1. State, in general terms, under what conditions one may expect the diffraction of matter waves to be important in determining the dynamics of a particle, and under what conditions diffraction is unimportant. 20%

2. Set up and solve the secular equations for the Hückel molecular orbitals of

   (a) the allyl radical, $H_2\dot{C} - \dot{C}H - \dot{C}H_2$;

   (b) the cyclopropenyl radical;

   (c) cyclobutadiene.

   (Hint: use the molecular symmetry to factor the 3×3 and 4×4 matrices so you have nothing larger than a quadratic to solve.) 20%

3. The energy, mass and volume of a system are extensive. How about the molar energy, molar mass, and molar volume? How about the energy and energy density? 10%

4. The entropy change ΔS for a phase transition equals $\Delta H/T$, where ΔH is the enthalpy change. Why is it that the entropy changes for a system in which a chemical reaction occurs spontaneously does not equal to $\Delta H/T$? 10%

5. Suppose that a volume V is subdivided into two compartments. One of these contains N'_A A molecules and N'_B B molecules; the other contains N''_A A molecules and N''_B B molecules. A valve between the compartment is opened and closed and one molecule transferred from the side marked ($'$) to the side marked ($''$). After a long time the valve is again opened and closed and one molecule transferred from ($''$) to side ($'$). What is the probability that the molecule transferred in both step is an A molecule. 20%

6. You perform some experiments for the reaction $A + B \longrightarrow C$ and determine the rate law has the form

$$\text{Rate} = k[A]^x$$

   Calculate the value of exponent x for each of the following.

   (a) $[A]$ is tripled and you observe no rate chane.

   (b) $[A]$ is doubled and the rate doubles.

   (c) $[A]$ is tripled and the rate goes up by a factor of 27.

20%

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