CHEM 145 Honor General Chemistry I Equations

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Gas

Kinetic Theory of Gas

Quantity	Unit	Definition
Pressure	$\mathrm{N/m^2}$	$P = \dfrac{F}{A}$
Mole fraction of a	-	$X_a = \dfrac{n_a}{n_{\text{total}}}$
Partial pressure of a	$\mathrm{N/m^2}$	$P_a = X_a P_{\text{total}}$
Pressure-volume work	J	$W = -P\Delta V$
Compressibility of gas	-	$z = \dfrac{PV}{nRT}$

Description	Equations
Ideal gas law	$PV = nRT$
Ideal gas constant and Boltzmann constant	$R = N_A k_B$
Average kinetic energy of one gas molecule	$\varepsilon = \dfrac{3}{2}k_B T$
Root mean square speed gas	$v_{\text{RMS}} = \sqrt{\dfrac{3RT}{\mathcal{M}}} = \sqrt{\dfrac{3k_B T}{m}}$
Mean speed of gas	$\bar{v} = \sqrt{\dfrac{8RT}{\pi\mathcal{M}}} = \sqrt{\dfrac{8k_B T}{\pi m}}$

Description	Equations
Most probable speed of gas	$v_{\mathrm{mp}} = \sqrt{\dfrac{2RT}{\mathcal{M}}} = \sqrt{\dfrac{2k_B T}{m}}$
Maxwell-Boltzmann speed distribution	$f(v) = 4\pi\left(\dfrac{m}{2\pi k_B T}\right)v^2 \exp\left(\dfrac{-mv^2}{2k_B T}\right)$
Van der Waals equation of state	$\left(P + a\dfrac{n^2}{V^2}\right)(V - bn) = nRT$
Lennard-Jones potential	$V_{\mathrm{LJ}} = 4\varepsilon\left(\left(\dfrac{\sigma}{R}\right)^{12} - \left(\dfrac{\sigma}{R}\right)^6\right)$

Molecular Collisions and Rate Processes

Description	Equations
Molecule collision rate with wall	$Z_w \propto \dfrac{1}{4}\dfrac{N}{V}\bar{v}A = \dfrac{1}{4}\dfrac{N}{V}\sqrt{\dfrac{8RT}{\pi\mathcal{M}}}A$
Graham's law of effusion	$\dfrac{\text{rate of effusion of A}}{\text{rate of effusion of B}} = \dfrac{N_A}{N_B}\sqrt{\dfrac{\mathcal{M}_B}{\mathcal{M}_A}}$
Molecule-molecule collision rate	$Z_1 = 4\dfrac{N}{V}d^2\sqrt{\dfrac{\pi RT}{\mathcal{M}}}$
Mean free path	$\lambda = \dfrac{\bar{v}}{Z_1} = \dfrac{V}{\sqrt{2}\pi d^2 N}$
Mean square displacement of diffusion in 3D	$\overline{\Delta r}^2 = 6Dt$
Gas diffusion constant	$D = \dfrac{3}{8}\sqrt{\dfrac{RT}{\pi\mathcal{M}}}\dfrac{V}{Nd^2}$

Intermolecular Interactions

Quantity	Unit	Definition
Electrostatic force	N	$F = \dfrac{q_1 q_2}{4\pi\varepsilon r^2}$
Electrostatic potential energy	N	$V = \dfrac{q_1 q_2}{4\pi\varepsilon r}$
Dipole moment	$\mathrm{C}\cdot\mathrm{m}$	$\mu = qd$
Polarizability	$\mathrm{C}\cdot\mathrm{m}^2/\mathrm{V}$	$\alpha = \dfrac{\mu}{E}$
Induced dipole moment	$\mathrm{C}\cdot\mathrm{m}$	$\mu^* = \alpha E$

Description	Equations

Description	Equations
Ion-ion interactions	$E \propto \dfrac{q_1 q_2}{r}$
Ion-dipole interactions	$E \propto -\dfrac{q\mu}{r^2}$
Dipole-dipole interactions	$E \propto -\dfrac{\mu_1 \mu_2}{r^3}$
Induced-dipole-induced-dipole (London)	$E \propto -\dfrac{\alpha_1 \alpha_2}{r^6}$
Dipole-induced-dipole	$E \propto -\dfrac{\mu_1^2 \alpha_2}{r^6}$
Rotating fixed dipole (Keesom)	$E \propto -\dfrac{\mu_1^2 \mu_2^2}{r^6}$

Thermodynamics

First law of thermodynamics

Quantity	Unit	Definition
Specific heat capacities	$J \cdot kg^{-1} \cdot K^{-1}$	$q = mc_s \Delta T = n\bar{c}\Delta T$
Heat capacity	J/K	$q = C\Delta T$
Molar heat capacities	$J \cdot mol^{-1} \cdot K^{-1}$	$q_V = nc_V \Delta T$ $q_P = nc_P \Delta T$
Enthalpy	J	$H = U + PV$

Description	Equations
First law of thermodynamics	$\Delta U = q + w$ $dU = đq + đw$ $\Delta U_{\text{univ}} = \Delta U_{\text{sys}} + \Delta U_{\text{surr}} = 0$
Enthalpy change	$q_P = \Delta(U + PV) = \Delta H$
Molar heat capacity of monoatomic ideal gas at constant volume	$c_V = \dfrac{3}{2}R$
Molar heat capacity of any ideal gas at constant pressure	$c_P = c_V + R = \dfrac{5}{2}R$
Internal energy change of any ideal gas	$\Delta U = nc_V \Delta T$
Enthalpy change of any ideal gas	$\Delta H = nc_P \Delta T$ $= \Delta U + \Delta(PV)$ $= nc_V \Delta T + nR\Delta T$

Description	Equations
Hess's law	$\Delta H^\circ = \sum_i^{\text{prod}} n_i \Delta H_i^\circ - \sum_j^{\text{react}} n_j \Delta H_j^\circ$
Molality	$b = \dfrac{n_{\text{solute}}}{m_{\text{solvent}}}$
Boiling point elevation (i is vant's Hoff dissociation factor)	$\Delta T_{\text{boil}} = ibK_{\text{boil}}$
Freezing point depression (i is vant's Hoff dissociation factor)	$\Delta T_{\text{freeze}} = ibK_{\text{freeze}}$
Reversible isothermal process of ideal gas	$\Delta T = 0$ $\Delta U = 0$ $\Delta H = 0$ $w = -\displaystyle\int_{V_1}^{V_2} P \, dV = -nRT \ln \dfrac{V_2}{V_1}$ $q = -w$
Reversible adiabatic process of ideal gas	$q = 0$ $\Delta U = nc_V \Delta T = w$ $\Delta H = nc_P \Delta T$ $\gamma = \dfrac{c_P}{c_V}$ $T_1 V_1^{\gamma-1} = T_2 V_2^{\gamma-1}$ $P_1 V_1^{\gamma} = P_2 V_2^{\gamma}$

Second law of thermodynamics

Description	Equations
Entropy	$S = k_B \ln \Omega$
Entropy change	$\Delta S = \displaystyle\int_i^f \dfrac{dq_{\text{rev}}}{T}$
ΔS_{sys} for reversible isothermal process	$\Delta S = \displaystyle\int_i^f \dfrac{dq_{\text{rev}}}{T} = \dfrac{1}{T}\int_i^f dq_{\text{rev}} = \dfrac{q_{\text{rev}}}{T}$
ΔS_{sys} for reversible isothermal process - compression/expansion of ideal gas	$q_{\text{rev}} = nRT \ln\left(\dfrac{V_2}{V_1}\right)$ $\Delta S = nR \ln\left(\dfrac{V_2}{V_1}\right)$
ΔS_{sys} for reversible isothermal process - phase transitions	$q_{\text{rev}} = \Delta H_{\text{fus}}$ $\Delta S_{\text{fus}} = \dfrac{q_{\text{rev}}}{T_{\text{fus}}} = \dfrac{\Delta H_{\text{fus}}}{T_{\text{fus}}}$
ΔS_{sys} for reversible adiabatic process	$q = 0$ $\Delta S = 0$

Description	Equations
ΔS_{sys} for reversible isochoric process	$\Delta V = 0$ $dq_{\text{rev}} = nc_V dT$ $\Delta S = nc_V \int_{T_1}^{T_2} \frac{dT}{T} = nc_V \ln\left(\frac{T_2}{T_1}\right)$
ΔS_{sys} for reversible isobaric process	$\Delta P = 0$ $dq_{\text{rev}} = nc_P dT$ $\Delta S = nc_P \int_{T_1}^{T_2} \frac{dT}{T} = nc_P \ln\left(\frac{T_2}{T_1}\right)$
Entropy change of surrounding	$\Delta S_{\text{surr}} = \frac{-\Delta H_{\text{sys}}}{T_{\text{surr}}}$
Second law of thermodynamics	$\Delta S \geq \frac{q_{\text{rev}}}{T}$
Enthalpy of spontaneous process	$\Delta S_{\text{total}} = \Delta S_{\text{sys}} + \Delta S_{\text{surr}} > 0$
Standard molar entropy	$S^\circ = \int_{0K}^{298.15K} \frac{c_P}{T} dT +$ $\Delta S(\text{phase changes between 0K and 298.15K})$
Gibbs free energy for reaction at constant temperature	$\Delta G = \Delta H - T\Delta S$
Efficiency of Carnot engines	$\epsilon = \frac{\text{work on surrounding}}{\text{heat into system}}$ $= \frac{T_{\text{high}} - T_{\text{low}}}{T_{\text{high}}} = 1 - \frac{T_{\text{low}}}{T_{\text{high}}}$
Relationship between heat and temperature in Carnot cycle	$\frac{q_{\text{high}}}{T_{\text{high}}} + \frac{q_{\text{low}}}{T_{\text{low}}} = 0$
Work done by Carnot cycle in one cycle	$w_{\text{cycle}} = -nR(T_{\text{hot}} - T_{\text{cold}}) \ln \frac{V_B}{V_A}$

Equilibrium

Description	Equations
Law of mass action - partial pressure	$K = \dfrac{\prod\limits_{j}(P_{\text{product } j}/P_{\text{ref}})_{eq}^{b_j}}{\prod\limits_{i}(P_{\text{reactant } i}/P_{\text{ref}})_{eq}^{a_i}}$
Law of mass action - concentration	$K = \dfrac{\prod\limits_{j}(c_{\text{product } j}/c_{\text{ref}})_{eq}^{b_j}}{\prod\limits_{i}(c_{\text{reactant } i}/c_{\text{ref}})_{eq}^{a_i}}$
Gibbs free energy of isothermal reactions	$\Delta G = -T\Delta S = nRT \ln \frac{P_2}{P_1}$

Description	Equations
Equilibrium expression: relationship between Gibbs free energy and equilibrium constant (gas phase reaction)	$\Delta G^{\circ} = -RT \ln K$
Equilibrium expression: alternative form	$\ln K = -\dfrac{\Delta G^{\circ}}{RT} = -\dfrac{\Delta H^{\circ}}{RT} + \dfrac{\Delta S}{R}$
Change in Gibbs free energy at non-standard conditions	$\Delta G = \Delta G^{\circ} + RT \ln Q = RT \ln \dfrac{Q}{K}$
Reaction quotient - partial pressure	$Q = \dfrac{\prod\limits_{j}(P_{\text{product } j}/P_{\text{ref}})^{b_j}}{\prod\limits_{i}(P_{\text{reactant } i}/P_{\text{ref}})^{a_i}}$
Reaction quotient - concentration	$Q = \dfrac{\prod\limits_{j}(c_{\text{product } j}/c_{\text{ref}})^{b_j}}{\prod\limits_{i}(c_{\text{reactant } i}/c_{\text{ref}})^{a_i}}$
vant's Hoff equation temperature dependence of equilibrium constant of a reaction	$\ln \dfrac{K_2}{K_1} = -\dfrac{\Delta H^{\circ}}{R}\left(\dfrac{1}{T_2} - \dfrac{1}{T_1}\right)$
Clapeyron equation for two phase in equilibrium, construct phase diagram by finding change of pressure as a function of temperature	$\left(\dfrac{dP}{dT}\right)_{eq} = \dfrac{\Delta S}{\Delta V} = \dfrac{\Delta H}{T \Delta V}$
Clausius-Clapeyron equation temperature dependence of vapor pressure for condensed phase and gas phase in equilibrium	$\ln \dfrac{P_2}{P_1} = -\dfrac{\Delta H_{\text{vap}}}{nR}\left(\dfrac{1}{T_2} - \dfrac{1}{T_1}\right)$
Clausius-Clapeyron equation for $P_1 = P^{\circ}$; $\Delta S^{\circ} = \dfrac{\Delta H^{\circ}}{T^{\circ}}$	$\ln \dfrac{P_2}{P^{\circ}} = -\dfrac{\Delta H_{\text{vap}}}{nRT_2} + \dfrac{\Delta S^{\circ}_{\text{vap}}}{nR}$