

1. Properties of gases

- 1.1. Ideal gas: variables of state, equations of state
- 1.2. The kinetic model: collisions, real gases: deviations from perfect behavior, van der Waals equation

2. The first law of thermodynamics

- 2.1. Internal energy: work, heat and energy, the definition of internal energy, expansion work, heat transactions
- 2.2. Enthalpy: definition, the variation of enthalpy on temperature
- 2.3. Thermochemistry: standard enthalpy changes, standard enthalpies of formation, the temperature dependence of reaction enthalpies, experimental techniques
- 2.4. State functions and exact differentials: exact and inexact differentials, changes in internal energy, changes in enthalpy, the Joule-Thomson effect
- 2.5. Adiabatic changes: changes in temperature and pressure

3. The second and third laws of thermodynamics

- 3.1. Entropy: the second law of thermodynamics, the definition of entropy, the entropy as a state function; entropy changes accompanying selected processes (expansion, phase changes, heating, composite processes), the measurement of entropy, third law of thermodynamics
- 3.2. Thermodynamics of the system: the Helmholtz and Gibbs energies, standard molar Gibbs energies
- 3.3. Combining the first and second laws of thermodynamics: properties of internal energy and Gibbs energy

4. Physical transformations of pure substances

- 4.1. Phase diagrams of pure substances: the stabilities of phases, phase boundaries, representative phase diagrams
- 4.2. Thermodynamic aspects of phase transitions: the dependence of stability on the conditions, the location of phase boundaries

5. Simple mixtures

- 5.1. Simple mixtures: the thermodynamic description of mixtures, partial molar quantities, the thermodynamics of mixing, the chemical potentials of liquids
- 5.2. The properties of solutions: liquid mixtures, colligative properties
- 5.3. Phase diagrams of binary systems: vapor pressure diagrams, temperature-composition diagrams, liquid-liquid phase diagrams, liquid-solid phase diagrams; solids: eutectics, systems in which reactions take place, incongruent melting
- 5.4. Phase diagrams of ternary systems: triangular phase diagrams, ternary systems
- 5.5. Activities: the solvent activity, the solute activity, the activities of regular solutions, the activities of ions (mean activity coefficients, the Debye-Hückel theory)

6. Chemical equilibrium

- 6.1. The equilibrium constant: the Gibbs energy minimum, the description of equilibrium
- 6.2. The response of equilibria to the conditions (pressure and temperature)
- 6.3. Electrochemical cells: half-reactions and electrodes, varieties of cells, the cell potential, the determination of thermodynamic functions
- 6.4. Electrode potentials: standard potentials, applications of standard potentials

7. Quantum theory

- 7.1. Energy quantization: black-body radiation, heat capacity, atomic and molecular spectra, wave-particle duality: the particle character of electromagnetic radiation, the wave character of particles
- 7.2. Dynamics of microscopic systems: the Schrödinger equation, the Born interpretation of the wavefunction (normalization, constraints on the wavefunction, quantization)
- 7.3. The principles of quantum theory: operators (eigenvalue equations, the construction of operators, Hermitian operators, orthogonality), superpositions and expectation values, the uncertainty principle, the postulates of quantum mechanics
- 7.4. Translation: free motion in one dimension, confined motion in one dimension (the acceptable solutions, the properties of the wavefunctions, energy properties, motion in limited two- and three-dimensional space (energy levels and wavefunctions, degeneracy, tunneling)
- 7.5. Vibrational motion: harmonic oscillator (the energy levels, the wavefunctions) properties of a harmonic oscillator (mean values, tunneling)
- 7.6. Rotational motion: rotation in two dimensions (the qualitative origin of quantized rotation, the solution of the Schrödinger equation, quantization of angular momentum), rotation in three dimensions (the wavefunctions, the energies, angular momentum, the vector model)

8. Atomic structure and spectra

- 8.1. Hydrogenic atoms: structure of hydrogenic atoms, atomic orbitals and their energies
- 8.2. Many-electron atoms: the orbital approximation, the Pauli exclusion principle, principle of expansion of electron shells, self-consistent field orbitals
- 8.3. Atomic spectra of hydrogenic atoms and complex atoms (singlet and triplet states, spin-orbit coupling, term symbols, Hund's rules, selection rules)

9. Molecular structure

- 9.1. The Born-Oppenheimer approximation
- 9.2. Valence-bond theory, diatomic molecules (basic formulation, resonance), polyatomic molecules (promotion, hybridization)
- 9.3. Principles of molecular orbital theory: linear combination of atomic orbitals (the construction of linear combinations, bonding and antibonding orbitals), orbital notations
- 9.4. Homonuclear diatomic molecules, electron configurations (σ and π orbitals, the overlap integral, period 2 diatomic molecules), photoelectron spectroscopy
- 9.5. Heteronuclear diatomic molecules: polar bond (the molecular orbital formulations, electronegativity), the variation principle (the procedure, the features of the solutions)
- 9.6. Polyatomic molecules: the Hückel approximation (an introduction to the method, the matrix formulation of the method), applications (π -electron binding energy, benzene and aromatic stability),
- 9.7. Computational chemistry (semi-empirical and ab initio methods, density functional theory, graphical representation of molecules)

10. Molecular symmetry

- 10.1. Shape and symmetry: symmetry operations and symmetry elements, the symmetry classification of molecules, immediate consequences of symmetry (polarity and chirality)
- 10.2. Applications of symmetry: vanishing integrals, applications to molecular orbital theory, selection rules

11. Molecular spectroscopy

- 11.1. General features of molecular spectroscopy: the absorption and emission of radiation, spectral linewidths, experimental techniques
- 11.2. Rotational spectroscopy: rotational energy levels, microwave spectroscopy, rotational Raman spectroscopy, nuclear statistics and rotational states
- 11.3. Vibrational spectroscopy of diatomic molecules: vibrational motion, infrared spectroscopy, anharmonicity, vibration-rotation spectra, vibrational Raman spectra
- 11.4. Vibrational spectroscopy of polyatomic molecules: normal vibrations, infrared absorption spectra, vibrational Raman spectra
- 11.5. Symmetry analysis of vibrational spectra: classification of normal modes according to symmetry, symmetry of vibrational wavefunctions
- 11.6. Electronic spectra of two- and polyatomic molecules
- 11.7. Decay of excited states: fluorescence and phosphorescence, dissociation and predissociation, lasers

12. Magnetic resonance

- 12.1. General principles: nuclear magnetic resonance, electron paramagnetic resonance
- 12.2. Features of NMR spectra: the chemical shift, the origin of shielding constants, the fine structure, exchange processes, solid-state NMR
- 12.3. Pulse techniques in NMR: the magnetization vector, spin relaxation, spin decoupling, the nuclear Overhauser effect
- 12.4. Electron paramagnetic resonance: the g-value, hyperfine structure

13. Statistical thermodynamics

- 13.1. The Boltzmann distribution: macro states of the system and thermodynamic probability, relative occupancy of states
- 13.2. Molecular partition functions: significance and contributions to the partitions function
- 13.3. Molecular energies: the basic equations, contributions of the fundamental modes of motion
- 13.4. The canonical ensemble: the concept of ensemble, the mean energy of the system, independent molecules, the variation of the energy with volume
- 13.5. Internal energy and entropy and derived thermodynamic functions

14. Molecular interactions

- 14.1. Electric properties of molecules: electric dipole moment, polarizabilities, polarization
- 14.2. Interactions between molecules: the interactions of dipoles, hydrogen bonding, the hydrophobic interactions, the total interaction
- 14.3. Liquids: molecular interactions in liquids, the liquid-vapor interface, surface films, condensation
- 14.4. Macromolecules: average molar masses, the different levels of structure, random coils, mechanical properties, thermal properties
- 14.5. Self-assembly: colloids, micelles and biological membranes

15. Solids

- 15.1. Crystal structure: periodic crystal lattices, the identification of lattice planes
- 15.2. Diffraction techniques: X-ray crystallography, neutron and electron diffraction
- 15.3. Bonding in solids: metals, ionic solids, covalent and molecular solids
- 15.4. Electrical properties of solids: metallic conductors, insulators and semiconductors, superconductors
- 15.5. Magnetic properties of solids: magnetic susceptibility, permanent and induced magnetic moments, magnetic properties of superconductors

16. Molecules in motion

- 16.1. Transport quantities of a perfect gas: the phenomenological equations, the transport parameters
- 16.2. Motion in liquids, diffusion (thermodynamic approach, diffusion equation, the statistical view)

17. Chemical kinetics

- 17.1. The rates of chemical reactions: monitoring the progress of a reaction, the rates of reactions
- 17.2. Integrated rate laws: zeroth-order reactions, first-order reactions, second-order reactions
- 17.3. Reactions approaching equilibrium: first-order reactions approaching equilibrium
- 17.4. The Arrhenius equation: the temperature dependence of reaction rates, the interpretation of the Arrhenius parameters
- 17.5. Reaction mechanisms: elementary reactions, consecutive elementary reactions, the steady-state approximation, the rate-limiting step, pre-equilibria, kinetic and thermodynamic control of reactions
- 17.6. Examples of reaction mechanisms: unimolecular reactions, polymerization kinetics, enzyme-catalyzed reactions
- 17.7. Photochemistry: photochemical processes, the primary quantum yield, mechanism of decay of excited singlet states, quenching, resonance energy transfer

18. Reaction dynamics

- 18.1. Collision theory: reactive encounters, the Rice–Ramsperger–Kassel model
- 18.2. Diffusion-controlled reactions: reactions in solution, the material-balance equation
- 18.3. Transition state theory: the Eyring equation, thermodynamic aspects, the kinetic isotope effect

19. Processes at solid surfaces

- 19.1. Surface growth, physisorption and chemisorption, experimental techniques
- 19.2. Adsorption and desorption: adsorption isotherms, adsorption and desorption rates
- 19.3. Heterogeneous catalysis: mechanisms of heterogeneous catalysis, catalytic activity at surfaces
- 19.4. Processes at electrodes: the electrode-solution interface, the current density at an electrode, voltammetry, electrolysis, working galvanic cells