Modeling the Pi-electrons of Benzene as Particles in a Ring

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In this exercise benzene's six π electrons will be modeled as particles in a ring or circular corral. Schrödinger's equation in plane polar coordinates and its energy eigenvalues are given below. R is the ring radius and C the ring circumference.

$$\frac{-h^2}{8\cdot\pi^2\cdot m_e}\cdot\left(\frac{d^2}{dr^2}\Psi(r)+\frac{1}{r}\cdot\frac{d}{dr}\Psi(r)-\frac{L^2}{r^2}\cdot\Psi(r)\right)=E\cdot\Psi(r) \qquad E_{n,L}=\frac{(Z_{n,L})^2\cdot h^2}{8\cdot\pi^2\cdot m_e\cdot R^2}=\frac{(Z_{n,L})^2\cdot h^2}{2\cdot m_e\cdot C^2}$$

J_L is the L^{th} order Bessel function, L is the angular momentum quantum number, n is the principle quantum number, $Z_{n,L}$ is the n^{th} root of J_L. Dirac notation is used to describe the electronic states, |n,L>. The roots of the Bessel function are given below in terms of the n and L quantum numbers.

L quantum number

Z :=

0	1	2	3	4	5	6	7	"n"
2.405	3.832	5.316	6.380	7.588	8.771	9.936	11.086	1
5.520	7.016	8.417	9.761	11.065	12.339	13.589	14.821	2
8.654	10.173	11.620	13.015	14.373	15.700	17.004	18.288	3
11.792	13.324	14.796	16.223	17.616	18.980	20.321	21.642	4
14.931	16.471	17.960	19.409	20.827	22.218	23.586	24.935	5

n quantum number

The manifold of allowed energy levels up to the LUMO is shown below and is populated with 6 π electrons. Note that the states with L > 0 are doubly degenerate.

					$Z_{n,L}$	
LUMO	(1,2)	(1,−2)	____	____	5.316	
HOMO	(1,1)	(1,−1)	_xo_	_xo_	3.832	6
	(1,0)		_xo_		2.405	2

The photon wavelength required for the first electronic transition involving the π electrons is now calculated. The ring circumference is approximated as six benzene carbon-carbon bond lengths.

$h := 6.6260755\cdot10^{-34}\cdot joule\cdot sec \qquad c := 2.99792458\cdot10^{8}\cdot\frac{m}{sec} \qquad m_e := 9.1093897\cdot10^{-31}\cdot kg \qquad pm := 10^{-12}\cdot m$

$$C := 6\cdot140\cdot pm \qquad \frac{(Z_{1,1})^2\cdot h^2}{2\cdot m_e\cdot C^2}+\frac{h\cdot c}{\lambda}=\frac{(Z_{1,2})^2\cdot h^2}{2\cdot m_e\cdot C^2}\ \Big|\begin{matrix}solve,\lambda\\ float,3\end{matrix}\rightarrow\frac{4.28e\text{-}8\cdot kg\cdot m^3}{joule\cdot sec^2}=42.8\cdot nm$$

Benzene has a strong electronic transition at about 200 nm.