

Water

1. Problem involving multiplication factor:

$$\text{Multiplication factor} = \frac{\text{equivalent mass of CaCO}_3}{\text{Equivalent mass of hardness causing impurity}}$$

$$\text{Equivalent hardness of CaCO}_3 = \text{mass of hardness causing impurity} \times \text{multiplication factor}$$

$$= \text{mass of impurity} \times \frac{\text{equivalent mass of CaCO}_3}{\text{equivalent mass of impurity}}$$

$$1 \text{ PPM} = 1 \text{ mg/L} = 0.1 \text{ French} = 0.07 \text{ Clarke}$$

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 x 2 mg of MgCl₂ will be present in 1 litre soln

Hardness of MgCl₂ = 19 ppm

$$\text{Equivalent hardness of CaCO}_3 = 19 \times \frac{100}{95} = 20 \text{ ppm}$$

2. Problem involving Temporary, permanent and Total hardness

Calculate the temporary, permanent and total hardness 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 = 6.8 ppm, CO₂ = 22 ppm, HCl = 3.65 ppm, Ca(NO₃)₂ = 4.1 ppm, SiO₂ = 10 ppm, KNO₃ = 15 ppm, MgCl₂ = 3.8 ppm, MgCl₂ = 3.8 ppm, Al₂(SO₄)₃ = 11.4 ppm, NaHCO₃ = 10 ppm

Name of impurity	Amount present in ppm	Multiplication factor	Equivalent hardness of CaCO ₃	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

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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

= $30 \times (5/2 \text{ mg of } \text{CaCO}_3)$

= 75 mg of CaCO_3 Therefore,

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

= 1500 ppm

Also,

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

= 28×2.5 mg of CaCO_3

Permanent Hardness= $70 \times (1000/100) = 700$ ppm

3. Problem involving lime soda calculation

Name of Impurities	Reaction with Lime	Reaction With Soda	L & S Requirement
1.Temp i)Temp Ca	$\text{Ca(OH)}_2 + \text{Ca(HCO}_3)_2 \rightarrow 2\text{CaCO}_3 + 2\text{H}_2\text{O}$	No Reaction	L
ii)Temp Mg	$\text{Mg(HCO}_3)_2 + 2\text{Ca(OH)}_2 \rightarrow \text{Mg(OH)}_2 + 2\text{CaCO}_3 + 2\text{H}_2\text{O}$	No Reaction	2L
2 Perm i)Mg	$\text{Ca(OH)}_2 + \text{MgSO}_4 \rightarrow \text{CaSO}_4 + \text{Mg(OH)}_2$	$\text{CaSO}_4 + \text{Na}_2\text{CO}_3 \rightarrow \text{CaCO}_3 + \text{Na}_2\text{SO}_4$	L + S
ii)Perm Al	$3\text{Ca(OH)}_2 + \text{Al}_2(\text{SO}_4)_3 \rightarrow 2\text{Al(OH)}_3 + 3\text{CaSO}_4$	$\text{CaSO}_4 + \text{Na}_2\text{CO}_3 \rightarrow \text{CaCO}_3 + \text{Na}_2\text{SO}_4$	L + S
iii)Perm Fe	$\text{Ca(OH)}_2 + \text{FeCl}_2 \rightarrow \text{Fe(OH)}_2 + \text{CaCl}_2$	$\text{CaCl}_2 + \text{Na}_2\text{CO}_3 \rightarrow \text{CaCO}_3 + 2\text{NaCl}$	L + S
iv).Perm Ca		$\text{CaSO}_4/\text{CaCl}_2 + \text{Na}_2\text{CO}_3 \rightarrow \text{CaCO}_3 + \text{Na}_2\text{SO}_4/2\text{NaCl}$	S
3. CO2	$\text{CO}_2 + \text{Ca(OH)}_2 \rightarrow 2\text{CaCO}_3 + 2\text{H}_2\text{O}$	No Reaction	L
4. NaHCO3	$2\text{NaHCO}_3 + \text{Ca(OH)}_2 \rightarrow \text{CaCO}_3 + \text{Na}_2\text{CO}_3 + 2\text{H}_2\text{O}$	No Reaction	L - S

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5. NaAlO ₂	NaAlO ₂ + H ₂ O -----> Al(OH) ₃ + NaOH		(-L)eq to Ca(OH) ₂
6. Acid			
-i) HCl	2HCl + Ca(OH) ₂ -----> 2 H ₂ O + CaCl ₂	CaCl ₂ + Na ₂ CO ₃ ---->2 NaCl +CaCO ₃	L + S
ii) H ₂ SO ₄	H ₂ SO ₄ + Ca(OH) ₂ ----> 2 H ₂ O + CaSO ₄	CaSO ₄ +Na ₂ CO ₃ ----->CaCO ₃ + Na ₂ SO ₄	L +S

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

+ Acid (HCl, H₂SO₄,...) + CO₂

+ NaHCO₃ – NaAlO₂] all in terms of CaCO₃ hardness

X (vol of water / 10⁶) x (100 / % purity)

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

+ Acid (HCl, H₂SO₄,...) - NaHCO₃] all in terms of CaCO₃ hardness

X (vol of water / 10⁶) x (100 / % purity)

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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(HCO₃)₂ = 8.1 ppm Mg(HCO₃)₂ = 3.9 ppm, CO₂ = 11 ppm HCl = 7.3 ppm

NaHCO₃ = 2.2 ppm, NaAlO₂ = 3.24 ppm. CaSO₄ = 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

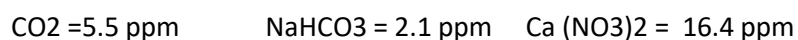
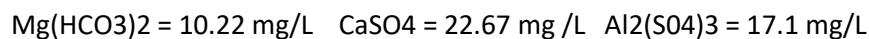
$$\text{Lime reqd} = 74 / 100 \times [44.68] \times 10^6 / 10^6 \times 100 / 80$$

$$= 41.33 \text{ kg}$$

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

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

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



Impurity	Amt present in mg/L	M.F	Equivalence of CaCO3 hardness	Lime	Soda
Mg(HCO3)2	10.22	100/146	7	2 x7 (2 x L)	-
CaSO4	22.67	100/136	16.67	-	16.67(S)
Al2(SO4)3	17.1	(100/2)/(342/6) =100/114	15	15	15
CO2	5.5	100/44	12.5	12.5	
NaHCO3	2.1	100/84 x 2	1.25	1.25	-1.25
Ca (NO3)2	16.4	100 /164	10	-	10
FeSO4.7H2O	2.78	100/278	1	1	1
HCl	3.65	100/36.5 x 2	5	5	5
SiO2	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

$$\begin{aligned}
 &= 75 \text{ litre of brine soln containing } 125 \text{ g /l NaCl} \\
 &= 75 \times 125 \text{ g of NaCl} \\
 &= 75 \times 125 \times 1000 \text{ mg of NaCl} \\
 &= 75 \times 125 \times 1000 \times (50/58.5) \text{ mg of CaCO}_3 \\
 \text{Therefore,} \\
 \text{Hardness X ppm} &= \frac{75 \times 125 \times 1000 \times 50}{58.5 \times 32000} \\
 \text{X} &= 250.4 \text{ ppm}
 \end{aligned}$$

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 of 50,000 liter of hard water = 200 liter of 0.1 N HCl solution

$$\begin{aligned}
 &= 200 \text{ lit of } 0.1 \text{ N CaCO}_3 \text{ solutions.} \\
 &= 20 \text{ lit of } 1 \text{ N CaCO}_3 \text{ solution} \\
 &= 20 \times 50 \text{ g of CaCO}_3 \\
 &= 1000 \times 1000 \text{ mg of CaCO}_3 \\
 \text{Therefore hardness} &= \frac{1000000}{20000} \\
 &= 50 \text{ ppm}
 \end{aligned}$$

5. Problem on Chemical Oxygen Demand

20 ml of sample of water was refluxed with 15 ml of K₂Cr₂O₇ 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.

$$\begin{aligned}
 \text{COD} &= \frac{(V_{\text{blank}} - V_{\text{sample}}) \times N_{\text{FAS}} \times 8000}{\text{Volume of water sample}} \\
 &= \frac{(48 - 22) \times 0.25 \times 8000}{20} \\
 &= 2600 \text{ ppm}
 \end{aligned}$$

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:

$$\begin{aligned}\text{BOD} &= (\text{DO}_1 - \text{DO}_5) \times \text{dilution factor} \\ &= (8.5 - 5.5) \times V_f/V_i \\ &= 3 \times 100/2 \\ &= 150 \text{ mg /lit}\end{aligned}$$

ENERGY

$$1 \text{ K cal} = 2.2 \text{ C.H.U} = 3.968 \text{ B.T.U}$$

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:

$$\begin{aligned}\text{GCV} &= 1/100 [8080 \times \%C + 34500 (\text{H}-\text{O}/8) + 2240 \times \text{S}] \\ &= 1/100 [8080 \times 74 + 34500 (10-5/8) + 2240 \times 6] \\ &= 9347.97 \text{ Kcal /Kg}\end{aligned}$$

$$\begin{aligned}\text{NCV} &= \text{GCV} - 9/100 \times \% \text{H} \times 587 \\ &= 9347.97 - 0.09 \times 10 \times 587 \\ &= 8819.67 \text{ Kcal/Kg}\end{aligned}$$

2. _Proximate analysis

i) 1.5 gram of coal was subjected for proximate analysis. The weight of coal after heating at 100 ° C for 60 minutes was found to be 1.28 g. This was further heated in muffle furnace at 925 ° C for 7 minutes, the weight after heating was found 1.08 g. Finally, the coal is heated further at 750 ° 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 = $W_1 = 1.5$ g
 Weight of coal after heating 100°C for 60 minutes = $W_2 = 1.28$ g
 Weight of coal after heating in furnace at 925°C for 7 minute= $W_3= 1.08$ g
 Weight of coal after heating in furnace at 750°C for 30 min= $W_4= 0.35$ g

Formula:

$$\begin{aligned}\% \text{ Moisture} &= \frac{W_1 - W_2}{W_1} \times 100 \\ &= \frac{1.5 - 1.28}{1.5} \times 100 \\ &= 14.66\end{aligned}$$

$$\begin{aligned}\% \text{ V.M} &= \frac{W_2 - W_3}{W_1} \times 100 \\ &= \frac{1.28 - 1.08}{1.5} \times 100 \\ &= 13.33\%\end{aligned}$$

$$\begin{aligned}\% \text{ Ash} &= \frac{W_4}{W_1} \times 100 \\ &= \frac{0.35}{1.5} \times 100 \\ &= 23.33\%\end{aligned}$$

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 CaCl_2 tube and KOH bulb. The increase in mass of CaCl_2 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 CaCl_2 tube = 0.35 g

Increase in mass of KOH bulb = 0.68 g

$$\begin{aligned}\% \text{ Carbon} &= \frac{\text{increase in mass of KOH bulb}}{\text{Mass of coal}} \times \frac{12}{44} \times 100 \\ &= \frac{0.35 \times 12 \times 100}{1.8 \times 44} \\ &= 5.3\end{aligned}$$

$$\begin{aligned}
 \% \text{ Hydrogen} &= \frac{\text{increase in mass of CaCl}_2 \text{ tube}}{\text{Mass of coal}} \times \frac{2}{18} \times 100 \\
 &= \frac{0.68 \times 2 \times 100}{1.8 \times 18} \\
 &= 4.19 \%
 \end{aligned}$$

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 0.25 N KOH for neutralization. Calculate % Nitrogen in coal.

$$\begin{aligned}
 \% \text{ Nitrogen} &= \frac{(V_{\text{blank}} - V_{\text{Sample}}) \times N_{\text{KOH}} \times 1.4}{\text{Mass of coal}} \\
 &= \frac{(48 - 18) \times 0.25 \times 1.4}{1.35} \\
 &= 7.77 \%
 \end{aligned}$$

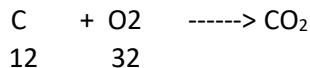
iii) Problem on Sulphur content:

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:

$$\begin{aligned}
 \% \text{ Sulphur} &= \frac{\text{mass of BaSO}_4 \text{ residue}}{\text{Mass of coal}} \times \frac{32}{233} \times 100 \\
 &= \frac{0.69 \times 32 \times 100}{1.1 \times 233} \\
 &= 8.61 \%
 \end{aligned}$$

4. Oxygen requirement for combustion for SOLID COAL:

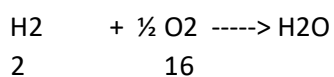


Therefore,

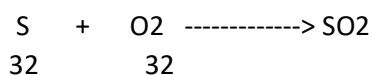
12 gram of carbon required = 32 gram of oxygen for combustion

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

Similarly,



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



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 = 0.30
Hydrogen	0.03 Kg	16/2	= 0.03 x 16/2 = 0.24
Sulphur	0.025 Kg	32/32	= 0.025 x 32/32 = 0.025
Nitrogen	0.025 kg	- (does not burn)	-
Ash	0.05 kg	- (does not burn)	-
Oxygen	0.07 kg	1	- 0.07 (subtract from total)
Total oxygen required for burning 1 Kg Coal			= 0.30 + 0.24 + 0.025 +(-0.07) = 0.495 Kg

Total oxygen required for burning 1 kg coal = 0.495 kg

100 Kg of air contains = 23 kg of oxygen

Therefore,

Multiplying factor for converting oxygen to air = 100/23

$$\begin{aligned} 0.495 \text{ kg of oxygen} &= 0.495 \times 100/23 \\ &= 2.152 \text{ Kg} \end{aligned}$$

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

$$\begin{aligned} \text{Amount of air required if 20\% excess air is supplied} &= 2.152 \times 120/100 \\ &= 2.5824 \text{ Kg} \end{aligned}$$

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:

CH₄ = 20%, C₃H₆ = 15%, H₂=30%, CO=5%, H₂O=8%, C₂H₆=12%, oxygen remaining.

Gaseous Component	Volume present in 1 m ³	Combustion reaction	Multiplication Factor	Volume of Oxygen required for
CH ₄	0.20 m ³	CH ₄ + 2 O ₂ -----> CO ₂ + 2 H ₂ O	2	= 0.20 x 2 = 0.40 dm ³
C ₃ H ₆	0.15 m ³	C ₃ H ₆ + 9/2 O ₂ -----> 3 CO ₂ + 3H ₂ O	9/2	= 0.15 x 9/2 = 0.675 dm ³
H ₂	0.30 m ³	H ₂ + ½ O ₂ -----> H ₂ O	½	=0.30 x ½ = 0.15 dm ³
CO	0.05 m ³	CO + ½ O ₂ -----> CO ₂	½	=0.05 x ½ = 0.025 dm ³
H ₂ O	0.08 m ³	No reaction	-	-
C ₂ H ₆	0.10 m ³	C ₂ H ₆ + 7/2 O ₂ -----> 2CO ₂ + 3 H ₂ O	7/2	= 0.10 x 7/2 =0.35 dm ³
O ₂	0.10 m ³		-1	-0.10 dm ³
Volume of oxygen required for combustion of 1 dm ³ of fuel				= 0.40

$ \begin{aligned} &+0.675+0.15+0.025+ \\ &0.35-0.10 \\ &= 1.5 \text{ dm}^3 \end{aligned} $
--

Therefore,

Volume of oxygen required for combustion of 1 dm³ of fuel = 1.5 dm³

Volume of air:

100 dm³ of air contains = 21 dm³ of oxygen

Therefore,

1.5 dm³ of oxygen will be = $1.5 \times 100/21$

= 7.142 dm³ of air

Volume of oxygen required for combustion of 1 dm³ of fuel = 7.142 dm³ of air

UV-Vis SPECTROSCOPY

1. The transmittance of 2×10^{-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:

$$A = 2 - \log(\%T)$$

$$\begin{aligned}
 A &= 2 - \log(76.2) \\
 &= 2 - 1.8819 \\
 &= 0.1181
 \end{aligned}$$

$$A = \epsilon \cdot b \cdot C$$

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

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

$$= 590 \text{ dm}^3 \text{ mol}^{-1} \text{ cm}^{-1}$$

$$\begin{aligned} \frac{A_1}{A_2} &= \frac{\epsilon b_1 C}{\epsilon b_2 C} & \text{OR} & & A_2 &= \epsilon b_2 \cdot C \\ & & & & &= 590 \times 2 \times 2 \times 10^{-4} \\ A_2 &= (b_2/b_1) \cdot A_1 & & & &= 0.236 \\ &= (2/1) \cdot 0.1181 \\ &= 0.2362 \end{aligned}$$

$$A = 2 - \log(\%T)$$

$$\begin{aligned} \log(\%T) &= 2 - 0.2362 \\ &= 1.7638 \end{aligned}$$

$$\% T = 58.1\%$$

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

$$\% T = 90\%$$

$$\begin{aligned} A &= 2 - \log(90) \\ &= 2 - 1.9542 = 0.0458 \end{aligned}$$

$$\begin{aligned} A &= \epsilon b C \\ \epsilon &= A / b \cdot c \\ &= \frac{0.0458}{1 \times 10^{-3}} \\ &= 45.8 \text{ dm}^3 \text{ mol}^{-1} \text{ cm}^{-1} \end{aligned}$$

$$\% T_2 = 10 \% \text{ (since 90\% of incident light absorbed)}$$

$$\begin{aligned} A_2 &= 2 - \log(10) \\ &= 2 - 1 \\ &= 1 \end{aligned}$$

$$\begin{aligned} A_2 &= \epsilon b C_2 \\ C_2 &= A_2 / \epsilon b \\ &= 1 / 1 \times 45.8 \\ &= 2.18 \times 10^{-2} \text{ mol/dm}^3 \end{aligned}$$

IR Spectroscopy

3. Problem on total theoretical mode of vibration:

Formula:

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

Total Theoretical mode of vibration = $3N - 6$
for non-linear molecule

Where, N = total number of atom in molecule

for e.g.

Calculate total possible theoretical mode of vibration for ammonia (NH_3) molecule.

Soln:

Ammonia is sp^3 hybridized molecule hence it is non-linear

Therefore,

$$\begin{aligned}\text{Total possible mode of vibration} &= 3N - 6 \\ &= 3 \times 4 - 6 \\ &= 6\end{aligned}$$

Calculate total possible modes of vibration in acetylene (C_2H_2)

Soln:

Acetylene is SP hybridized hence it is linear molecule

Therefore,

$$\text{Total possible mode of vibration} = 3N - 5 = 3 \times 2 - 5 = 1$$

Characteristic IR Absorption Frequencies of Organic Functional Groups

Functional Group	Type of Vibration	Characteristic Absorptions (cm^{-1})	Intensity
Alcohol			
O-H	(stretch, bonded) H-	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			
$\text{C}\equiv\text{C}-$	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

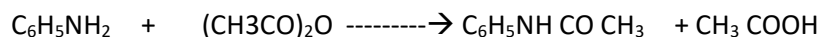
IR Absorption Frequencies of Functional Groups Containing a Carbonyl (C=O)

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:



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 x 10³ Calculate Mn, Mw and PDI.

Soln:

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

$$= 5.35 \times 10^3$$

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

$$= 9.4 \times 10^3$$

$$\text{P.D.I} = \text{Mw} / \text{Mn}$$

$$= \frac{9.4 \times 10^3}{5.35 \times 10^3}$$

$$= 1.757$$