

CHEM 145 Honor General Chemistry I Equations

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Gas

Kinetic Theory of Gas

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

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	$\varepsilon = \frac{3}{2} k_B T$
Root mean square speed gas	$v_{\text{RMS}} = \sqrt{\frac{3RT}{\mathcal{M}}} = \sqrt{\frac{3k_B T}{m}}$
Mean speed of gas	$\bar{v} = \sqrt{\frac{8RT}{\pi \mathcal{M}}} = \sqrt{\frac{8k_B T}{\pi m}}$

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

Molecular Collisions and Rate Processes

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

Intermolecular Interactions

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

Description Equations

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

Thermodynamics

First law of thermodynamics

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

Description	Equations
First law of thermodynamics	$\Delta U = q + w$ $dU = \delta q + \delta w$ $\Delta U_{\text{univ}} = \Delta U_{\text{sys}} + \Delta U_{\text{surr}} = 0$
Enthalpy change	$q_P = \Delta(U + PV) = \Delta H$
Molar heat capacity of monoatomic ideal gas at constant volume	$c_V = \frac{3}{2}R$
Molar heat capacity of any ideal gas at constant pressure	$c_P = c_V + R = \frac{5}{2}R$
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	$b = \frac{n_{\text{solute}}}{m_{\text{solvent}}}$
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	$\Delta T = 0$ $\Delta U = 0$ $\Delta H = 0$ $w = - \int_{V_1}^{V_2} P dV = -nRT \ln \frac{V_2}{V_1}$ $q = -w$
Reversible adiabatic process of ideal gas	$q = 0$ $\Delta U = nc_V \Delta T = w$ $\Delta H = nc_P \Delta T$ $\gamma = \frac{c_P}{c_V}$ $T_1 V_1^{\gamma-1} = T_2 V_2^{\gamma-1}$ $P_1 V_1^\gamma = P_2 V_2^\gamma$

Second law of thermodynamics

Description	Equations
Entropy	$S = k_B \ln \Omega$
Entropy change	$\Delta S = \int_i^f \frac{dq_{\text{rev}}}{T}$
ΔS_{sys} for reversible isothermal process	$\Delta S = \int_i^f \frac{dq_{\text{rev}}}{T} = \frac{1}{T} \int_i^f dq_{\text{rev}} = \frac{q_{\text{rev}}}{T}$
ΔS_{sys} for reversible isothermal process - compression/expansion of ideal gas	$q_{\text{rev}} = nRT \ln \left(\frac{V_2}{V_1} \right)$ $\Delta S = nR \ln \left(\frac{V_2}{V_1} \right)$
ΔS_{sys} for reversible isothermal process - phase transitions	$q_{\text{rev}} = \Delta H_{\text{fus}}$ $\Delta S_{\text{fus}} = \frac{q_{\text{rev}}}{T_{\text{fus}}} = \frac{\Delta H_{\text{fus}}}{T_{\text{fus}}}$
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	$K = \frac{\prod_j (P_{\text{product } j} / P_{\text{ref}})_{eq}^{b_j}}{\prod_i (P_{\text{reactant } i} / P_{\text{ref}})_{eq}^{a_i}}$
Law of mass action - concentration	$K = \frac{\prod_j (c_{\text{product } j} / c_{\text{ref}})_{eq}^{b_j}}{\prod_i (c_{\text{reactant } i} / c_{\text{ref}})_{eq}^{a_i}}$
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	$\ln K = -\frac{\Delta G^\circ}{RT} = -\frac{\Delta H^\circ}{RT} + \frac{\Delta S}{R}$
Change in Gibbs free energy at non-standard conditions	$\Delta G = \Delta G^\circ + RT \ln Q = RT \ln \frac{Q}{K}$
Reaction quotient - partial pressure	$Q = \frac{\prod_j (P_{\text{product } j} / P_{\text{ref}})^{b_j}}{\prod_i (P_{\text{reactant } i} / P_{\text{ref}})^{a_i}}$
Reaction quotient - concentration	$Q = \frac{\prod_j (c_{\text{product } j} / c_{\text{ref}})^{b_j}}{\prod_i (c_{\text{reactant } i} / c_{\text{ref}})^{a_i}}$
vant's Hoff equation temperature dependence of equilibrium constant of a reaction	$\ln \frac{K_2}{K_1} = -\frac{\Delta H^\circ}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right)$
Clapeyron equation for two phase in equilibrium, construct phase diagram by finding change of pressure as a function of temperature	$\left(\frac{dP}{dT} \right)_{eq} = \frac{\Delta S}{\Delta V} = \frac{\Delta H}{T \Delta V}$
Clausius-Clapeyron equation temperature dependence of vapor pressure for condensed phase and gas phase in equilibrium	$\ln \frac{P_2}{P_1} = -\frac{\Delta H_{\text{vap}}}{nR} \left(\frac{1}{T_2} - \frac{1}{T_1} \right)$
Clausius-Clapeyron equation for $P_1 = P^\circ$; $\Delta S^\circ = \frac{\Delta H^\circ}{T^\circ}$	$\ln \frac{P_2}{P^\circ} = -\frac{\Delta H_{\text{vap}}}{nRT_2} + \frac{\Delta S_{\text{vap}}^\circ}{nR}$