Major Concepts for Exam 1

Quantum Mechanics

- Energy is quantized.
- Atoms and molecules can put energy into different types of motion (e.g., translation or vibration).
- Given models for translation, vibration, rotation, etc. we can solve the Schrödinger equation for the energy levels.
- Energy can be converted to wavelength, wavenumber, and frequency.
- Degrees of freedom
- Relative energy spacings

Gas Laws

- There are different gas laws to describe non-ideality of gases. Some are empirical (van der Waals, Redlich-Kwong, Peng-Robinson, etc) and some are purely statistical/theoretical in nature (virial expansion). [Know about these laws and how to use them!]
- The ideal gas law is valid under certain conditions (i.e., the assumptions used to derive the law are valid under these conditions.)
- Attractive and repulsive forces (interactions) are one reason for non-ideality.
- Cubic equations of state and the critical point
- Law of corresponding states
- The second virial coefficient is the first deviation from non-ideality and can be related to the real and ideal molar volume.
- Interaction potentials and Lennard-Jones

Boltzmann/Partition Functions for Ideal Gases

- Statistical mechanics can tie the microscopic and macroscopic together.
- Boltzmann's equation (for probability) is one of the key equations in p chem.
- Changes in temperature and energy level spacing will change the partition function.
- From the partition function, one can find any thermodynamic quantity. [Know how! Also have some sense of what those quantities mean.]
- If a system follows Boltzmann's statistics, the molecular partition function is related to the total partition function by $Q = q^N/N!$ [Know when Boltzmann's statistics is true]
- Sometimes is more convenient to sum over levels and sometimes more convenient to sum over states when finding the partition function.
- The energy of a system is one of the key components of the partition function equation.
- It is convenient to express the vibrational and rotational partition functions in terms of vibrational or rotational temperatures. [Understand how these relate to bonding, strength of vibration, etc]
- The rotational partition function includes a symmetry number.
- Molecular shape effects the rotational and vibrational partition functions
- Rotational, vibrational, electronic and translational energies make contributions to the total partition function