Topics for Final Exam (Physical Chemistry II)

1. **Information and Probability**
   Statistical entropy, thermodynamic entropy, reason for logarithmic term ***Ln*** *p.*
   Combinatorics with large numbers of objects, Stirling's formula for *N*!
   Relation of entropy with number of states.

2. **Stationary Equilibrium States**
   Why is entropy at maximum, is that necessary for stationary state?
   H-Theorem, phase space, spontaneous equilibration processes.
   How to calculate the set of probabilities *p* with constraints?
   Lagrange multipliers method. Origin of Boltzmann factor.
   Extensivity of energy variables and entropy.
   Connection with free energies (minimum), Helmholtz and Gibbs
   Application to chemical reactions, chemical potential → dependence on *T*, *p*

3. **Partition Functions for different ensembles**
   Hierarchy of pf's. Grand canonical → canonical → micro canonical
   Product form for independent d.o.f., independent particles
   Occupation factor, degeneracy, fugacity/affinity factors.
   Derivation of thermodynamic properties from pf, like <E>, <p>, C_v, C_p,
   Partial derivatives with some variables held constant.

4. **Molecular Partition Functions**
   Classical point particles, single-atom, continuous translational pf,
   Maxwell-Boltzmann energy spectrum
   Quantum features, classical limit
   Diatomic d.o.f. vibrations and rotations, integral formulations,
   Equipartition theorem

5. **Quantum Gases**
   Fermi gas, Fermi partition functions and derivatives.
   Applications for electrons in metals, semiconductors.
   Bose statistics, photon gases,
   Radiation laws, Bose-Einstein Condensate

6. **Three Phenomenological Laws of Thermodynamics**

   Ideal gas laws, simple processes
   Thermodynamic entropy, work and heat energy, cyclic processes
   Applications to terrestrial weather phenomena
   Carnot and Otto thermal engines
   Extent of reaction variable ξ.
   Helmholtz and Gibbs energies,
   Chemical potential in reactions, equilibrium constant, mass-action law

7. **Real Substances**

   Lennard-Jones interaction potential
   Origin of corrections to ideal gas laws, van der Waals EoS.
   Compressibility, critical features, phase diagram
   Law of Corresponding States
   Thermodynamic state functions, relations
   Activity and fugacity

8. **Sample Evaluations and Numerical Calculations**

   Relating tabulated energies/enthalpies to equilibrium chemical reactions.
   Extrapolating thermodynamic functions with changing pressure or temperature
   Estimating efficiencies of thermal engines from operational parameters.
   Using virial expansions of thermodynamic functions such as heat capacity and applications,
   Applying model EoS for evaluation of critical pressures, temperatures