Lincoln College Biochemistry Tutorials
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1st years, Hilary Term, Tutorial 1

Title: Biophysical Chemistry – QM & MO (Lincoln)

You should ensure you have notes on the following areas:

Classical & Quantum Mechanics:

1. Building blocks of matter, fundamental particles. Forces between particles. Electrostatics, Coulomb's Law.
2. Classical mechanics. Particles and waves. Bond energy. Electrostatics and dielectric constant. Newton's Laws. Molecular modelling. Effects of electric fields, electrophoresis.
3. Breakdown of classical mechanics. Wave-particle duality of matter and wavefunctions. De Broglie's relationship. Heisenberg's Uncertainty Principle. Zero-point energy.
4. Boundary conditions and quantisation of energy. Particle in a box. Quantum numbers. Schrödinger's equation. Energy levels in molecules. Boltzmann and Maxwell-Boltzmann distribution.
5. Atomic orbitals and quantum numbers. Orbital energies. Aufbau principle.

Bonding in Molecules I:

1. Types of bonding, electrons in molecules. Crystal field theory.
2. Molecular orbital theory. Simple diatomics.
3. More complex examples of molecular orbital theory.

References

N.C. Price, R.A. Dwek, R.G. Ratcliffe and M.R. Wormald (2001) "Principles and Problems in Physical Biochemistry for Biochemists", pub. Oxford – *the best basic text for biochemists.*
S.R. Logan, (1998) "Physical Chemistry for the Biomedical Sciences", pub. Taylor & Francis.
P.W. Atkins and J. de Paula, (2006) "Physical Chemistry for the Life Sciences", pub. Oxford..
R. McWeeny, (1979) "Coulson's Valence", pub. Oxford – *updated version of "Valence" by Coulson, more advanced*.
K.F. Purcell and J.C. Kotz, (1977) "Inorganic chemistry" – *sections on bonding and crystal field theory*.

Problems

All submitted material to be attached as one bundle from each separate student, to be clearly marked with the title of the tutorial, the date, the name of the student, and to clearly display "FAO Dr. Mark Leake, Clarendon Lab" on the first page. To be handed in to either the receptionist, or placed in the "L" pigeon-hole,

of the Clarendon Laboratory, Dept of Physics by *12 noon* the day before the tutorial.

1). When and why does the quantisation of energy occur?   [5]

Sketch the first two allowed waves for a particle in a one-dimensional box. [3]

Starting from the de Broglie's relationship, $\lambda = h/mv$ here m is the mass of the particle, v is its velocity and λ is its wavelength, derive a general equation for the kinetic energy (K.E. $= mv^2/2$) of a particle localised in a one-dimensional box.   [5]

An electron can become trapped in a hole inside a NaCl crystal (called a colour centre, because it makes the crystal coloured). This electron behaves in a similar fashion to a particle in a box.
If the lowest energy absorption peak of the electron is at a wavelength of 550 nm, calculate the effective size of the hole in the crystal in which the electron is trapped.   [8]

If an electron were trapped in a hole in a KCl crystal, where the holes are bigger, would the lowest energy absorption peak shift to lower or higher wavelength? Give your reasons.   [4]

The mass of an electron is 9.1 x 10^{-31} kg and the speed of light is 2.99 x 10^8 m s^{-1}

2) Describe briefly the molecular orbital theory of bonding, highlighting any advantages over other bonding theories.   [10]

Explain **THREE** of the following observations in terms of molecular orbital theory.
                                                                        3x[5]
(i) The bond length of O_2^+ is shorter than in O_2 whereas the bond length in N_2^+ is longer than in N_2.
(ii) CO binds to metal ions via its carbon and NO binds to metal ions via its nitrogen.
(iii) The species $CH_2=CH-CH=CH_2$ is planar and exists as two isomers.
(iv) The rate of cis-trans isomerisation of double bonds (e.g.
cis-CHF=CHF $\leftrightarrow$ trans-CHF=CHF) is increased by light but not by heat.