

## Exam topics

### Part 1: Thermodynamics basics

#### 1 Properties of gases

state properties of gases: amount of matter, pressure, volume, temperature; pressure units, temperature scales (Fahrenheit, Celsius, Kelvin), Zeroth Law of thermodynamics, equation of state of ideal gases, partial pressure, Dalton's Law

#### 2 Real gases

compression factor, compression diagram, Boyle temperature, virial equation of state, van der Waals equation, isotherms of ideal gases, isotherms of real gases, definition of the critical constants, gas state and vapour state, isotherms of  $\text{CO}_2$

#### 3 Basic notions of thermodynamics

system, surroundings, boundary; open, closed and isolated systems; thermodynamic function; state functions and path functions; intensive and extensive properties; reversible and irreversible processes; work, heat, internal energy; First Law of thermodynamics, sign convention of energy change, perpetuum mobile of the first and second kind

#### 4 Change of internal energy and enthalpy

expansion work, definition and properties of enthalpy, exact differentials of  $U(T,V)$  and  $H(T,p)$ , the meaning of a partial derivative, the Joule experiment, the isothermal and the adiabatic Joule–Thomson experiments; inversion temperature, practical applications of the Joule–Thomson effect, heat capacity in general, definition of  $c_p$  and  $c_v$ , relation of  $c_p$  and  $c_v$ , temperature dependence of enthalpy

#### 5 Thermochemistry

exothermic and endothermic processes, stoichiometric coefficient, standard state, thermochemical equation, standard reaction enthalpy, standard molar enthalpy of formation, reference state element, calculation of reaction enthalpy, Hess's Law, Kirchhoff's Law

#### 6 The Second Law of thermodynamics

equivalent statements of the 2<sup>nd</sup> Law; definition and properties of entropy; interpretation of the entropy, Entropy theorem, Clausius inequality and its interpretation

#### 7 Heat engines

definition of a heat engine, calculation of the maximal efficiency of a heat engine, Carnot efficiency, Carnot cycle with ideal gas, thermodynamic temperature scale; refrigerator, air conditioner and heat pump

#### 8 The Third Law of thermodynamics and beyond

statistical interpretation of entropy, Boltzmann equation, Third Law of thermodynamics, the lowest temperature, combining the First and Second Laws

#### 9 Thermodynamic potential functions

thermodynamic potential functions at the various conditions; definition, calculation, and properties of the Helmholtz and Gibbs free energies, pressure and temperature dependence of the Gibbs free energy; Gibbs-Helmholtz equation; thermochemistry with Gibbs free energy; standard reaction Gibbs free energy, standard molar Gibbs free energy of formation; direction of chemical reactions

## **Part 2: Multiphase and multicomponent systems**

### **1 Phase change**

homogeneous, inhomogeneous and heterogeneous systems; phase and phase equilibrium; Clapeyron equation, Clausius–Clapeyron equation; boiling point, melting point and triple point; change of boiling point with pressure

### **2 Phase diagrams**

phase diagram, characteristic points and lines on phase diagrams, the phase diagram of CO<sub>2</sub> and H<sub>2</sub>O, number of phases, number of components, degrees of freedom (variance of a system), Gibbs' phase rule

### **3 Mixtures**

mixtures, limited/unlimited mixing and solubility; concentration units, change of extensive properties at mixing, ideal mixtures, change of  $G$ ,  $H$ ,  $V$  and  $S$  at the formation of ideal mixtures

### **4 Partial molar quantities**

Calculation and features of partial molar quantities, chemical potential, applications of the chemical potential, chemical potential of a component in an ideal mixture, chemical potential of a component in a mixture of ideal gases, chemical potential of a component in a real mixture, activity and fugacity

### **5 Colligative properties**

common features and common origin of all colligative properties, the common reason of the elevation of boiling point and the depression of freezing point, the calculation of the ebullioscopic and cryoscopic constants, osmotic pressure, derivation of the van't Hoff equation for the calculation of osmotic pressure

### **6 Vapour pressure above mixtures and eutectics**

Raoult's and Henry's laws, eutectic mixture, eutectic point, the temperature–composition phase diagram of eutectics, famous eutectics, features of eutectics

### **7 Chemical equilibrium**

Definition of the equilibrium constants of various types; change of  $G$  at approaching a chemical equilibrium, extent of reaction, thermodynamic condition of chemical equilibrium, calculation of  $K_x$  and  $K_p$  from thermodynamic data, relation of  $K_x$  and  $K_p$ , temperature and pressure dependence of  $K_x$  and  $K_p$ , the origin of the Equilibrium Law (Le Chatelier's principle)

### **8 Surface-related phenomena**

surface tension, surface energy, vapour pressure of curved surfaces, Kelvin equation, formation of rain droplets and hailstones, capillary rise, Eötvös rule, adsorption, absorption, physisorption, chemisorption, active site, fractional coverage, adsorption isotherm, Langmuir isotherm, BET isotherm

### **9 Transport phenomena**

definition, interpretation and temperature dependence of viscosity; Stokes' relation, diffusion, convection, diffusion flux, Fick's 1<sup>st</sup> and 2<sup>nd</sup> law of diffusion, 1D partial differential equation for diffusion, convection and chemical reactions, heat conductivity, heat flux, Fourier's law, cross effects of transport phenomena, thermodiffusion

### **10 Basic notions of reaction kinetics**

production rate, reaction rate, rate equation, rate coefficient, reaction order with respect to a species, overall order of a reaction, law of mass action, generation and solution of kinetic differential equations; first order and second order reactions: rate equations, linear and non-linear integrated rate laws, half-lives; the units of rate coefficients; consecutive reactions, parallel reactions

### **11 Complex reaction mechanisms**

elementary reaction, molecularity, temperature dependence of the rate coefficient, Arrhenius equation, pre-exponential factor, activation energy, Arrhenius plot, overall reaction and the reaction mechanism, reaction kinetic simplifying principles: rate-determining step, quasi steady-state approximation, fast pre-equilibrium approximation, pool component approximation, classification of the reaction steps of a chain reaction: initiation, propagation, branching, inhibition, termination; chain carriers, H<sub>2</sub>–Br<sub>2</sub> reaction mechanism, open chain and branching chain reactions