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

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In this exercise the 20 π electrons of corannulene will be modeled as particles in a ring or circular corral. Corannulene is bowl-shaped not planar, so the model has some initial difficiencies.

Schrödinger's equation in plane polar coordinates and its energy eigenvalues are given below. R is the ring radius and C the ring circumference.

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

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

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

n quantum number

The manifold of allowed energy levels up to the LUMO is shown below and is populated with 20 π electrons. Note that the states for L > 0 are doubly degenerate.

					$Z_{n,L}$	
LUMO	(1,4)	(1,−4)	____	____	7.588	
HOMO	(2,1)	(2,−1)	_xo_	_xo_	7.016	20
	(1,3)	(1,−3)	_xo_	_xo_	6.380	16
	(2,0)		_xo_		5.520	12
	(1,2)	(1,−2)	_xo_	_xo_	5.316	10
	(1,1)	(1,−1)	_xo_	_xo_	3.832	6
	(1,0)		_xo_		2.405	2

Corannulene has a strong electronic transition at 280 nm. This information will be used to calculate its circumference.

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

$\lambda := 280 \cdot nm$ $\frac{(Z_{2,1})^2 \cdot h^2}{2 \cdot m_e \cdot C^2} + \frac{h \cdot c}{\lambda} = \frac{(Z_{1,4})^2 \cdot h^2}{2 \cdot m_e \cdot C^2} \left| \begin{matrix} \text{solve}, C \\ \text{float}, 3 \end{matrix} \right. \rightarrow \begin{pmatrix} -\frac{0.0000533 \cdot \sqrt{joule} \cdot \sqrt{nm} \cdot sec}{\sqrt{kg} \cdot \sqrt{m}} \\ \frac{0.0000533 \cdot \sqrt{joule} \cdot \sqrt{nm} \cdot sec}{\sqrt{kg} \cdot \sqrt{m}} \end{pmatrix} = \begin{pmatrix} -1.685 \times 10^{3} \\ 1.685 \times 10^{3} \end{pmatrix} pm$

This result is reasonable given that there are 15 c-c bonds on the circumference: $15 \cdot 140 \cdot pm = 2.1 \times 10^{3}\, pm$