BE564

Biophysics of Large Molecules

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Course syllabus, spring 2009

1. *Introduction.* Role of large molecules in biomedical engineering, molecular biology and biotechnology. Polyatomic molecules. Macromolecules. Examples: formaldehyde, benzene, buckminsterfullerene, polyethylene, polyenes, proteins, DNA, RNA.

2. *Basic principles of classical physics*. Symmetry of the space-time and conservation laws. Newton laws. Classical harmonic oscillator. Failure of classical physics to describe atoms and molecules. Triumph of modern (quantum) physics.

3. *Basic principles of quantum physics.* Operators and wavefunctions. Schrödinger equation. Free particle. De Broigle waves of matter. Heisenberg's uncertainty principle. A particle in a stationary external field. Spectrum of states. Harmonic oscillator. A particle in a box. Matrix elements. An electron in the Coulomb potential. Atomic orbitals. Pauli principle. Electronic structure of main "biological" elements: hydrogen, carbon, nitrogen and oxygen. Molecular orbitals. Hybridization. Covalent bonds. σ- and π- bonds.

4. *Polyatomic molecules*. Electronic and nuclear motions. Schrödinger equation for the molecule. Born-Oppenheimer (adiabatic) approximation. The Born-Oppenheimer parameter and its significance. Electronic terms. Nuclear vibrations. Zero-point vibrations. Normal modes. Ground and excited states. Time-dependent Schrödinger equation. Transitions between different states.

5. *Molecular photonics.* Photon absorption. The Beer-Lambert law. Transition probabilities. Electronic and vibrational spectra of polyatomic molecules. Selection rules. Singlet and triplet electronic terms. Luminescence, fluorescence and phosphorescence. Radiationless transitions. Excitation lifetime. Radiation width. Inhomogeneous broadening. Phonon broadening. Low-temperature spectra. Fluorescence resonance energy transfer (TRET). Spectra of biomolecules. Biomedical and biotechnology applications of molecular photonics. Photosynthesis and vision. Molecular photonics and genomics (fluorescence labels in DNA sequencing, molecular beacons, real time PCR).

6. *Group theory*. Group definition. Examples: digits, braids, symmetry operations, matrices, fundamental group, knot group. The representation theory. Reducible and irreducible representations. Characters.

7. *Molecular symmetry*. Symmetry groups and their representations. Example: formaldehyde. Classifications of electronic terms. Classification of normal modes. Selection rules. Symmetry forbidden transitions. Electronic and vibrational spectra of benzene. Optical spectra of biomolecules (proteins, nucleic acids, etc.).

8. *Basic principles of statistical physics.* Thermal motion and thermal equilibrium. Brownian motion. Energy and entropy. Gibbs distribution. Partition function. Classical statistical mechanics. Equipartition theorem. Quantum statistics: bosons and fermions. Blackbody radiation. Planck's equation. Heat capacity of solids. Role of statistical mechanics in understanding the behavior of polyatomic molecules and macromolecules.

9. *Macromolecules.* Role of the carbon atom. Polymerization and polycondensation. The nature of flexibility of the polymer chain. Theoretical models of polymers. Mean-square end-to-end distance. Kuhn statistical length. Persistence length. Analogy between the bodiless polymer chain and Brownian motion. Statistical coil. Role of entropy. Distribution function for the end-to-end distance. Excluded volume and second virial coefficient. Polymer swelling. Good and poor solvents.

10. *Polymer materials.* Crystallization and melting. Glass state. High elasticity. Nature of high elasticity. Polymer networks. Polymer gels.

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Textbook: T. Engel et al. *Physical Chemistry for the Life Sciences*, Pearson Prentice Hall, Upper Saddle River, N.J., 2008.