Introduction to Quantum Chemistry WS 2001/02 Exercises No. 1
Return before Mo evening, Nov. 5, wooden mail-box, AR-K6 left side wall.
Discussion hour on Mon. or Wed.?

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1) A bond is broken by photodissociation with UV light of $\lambda = 400\,\text{nm}$. Give wave number $1/\lambda$, energy in eV, in kJ/mol, in $k \cdot T$ (comp A11.10).

2) An electron moves with kinetic energy of 0.5 Hartree. What is its velocity, its deBroglie wavelength. Compare with the size of atoms. What is the mass, momentum and wave length of a photon of 0.5 hartree energy? Give all answers in a.u., and lengths also in SI units (comp. A11.5)

3 The modified box model for polyenes (C_nH_{n+2}) yields for the HOMO-LUMO transition from level $m = n/2$ to $m + 1$ the relation $\lambda = const \cdot (m + 1)/(1 + \delta m)$. Experimental values for λ in nm: Ethene - 162, Butadiene - 217, Hexatriene -257, Octatetraene - 290, Decapentaene - 317

a) Show that $1/\lambda$ scales linearly with $1/(n + 2)$

b) Plot $2000\,nm/\lambda$ versus $40/(n + 2)$

c) From which n upwards, polynenes will have a color?

d) What is the color of very long polyenes?

4) Discuss the stability of the HOMO-electrons, $E_m = m^2/2R^2$, of $(CH)_n$-rings, $n = 2$ to 11. The circumference is $2\pi R = n \cdot D_{cc}$. m is 0 to 3. The closed shell of F^-, Ne, Na^+, Mg^{2+} becomes more and more stable. But O^{2-}, N^{3-} are completely unstable in vacuum.

5) The vibrational quanta of H_2 are about 4000 cm^{-1}.

a) Determine the force constant in N/cm in atomic units: $\Delta E = \sqrt{k/\mu}$

b) $\psi = exp(-\sqrt{k\mu}(\Delta R)^2/2)$. For which values ΔR does the probablity take $1/e$ of the maximum value at $\Delta R = 0$? How many % of the $H - H$ separation of 86 pm is the vibrational width of $2 \cdot \Delta R$ at 0 K?