

## IT Skills for Chemist (Different Equations)

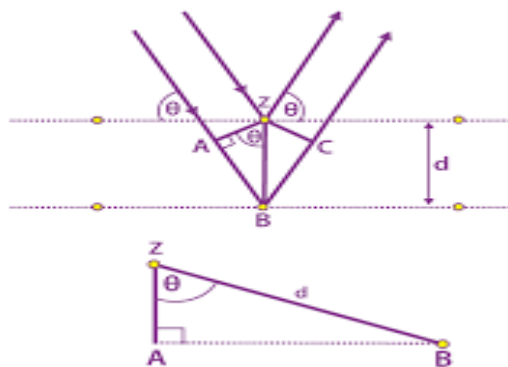
### 1. Maxwell-boltzmann distribution :

$$dn/N = 4\pi(M/2RT)^{3/2} c^2 \exp(-Mc^2/2RT) dc$$

Where  $N$  is the total number of molecules in the sample,  $dn/N$  is the fraction of molecules with speed between  $c$  and  $c+dc$ ,  $M$  is the molecular weight in kg/mole,  $T$  is the temperature in K and  $R$  the gas constant (J/K)

### 2. Brag's Law:

Brag's Law states the following: When the X-ray is incident onto a crystal surface, its angle of incidence,  $\theta$ , will reflect with the same angle of scattering,  $\theta$ . And, when the path difference,  $d$  is equal to a whole number,  $n$ , of wavelength,  $\lambda$ , constructive interference will occur.



$$\text{Brag's equation : } n\lambda = 2d\sin\theta$$

### 3. van der Waals equation:

$$P = \frac{RT}{V - b} - \frac{a}{V^2}$$

$P$  = pressure

$R$  = universal gas constant

$T$  = absolute temperature

$V$  = molar volume

$b$  = gas constant  $b$

$a$  = gas constant  $a$

$V$  = molar volume

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### 4. Planck's distribution law:

This law describes the intensity of the radiation per unit surface area emitted by a black body as a function of wavelength (cm) and surface temperature ( $^{\circ}\text{K}$ )

$$B_{\lambda}(\lambda, T) = \frac{2hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1}$$

where,  $B(\lambda, T)$  is the energy intensity emitted at wavelength (cm) and **temperature**  $T$  (Kelvin)

### 5. Molar extinction coefficients:

The Lambert- Beer law, states :

$$\log I/I_0 = \epsilon cl$$

where  $\epsilon$  is called the "Molar Absorptivity" or molar extinction coefficient of the compound. It is a function of wavelength specific for each molecule. With the path length normally given in cm, and  $C$  is in Molarity units, mol/L,  $\epsilon$  has the units  $\text{L}\cdot\text{mol}^{-1}\cdot\text{cm}^{-1}$ . If alternatively  $C$  is in mol/mL, then  $\epsilon$  will have the units  $\text{cm}^2\cdot\text{mol}^{-1}$

The Absorbance,  $A$ , is defined as

$$A = \log I/I_t$$

$$\text{Therefore } A = \epsilon cl$$

**$A$  vs  $C$  graph will be straight line passing through the origin.**

### 6. Molar enthalpy of vaporization:

The Clapeyron equation for any system of one substance and two phases can be written as

$$dP/dT = \Delta H_m / T \Delta V_m$$

where  $P$  is the pressure,  $\Delta H_m$  is the molar enthalpy change of the phase transition,  $T$  is the absolute temperature, and  $\Delta V_m$  is the change of molar volume of the phase



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transition. If  $\Delta V_m$  is known and the value of the derivative  $dP/dT$  can be evaluated, then the enthalpy change of vaporization can be calculated.

If we assume that the molar volume of the liquid is negligible compared to that of the gas we get

$$\Delta V_m = \Delta V_m (\text{gas}) - \Delta V_m (\text{liquid}) \approx \Delta V_m (\text{gas}) \approx RT/P$$

$$\text{so that } dP/dT = P\Delta H_m/RT^2$$

Dividing by  $P$  and carrying out an indefinite integration, we obtain the *Clausius - Clapeyron* equation :

$$\ln(P) = - (\Delta H_m/RT^2) + C \text{ where } C \text{ is the integration constant.}$$

Thus there is a linear relation between  $\ln P$  and  $1/T$

\*\*\*\*\*End\*\*\*\*\*