Chemistry 366

Spring 2008



Concepts of Chemistry Advanced Section

From "Physical Chemistry" by T. Engel and P. Reid, Pearson:San Francisco, 2007.



FUNDAMENTAL CONCEPTS

Why Thermodynamics? Basic definitions Thermometry Equation of state and the ideal gas

HEAT, WORK, INTERNAL ENERGY AND ENTHALPY

Work and heat Reversibility Irreversible work Calculations of q, w, DU and DH.

STATE FUNCTIONS

Mathematical properties of state functions Variation of Enthalpy with temperature and constant pressure $C_{\rm V}$ and $C_{\rm P}$ Joule-Thompson effect

THERMOCHEMISTRY

Internal energy and enthalpy changes and chemical reactions Hess's Law Temperature dependence of reaction enthalpy Experimental determination of DU and DH Differential Scanning Calorimetry

ENTROPY

Heat engines and the second law of thermodynamics Calculating entropy changes Clausius inequalities Third law of thermodynamics Entropy changes in chemical reactions

CHEMICAL EQUILIBRIUM

Gibbs and Helmholtz energies Differential forms of U, H, G, and A Gibbs energy of a reaction mixture Gibbs energy of a gas mixture DG_{rxn} and the equilibrium constant Variations of K with temperature

REAL GASES

Real gases Equations of states Compression factor Law of corresponding states Fugacity

PHASE DIAGRAMS

Pressure-temperature phase diagram Pressure-volume phase diagram Clapeyron equation and vapor pressure

IDEAL AND REAL SOLUTIONS

Ideal solutions Binary solutions Temperature-composition diagram Gibbs-Duhem equation Colligative properties Activities and real solutions Henry's and Raoult's laes

BOLTZMAN DISTRIBUTION

Microstates and configuration Derivation of the Boltzmann distribution Physical meaning of the Boltzmann distribution

ENSEMBLE AND PARTITION FUNCTION

Canonical ensemble Translational partition function Rotational partition function Vibrational partition function Equipartition theorem Electronic partition function

STATISTICAL MECHANICS

Energy and molecular degrees of freedom Heat capacity Entropy Other thermodynamic functions Chemical equilibrium