 100$$

$$= \frac{0.68 \times 2 \times 100}{1.8 \times 18}$$

$$= 4.19\ \%$$

**ii) Kjeldahl Method for determination of Nitrogen:**

1.35 gram of coal was heated in Kjeldahl flask for nitrogen determination. The liberated ammonia was dissolved in 45 ml of 0.25 N H2SO4 solution. The excess acid required 18 ml of 0.25 N KOH solution for neutralization. while the 50 ml of distilled water required 48 ml of o.25 N KOH for neutralization. Calculate % Nitrogen in coal.

$$\% \text{ Nitrogen} = \frac{(V_{blank} - V_{Sample}) \times N_{KOH} \times 1.4}{\text{Mass of coal}}$$

$$= \frac{(48 - 18) \times 0.25 \times 1.4}{1.35}$$

$$= 7.77\ \%$$

**iii) Problem on Sulphur content:**

1.1 gram of coal in bomb calorimeter experiment gave of BaSO4 residue which on heating in furnace and cooling in desiccator gave 0.69 g of residue. Calculate % S in coal sample.

Soln:

$$\% \text{ Sulphur} = \frac{\text{mass of BaSO4 residue}}{\text{Mass of coal}} \times \frac{32}{233} \times 100$$

$$= \frac{0.69 \times 32 \times 100}{1.1 \times 233}$$

$$= 8.61\ \%$$

**4. Oxygen requirement for combustion for SOLID COAL:**

$$\underset{12}{C} + \underset{32}{O_2} \longrightarrow CO_2$$

Therefore,

12 gram of carbon required = 32 gram of oxygen for combustion

Hence multiplication factor for oxygen required = $\frac{12}{32}$

Similarly,

$H_2 + \frac{1}{2} O_2 \longrightarrow H_2O$

2 16

Hence , multiplication factor for oxygen required = $\frac{16}{2}$

$S + O_2 \longrightarrow SO_2$

32 32

Multiplication factor for oxygen required = $\frac{32}{32}$

= 1

| Element | Multiplication Factor |
|---|---|
| Carbon | 32/12 |
| Hydrogen | 16/2 |
| Nitrogen | - ( no reaction with oxygen) |
| Sulphur | 32/32 |
| Oxygen | -1 |

i) Calculate the amount of oxygen and air required for combustion of 1 Kg coal containing Carbon =80 %, N= 2.5 %H = 3%, S=2.5 % ash = 5 % .

% O = 100 – (80 + 2.5 +3+2.5+5)

= 7 %

| Element | Quantity present in **1 Kg** | Multiplication Factor | Amount of O2 required |
|---|---|---|---|
| Carbon | 0.80 Kg | 12 /32 | = 0.80 x 12/32<br>= 0.30 |
| Hydrogen | 0.03 Kg | 16/2 | = 0.03 x 16/2<br>= 0.24 |
| Sulphur | 0.025 Kg | 32/32 | = 0.025 x 32/32<br>= 0.025 |
| Nitrogen | 0.025 kg | - (does not burn) | - |
| Ash | 0.05 kg | - (does not burn) | - |
| Oxygen | 0.07 kg | 1 | - 0.07 (substract from total) |
| | Total oxygen required for burning 1 Kg Coal | | = 0.30 + 0.24 + 0.025 +(-0.07)<br>= 0.495 Kg |

Total oxygen required for burning 1 kg coal = o.495 kg

**100 Kg of air contains = 23 kg of oxygen**

Therefore,

**Multiplying factor for converting oxygen to air = 100/23**

0.495 kg of oxygen = 0.495 x 100/23
= 2.152 Kg

If in case, oxygen is supplied in excess for combustion of coal then we need to supply extra oxygen than what is calculated for combustion.
For e.g.
Suppose if there is 20% excess air is supplied for combustion

Amount of air required if 20% excess air is supplied = 2.152 x 120/100
= 2.5824 Kg

5. **Oxygen requirement for combustion for Gaseous Fuel:**
   i) Calculate volume of oxygen and air required for combustion of 1 m3 gaseous fuel containing following composition:
   $CH_4$ = 20%, $C_3H_6$ = 15%, $H_2$=30%, CO=5%, $H_2O$=8%, $C_2H_6$=12%, oxygen remaining.

| Gaseous Component | Volume present in 1 m3 | Combustion reaction | Multiplication Factor | Volume of Oxygen required for |
|---|---|---|---|---|
| $CH_4$ | 0.20 $m^3$ | $CH_4$ + 2 O2 ------> CO2 + 2 H2O | 2 | = 0.20 x 2<br>= 0.40 $dm^3$ |
| $C_3H_6$ | 0.15 $m^3$ | $C_3H_6$ + 9/2 O2 ------> 3 CO2 + 3H2O | 9/2 | = 0.15 x 9/2<br>= 0.675 $dm^3$ |
| $H_2$ | 0.30 $m^3$ | $H_2$ + ½ O2 ------> H2O | ½ | =0.30 x ½<br>= 0.15 $dm^3$ |
| CO | 0.05 $m^3$ | CO + ½ O2 ------> CO2 | ½ | =0.05 x ½<br>= 0.025 $dm^3$ |
| $H_2O$ | 0.08 $m^3$ | No reaction | - | - |
| $C_2H_6$ | 0.10 $m^3$ | $C_2H_6$ + 7/2 O2 ------> 2CO2 + 3 H2O | 7/2 | = 0.10 x 7/2<br>=o.35 $dm^3$ |
| O2 | 0.10 $m^3$ | | -1 | -0.10 $dm^3$ |
| Volume of oxygen required for combustion of 1 $dm^3$ of fuel | | | | = 0.40 |

| | |
|---|---|
| | +0.675+0.15+0.025+ 0..35-0.10 = 1.5 $dm^3$ |

Therefore,

Volume of oxygen required for combustion of 1 $dm^3$ of fuel = 1.5 $dm^3$

Volume of air:

100 $dm^3$ of air contains = 21 $dm^3$ of oxygen

Therefore,

1.5 $dm^3$ of oxygen will be = 1.5 x 100/21

=7.142 $dm^3$ of air

Volume of oxygen required for combustion of 1 $dm^3$ of fuel = 7.142 $dm^3$ of air

**UV-Vis SPECTROSCOPY**

1. The transmittance of 2 x $10^{-4}$M of solution was found to be 76.2% at a wavelength of 530 nm when placed in cuvette of path length 1 cm. Calculate absorbance, molar absorptivity and transmittance of sample when pathlength is 2 cm.
   Solution:
   Formula:

   A = 2- log(%T)

   A = 2 – log(76.2)
   = 2 – 1.8819
   = 0.1181

   A =ϵ. b . C

   $$\epsilon = \frac{A}{b.\ c}$$

$$= \frac{0.1181}{1 \quad x\ 2\ x\ 10^{-4}}$$

= 590 dm3 mol-1 cm-1

$$\frac{A1}{A2} = \frac{\epsilon\ b1\ C}{\epsilon\ b2\ C}$$

A2 = (b2/b1) . A1

= (2/1) . 0.1181

= 0.2362

OR

A2 = $\epsilon$ b2. C

= 590 x 2 x 2 x $10^{-4}$

= 0.236

A = 2- log(%T)

Log(%T) = 2- 0.2362

=1.7638

% T = 58.1%

2. An aqueous solution of $10^{-3}$ mol/$dm^3$ concentration absorbs 10% of incident radiation in path length 1cm. Calculate concentration of same substance that will absorb 90% of incident radiation is same path length of cell.

Soln: Since solution absorbs 10 % of incident radiation in path length of 1 cm cell

% T = 90%

A = 2- log(90)

= 2 -1.9542 = 0.0458

A = $\epsilon$ b C

$\epsilon$ = A / b.c

$$= \frac{0.0458}{1\ x\ 10\text{-}3}$$

= 45.8 $dm^3 mol^{-1} cm^{-1}$

% T2 = 10 % (since 90% of incident light absorbed)

A2 = 2 – log(10)

= 2-1

=1

A2 = $\epsilon$ b C2

C2 = A2/ $\epsilon$ b

= 1/ 1 x 45.8

=2.18 x 10-2 mol/$dm^3$

**3. Problem on total theoretical mode of vibration:**

Formula:
Total Theoretical mode of vibration = 3 N -5
for linear molecule

Total Theoretical mode of vibration = 3 N -6
for non-linear molecule
Where, N= total number of atom in molecule

for e.g.
Calculate total possible theoretical mode of vibration for ammonia (NH3) molecule.
Soln:
Ammonia is $sp^3$ hybridized molecule hence it is non-linear
Therefore,
Total possible mode of vibration = 3 N – 6
= 3 x 4 -6
= 6
Calculate total possible modes of vibration in acetylene (c2H2)
Soln:
Acetylene is SP hybridized hence it is linear molecule
Therefore,

Total possible mode of vibration = 3 N -5 = 3 x 4 -5 = 7

**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 (free O-H will give sharp peak) |
| **Alkane** | | | |
| C-H | stretch | 2850-3000 | strong |
| -C-H | bending | 1350-1480 | variable |
| **Alkene** | | | |
| C=C | stretch | 1620-1680 | variable |
| **Alkyne** | | | |
| $-C\equiv C-$ | 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) |

| | | | |
|---|---|---|---|
| **Aromatic** | | | |
| C=C | stretch | 1400-1600 | medium-weak, multiple 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** | (Peak for carbonyl +) | | |
| O-H | stretch | 2500-3300 | strong, very broad |
| **Aldehyde** | (Peak for carbonyl +) | | |
| =C-H | stretch | 2820-2850 & 2720-2750 | medium, two peaks |
| **Ester** | (Peak for carbonyl +) | | |
| C-O | stretch | 1000-1300 | two bands or more |

| **Functional Group** | **Type of Vibration** | **Characteristic Absorptions (cm-1)** | **Intensity** |
|---|---|---|---|
| | | | |
| Ether | | | |
| C-O | stretch | 1000-1300 | strong |
| Nitrile | | | |
| - CN | stretch | 2210-2260 | medium |

**Green Chemistry:**

Calculate the percentage atom economy of the following reaction with respect to aceanilide:

$C_6H_5NH_2$ + $(CH3CO)_2O$ ---------→ $C_6H_5NH\ CO\ CH_3$ + $CH_3\ COOH$

Soln:

$$\%\ \text{Atom Economy} = \frac{\text{mass of desired product}}{\text{Total mass of reactants}} \times 100$$

$$= \frac{135 \times 100}{(93 + 102}$$

$$= 69.23\ \%$$

A Polymer there are 100 molecules of molecular weight 100, 200 molecules with molecular weight 1000 and 300 molecule with molecular weight 10,000. 5.35 x1 0 3 Calculate Mn, Mw and PDI.

Soln:

$$Mn = \frac{100 \times 100 + 200 \times 1000 + 300 \times 10000}{100 + 200 + 300}$$

$$= 5.35 \times 1\,0^{3}$$

$$Mw = \frac{100 \times (100)^2 + 200 \times (1000)^2 + 300 \times (10000)^2}{100 \times 100 + 200 \times 1000 + 300 \times 10000}$$

$$= 9.4 \times 1\,0^{3}$$

P.D.I = Mw /Mn

$$= \frac{9.4 \times 1\,0^{3}}{5.35 \times 1\,0^{3}}$$

$$= 1.757$$