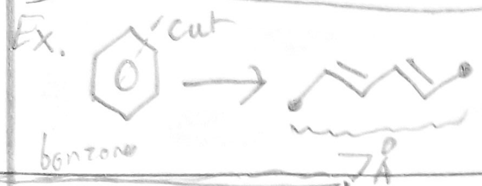
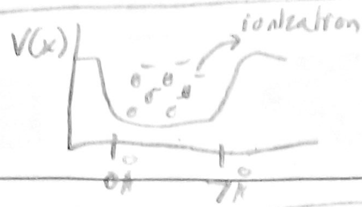
Lecture 9: Molecule as a box of electrons

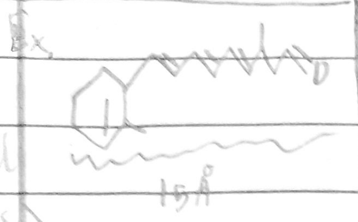
Ex.





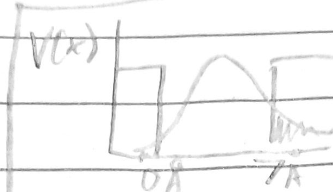
Potential higher when away from positive nuclei.

Ex.



retinal switches from cis to trans & back under light absorption, providing basis for vision.

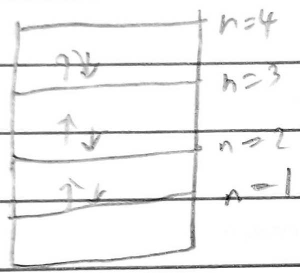
Is benzene colored or transparent? (Absorbs or doesn't absorb in 400–700 nm)



By logic/analogy, lowest E wavefunction has form like this.

- If sides of box are higher, shape will be same, but forbidden region penetration will be smaller.
- If walls are infinitely high, probability in classically-forbidden region is 0.

Fermions can't be in the same state, and spin is quantized, so $s=\frac{1}{2} \rightarrow \pm\frac{1}{2}$ ↑, ↓



6 pi e^-

$H\psi = E\psi$ $V(x),\ 0<x<7$ Å

$\left(\frac{-\hbar\,\partial^2}{2m\,dx^2}+0\right)\psi_n = E_n\psi_n$

$\psi=0$ at $x=0$, ↑ $\sin(ax)$ ~~$\cos(ax)$~~

$h\nu = E_4 - E_3 = \frac{h^2}{8mL^2}(4^2-3^2) \rightarrow$

$\rightarrow \nu = 1.3e15$ Hz

$\rightarrow \lambda = 231$ nm

Ultraviolet light, so benzene is transparent.

Need $\sin(aL)=0$. ← L is 7 Å for this example (benzene.)

$a = \frac{\pi \cdot n}{L}$

$n=1,2,3\ldots$ (not $n=0$, since that's trivial – no e^- present.)

$\psi_n(x) = \sin\left(\frac{n\cdot\pi}{L}\cdot x\right),\ n=1,2,3\ldots$

$\frac{-h^2}{8m\pi^2}\frac{\partial^2}{dx^2}\sin\left(\frac{n\pi}{L}\cdot x\right) = E_n \sin\left(\frac{n\pi}{L}\cdot x\right)$

$\frac{h^2}{8m\pi^2}\frac{n^2\pi^2}{L^2}\psi_n = E_n\psi_n$

$E_n = \frac{h^2n^2}{8mL^2} = \frac{p_n^2}{2m} \rightarrow p_n = \pm\frac{hn}{2L}$