Chem 442
Spring 2021

Exam 1

Useful numbers and plots you may need are at the end.
You must upload your answer (PDF or JPEG) by 10:55 on Moodle to get full credit.

1. (18 pts) **Calculate** the wavelength of light that will be absorbed by the molecule propene (it has a C-C=C backbone) by approximating its electronic structure by an "electron in a box."

a. (2) With d(C-C) = 1.54 Å and d(C=C) = 1.35 Å, **what is** the length L of the box, assuming the electron can move through the whole carbon skeleton?

b. (3+3) Of the three π electrons in propene, the first two will fill the n=1 energy level of the box, and the third electron, which will be excited by the light, will be in the n=2 level or "HOMO" (highest occupied molecular orbital). **Write down** the particle-in-a-box energy formula for the third electron in terms of n, h, m_e and L and **calculate** the energy of the n=2 electron in Joules.

c. (3+2) When light is absorbed, the electron goes to the $n = 3$ level. **Write down** the formula for the energy difference between the $n = 3$ *and* $n = 2$ states, and **calculate** the energy difference in Joules.

d.. (3+2) Finally, use Planck's law to convert the energy to a **wavelength in nm**. What part of the **electromagnetic spectrum** at the end of the exam is it?

2. (15 pts) The normalized wavefunction $\Psi(x) = \left(\frac{1}{\sqrt{2}}\right) e^{-|x|/2}$ is also known as a "1s orbital" for an electron whose nucleus sits at x=0. Here x is in Ångstrom units, treat the problem as 1-D.

a. (4+2+2) **Sketch** the wavefunction roughly between x= -5 to 5 Å, **labeling** the axes "x" and "Ψ" and **indicating** roughly where x=±2 lies on the x-axis.

b. (2+3+2) Calculate the probability of finding the electron at a <u>distance</u> of between 3 and 3.1 Å from the nucleus by first **writing down the integral** with correct integration limits, then **evaluating** the integral, and **plug in** the numbers to get the probability.

3. (10 pts) Someone plays the kettle drum.

a. (3+3) If they play on the kettle drum a "low "A" note at 110 Hz for 50 milliseconds (0.05 s), what is the uncertainty in the pitch Δv as a percentage of the frequency v? **Formula** and **value**.

b. (2+2) **Can they distinguish** the "A" from an "A#" at 116.5 Hz? In one sentence, **why do you think** orchestras use kettle drums, but not snare drums, to play bass melodies in symphonies?

4. (18 pts) If a quantum particle is in state $\Psi(x,t)$, let us show that the average value of the energy from many measurements is given by

$$\langle E \rangle = \bar{E} = \int_{-\infty}^{\infty} dx \Psi^*(x,t) \hat{H} \Psi(x,t),$$

a. (3+3) **Write down** the formula for $P(E = E_n) = ?$ from postulate 4, calling the energy eigenvalues E_n and the eigenfunctions $\varphi_n(x)$. Then recall from the \$ bills homework that $\bar{A} = \Sigma a_n P(A = a_n)$ for any observable A. **Combine these two equations** to write an expression for $\langle E \rangle$ in terms of the eigenvalues and eigenfunctions of $\hat{H}$.

b. (3) Now **write down** the same expression for $\langle E \rangle$ again, but multiply out the $||^2$ square modulus explicitly. Something like

$$\int_{-\infty}^{\infty} dx \Psi^*(x,t) \varphi_n(x) \int_{-\infty}^{\infty} dx' \varphi_n^*(x') \Psi(x',t)$$

should appear in your expression (the integral times its complex conjugate). It's always a good idea to give your integration variables <u>different</u> names (here x and x') when you have several integrals in an expression.

c. (1+2) Your expression for $\langle E \rangle$ has an "E_n" outside the first integral. Since E_n is a constant, you can stick it inside the integral in front of $\varphi_n(x)$, and play the reverse of a trick we have done in class several times: since $\hat{H}\varphi_n(x) = E\varphi_n(x)$, you can replace "$E_n$" **by what** in the integral? **Write down** the formula for $\langle E \rangle$ again, this time without E_n in it.

d. (3+3) Remember that any function can be expanded as a linear combination of a complete set of eigenfunctions. For example, $\Psi(x,t) = \Sigma c_m(t) \varphi_n(x)$, where $c_m(t) = \int_{-\infty}^{\infty} dx' \varphi_n^*(x') \Psi(x',t)$ is the "overlap integral" between $\varphi_n(x)$ and $\Psi(x,t)$. Look at your expression from part c., and replace one of the integrals by c_m, and **write down** the resulting formula for $\langle E \rangle = \bar{E}$. Finally **do the sum** $\Sigma c_m(t) \varphi_n(x)$, which equals $\Psi(x,t)$, and write down your final expression for $\langle E \rangle = \bar{E}$.

Congrats, in 1926 you would have won a Nobel Prize!

<u>Useful numbers:</u>
1 atomic mass unit = 1.66 x 10^{-27} kg; mass of electron m_e = 9.109 x 10^{-31} kg
Planck's constant h = 6.626 × 10^{-34} J·s; note that $\hbar = 2\pi h$ is about 6.28 times larger.
1 Å = 0.1 nm = 100 pm; $c \approx 3 \cdot 10^8$ m/s

ELECTROMAGNETIC SPECTRUM

Extreme ultraviolet (EUV) — Ultraviolet C (UVC) — Ultraviolet B (UVB) — Ultraviolet A (UVA) — Far-red

10 nm — 100 nm — 280 nm — 315 nm — 400 nm — 500 nm — 600 nm — 700 nm