

# Final Exam Review

19th May 2009

## 1 Kinetic Theory, Transport, Diffusion

- distributions, how to get various properties from distribution (Maxwell distribution of speeds; Maxwell-Boltzmann distribution of velocities)
- general considerations based on probability distributions; average property, most probable value of distribution, average of distribution
- Collisions, mean-free-path,
- diffusion concepts; given a probability distribution function for distance (position) at various times, how to determine position at time  $t$
- viscosity; what it is; what it measures; how it is transferred/transported in the context of kinetic theory formalism
- average distance = (time)  $\times$  (average velocity)
- root-mean-squared distance; equation and how to manipulate it to get different properties (time, diffusion constant, self-diffusion constant)
- sedimentation; know equations and how to use them
- Know location of Constants, Integrals, Equations, diameters, diffusion constants, etc (begin with section 8) in blue book

## 2 Kinetics

- write rate of change of species with time (based on concept of rate)
- write empirical rate expressions for elementary reactions
- Integrated rate expressions for elementary reactions (1st, 2nd, order reactions)

- linearize integrated rate expressions and determine order of reaction
- how to determine arrhenius parameters; idea behind Arrhenius temperature dependence
- transition state theory and activated processes
- Lindemann mechanism and steady state and equilibrium approximations.
- complex reaction mechanisms; deriving rate expressions for species (products; reactants)
- Michaelis - Menten kinetics

### 3 Quantum Mechanics

- Postulates, meaning of wavefunction, probability density, superposition, measurements
- operators, commutation,
- normalization of wavefunctions
- orthogonality of wavefunctions
- understanding of commutators as operators; reduction of complex commutators to simpler forms
- particle in a box wavefunctions; harmonic oscillator; rotational dynamics; angular momentum;
- Hydrogen atom wavefunctions and energies; relation to orbitals
- radial probability distribution
- spin and Pauli's principle
- Many electron atoms and many electron wavefunctions (Hartree-Fock model and orbital concept)
- breaking of degeneracy of principle levels in many electron atoms
- ionization potential determination
- variational principle; application to Helium atom energies
- configurations of atoms
- Atomic Terms; spin-orbit interactions (level); fine and hyperfine structure

- Hund's rules (no spin-orbit coupling); determining ground state term for a given configuration
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- Diatomic molecules; vibration-rotation spectroscopy
- Molecular electronic configurations; bond orders;