SISSA ISAS

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April 2010 – Entrance Examination: Physics and Chemistry of Biological Systems

Solve **one** of the following problems (no extra credit is given for attempts to solve more than one problem). Write out solutions clearly and concisely. State each approximation used. Diagrams welcome. Number page, problem, and question clearly. All essays/solutions should be written in English. Do not write your name on the problem sheet, but use extra envelope.

Problem n. 1 – Interconverting molecules

Consider an ensemble of identical, non-interacting molecules, each of them with three available internal states A, B and C. The total number of molecules ($N = N_A + N_B + N_C$) is kept constant and satisfies $N >> 1$. The transition rate for the process $A \to B$ is k_{BA}, whereas the transition rate for the process $B \to C$ is k_{CB}. All the other rates are negligible.

At time $t = 0$ all the N molecules in the ensemble are in state A.

1. Calculate N_A as a function of time.
2. Calculate N_A, N_B and N_C in the long time limit.
3. Sketch the time dependence of N_A, N_B and N_C.
4. Calculate the explicit expressions for N_B and N_C as a function of time.
5. Now assume that $k_{BA} = k_{CB} \equiv k$ and that, due to the action of an unspecified external force, state C can convert to state A with rate $k_{AC} = k$. Calculate N_A, N_B and N_C in the long time limit, and estimate the typical time required to reach the steady state from an arbitrary initial condition.

Problem n. 2 – Hueckel MO Theory

Using Hueckel MO theory a molecule can be tough as a set of 6 sites on each of which it is placed a C atom. Each C atom shares one electron in a delocalized p_z orbital. Considering the benzene and hexatriene molecules:

1. calculate the π-electron energies
2. draw an energy diagram for the electronic states.
3. indicate which orbitals are occupied
4. draw a picture of the molecular orbitals.
5. calculate the delocalization energy per π electron.
6. determine which 6 π electron systems is more stable