Chemistry C2407x
Some Free Formulas for Exams

Kinetic Theory of Gases

Impacts/sec = (1/6) (N/V) Ac {Impacts/sec = (1/4) (N/V) Ac}

Force = [2mc] [(1/6) (N/V) Ac]=(1/3) (N/V) mc^2A

Pressure=Force/A= (1/3) (N/V) mc^2 = [(2/3)] [(1/2) mc^2] [N/V]

$pV=nRT=(N/N_0)RT=(N/N_0)(N_0k)T=NkT$

m/k=M/R

[(1/2) mc^2]=(3/2) kT [(1/2) Mc^2]= (3/2)RT

$c_{rms}=(3kT/m)^{1/2}= (3RT/M)^{1/2}$ $c_{avge}=(8kT/\square\ m)^{1/2}= (8RT/\square\ M)^{1/2}$

$c_{mp}=(2kT/m)^{1/2} =(2RT/M)^{1/2}$

$c_{rms}=1.37x10^5$ cm/sec = $1.37x10^3$ meter/sec (for He at 300 K)

Effusion Rate: R=(1/6) (N/V) Ac {R=(1/4) (N/V) Ac}

dw=-pdV dE=dQ+dw

$C_p=(dQ/dT)_p$ $C_V=(dQ/dT)_V$

$C_V=(3/2)R$ $C_p=(3/2)R+R$ (Atoms)

$C_V=(5/2)R$ $C_p=(5/2)R+R$ (Linear molecules)

$z=\square\square^2c\ (N/V)$ $\{z=(2)^{1/2}\square\square^2c_{avge}\ (N/V)\}$

$\square=c/z= [\square\square^2\ (N/V)]^{-1}=[\square\square^2\ (pN_0/RT)]^{-1}$

$\{\square=c_{avge}/z= [(2)^{1/2}\square\square^2\ (N/V)]^{-1}=[(2)^{1/2}\square\square^2\ (pN_0/RT)]^{-1}\}$

$\square N/N = (4\square)(m/2\square kT)^{3/2}\ c^2 \exp[-mc^2/2kT]\ \square c$

Binary Collision Model

$\langle u_{rel} \rangle = (8kT/\pi\mu)^{1/2}$, $\mu = m_a m_b/(m_a + m_b)$

$z=\pi(\sigma_{AB})^2 \langle u_{rel} \rangle (N/V)$

$Z_{AB}=\pi(\sigma_{AB})^2 \langle u_{rel} \rangle (N_A/V)(N_B/V)$

$Z_{AA}=(1/2)\pi(\sigma_{AA})^2 \langle u_{rel} \rangle (N_A/V)(N_A/V)$

$Z_{AA}=(1/2)(2)^{1/2}\pi(\sigma_{AA})^2 (8kT/\pi m_A)^{1/2} (N_A/V)^2$

All or Nothing Model $P_R=0$ when $E<E_A$; $P_R=1$ when $E \geq E_A$

Arrhenius Model $P_R=0$ when $E<E_A$; $P_R=(1-E_A/E)$ when $E \geq E_A$

$R=k_R(N_A/V)(N_B/V)=PZ_{AB}\exp[-E_A/RT]$ {P is the steric factor}

$k_R = P\pi(\sigma_{AB})^2 \langle u_{rel} \rangle \exp[-E_A/RT]=A\exp[-E_A/RT]$ (Arrhenius Model)

$k_R = (N_0/1000)\, P\pi(\sigma_{AB})^2 \langle u_{rel} \rangle \exp[-E_A/RT]$ (molar units)

$-dC/dt=kC$, $C=C_0\exp(-kt)$, $t_{1/2}=(0.693/k)$

$-dC/dt=kC^2$, $1/C=[1/C_0] + kt$, $t_{1/2}=(1/kC_0)$

$k(T_2)/k(T_1)=\exp[-(E_A/R)(1/T_2-1/T_1)]$

$A+A \rightarrow A+A^*$, k_1 $A^*+A \rightarrow A+A$, k_{-1} $A^* \rightarrow P$, k_2

$k_{uni} = k_2 k_1 (A)/[k_{-1}(A) + k_2]$, $dP/dt=[A]k_{uni}$

$E+S \rightarrow ES$, k_1 $ES \rightarrow E+S$, k_{-1} $ES \rightarrow P$, k_2

$dP/dt=v_i= k_2(E_0)/[1+K_M/(S)]$, $K_M =[k_{-1}+k_2]/k_1$

$(1/v)=(1/v_{max}) + (K_M/v_{max})(1/[S])$

$d\ln k_A/dT=E_A/RT^2$ $d\ln k_{BC}/dT=\square_A/RT^2$ $\square_A=(1/2)RT+E_A$

(k_A is the Arrhenius rate constant and k_{BC} is the binary collision rate constant)

$\ln K_{eq} = -\Delta G^0/RT = \ln(k_f/k_r) = \ln(A_f/A_r) - (E_{Af} - E_{Ar})/RT$

$\ln(A_f/A_r) \approx \Delta S^0/R$ $\qquad$ $(E_{Af} - E_{Ar}) \approx \Delta H^0/RT$

$K_w = [H_3O^+][OH^-] = 10^{-14}$, $T = 25^0$ C and concentrations in M

$K_h = K_w/K_a$ (Hydrolysis constant or base constant, $K_b = K_h$, for a conjugate acid/base pair)

$K_a = [H_3O^+][A^-]/[HA] \Rightarrow pH = pK_a - \log_{10}\{[HA]/A^-]\}$

$K_I = [In^-][H_3O^+]/[HIn]$

$y = ax^2 + bx + c = 0$, $2ax = -b \pm (b^2 - 4ac)^{1/2}$

Thermodynamic Formulas (First Law)

$dE = dq + dw$ $\qquad$ $\Delta E = q + w$ $\qquad$ $dw = -p_{ex}dV$ $\qquad$ $w = -\int p_{ex}dV$

$w_{rev} = -\int p_{ex}dV = -\int p_{int}dV = -\int (nRT/V)dV = -nRT\ln(V_f/V_i)$ (Isothermal)

$w = -\int p_{ex}dV = -p_{ex}\int dV = -p_{ex}(V_f - V_i)$ (constant pressure)

$H = E + pV$ $\qquad$ $\Delta H = q_p$ $\qquad$ $\Delta E = q_V$

$\Delta H = \sum \Delta H_f°(\text{products}) - \sum \Delta H_f°(\text{reactants})$

$\Delta H(T_2) = \Delta H(T_1) + [\sum C_p(\text{products}) - \sum C_p(\text{reactants})][T_2 - T_1]$

Thermodynamic Formulas (Second Law)

$\Delta S = \int_1^2 (dq_{rev}/T) = (1/T)\int_1^2 dq_{rev} = (q_{rev}/T)$ (isothermal)

ΔS (isothermal, ideal gas) $= q_{rev}/T = -w_{rev}/T = nR\ln(V_f/V_i)$

$\Delta S = \int_1^2 (dq_{rev}/T) = \int_1^2 (nC_p/T)dT = nC_p\ln(T_f/T_i)$

$S_T = \int_0^T (C_p/T)dT$ (Absolute Entropy)

$$S_T = \int_0^{T_M} [C_p(\text{solid})/T]dT + \Delta H_{fus}/T_M$$

$$+ \int_{T_M}^{T} [C_p(\text{liquid})/T]dT$$ (Absolute Entropy/melting phase change)

$G=H-TS$ $\quad \Delta G=\Delta H-T\Delta S$ (Isothermal) $\quad \Delta G=q-q_{rev}$

$\Delta G=0$, const T,p (equilibrium, reversible)

$\Delta G<0$, const T,p (irreversible, spontaneous)

$G(T) = G°(T) + RT \ln p$ (p in atm.)

$\Delta G = [c\mu°_C + d\mu°_D - a\mu°_A - b\mu°_B] + cRT\ln p_C + dRT\ln p_D - aRT\ln p_A - bRT\ln p_B$

$\Delta G = \Delta G° + RT \ln \{(p_C)^c(p_D)^d/(p_A)^a(p_B)^b\}$

$\Delta G° = -RT \ln K_p$ $\qquad K_p = e^{-\Delta G°/RT} = e^{-\Delta H°/RT}\, e^{\Delta S°/R}$

Bonding Information

$\psi_{1s} = 1/(\pi)^{1/2}(1/a_0)^{3/2} \exp[-r/a_0]$, a_0=Bohr Radius = 0.529 Angstroms

Ne_2 configuration (Z=10): $(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2pz})^2(\pi_{2p})^4(\pi_{2p}^*)^4(\sigma_{2pz}^*)^2$

N_2 configuration (Z=7): $(\sigma_{2s})^2(\sigma_{2s}^*)^2(\pi_{2p})^4(\sigma_{2pz})^2$

Some Possibly Useful Units

R=0.082 l-atm/mole-deg=82 ml-atm/mole-deg=8.2×10^{-5} m^3-atm/mole-deg

R=1.98 cal/mole-deg=8.314 joules/mole-deg=8.314×10^{7} ergs/mole-deg

1 joule= 10^7 ergs

1atm=760 torr=1.01325×10^5 Pascals = 1.01325×10^6 gm/cm-sec^2

1 torr=133.322 Pascals=133.322 newton/m^2

1 torr=133.322 Kg/m-s^2 $\quad$ 1 bar=750.062 torr=10^5 Pa=0.986923 atm

Density of Hg=13.59 gm/ml=13.59 Kg/L; g=980.7 cm/sec^2=9.807 m/sec^2