

Topics Midterm Exam 2 Physical Chemistry II

1. Information and Probability

Statistical entropy, thermodynamic entropy, reason for logarithmic term $\ln p$.
From combinatorics with large numbers of objects, Stirling's formula $M!$
Relation of entropy with number of states.

2. Stationary Equilibrium States

Why is entropy maximum, is that necessary for stationary state?
H-Theorem, phase space, equilibration/randomization process
How to calculate the set of probabilities p with constraints? Lagrange multipliers
method. Origin of Boltzmann factor.
Extensivity of entropy,
Connection with free energies (minimum), Helmholtz and Gibbs
Application to chemical reactions, chemical potential \rightarrow dependence on T.

3. Partition Functions for different ensembles

Hierarchy of pf's. Grand canonical \rightarrow canonical \rightarrow micro canonical
Product form for independent d.o.f., independent particles
Occupation factor, degeneracy, fugacity/affinity factors.
Derivation of thermodynamic properties from pf, $\langle E \rangle$, $\langle p \rangle$, C_v , C_p ,
Partial derivatives with variables held constant.

4. Molecular Partition Functions

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. Sample Numerical Calculations