

Estimate the electron transition energy and wavelength of decapentaene using the particle-in-a-box model. Assume that decapentaene is a ten-carbon polyene dye that can be modeled as a box of length 15.1 Å.

Solution: The particle-in-a-box model for a polyene assumes that electrons are paired in each quantum level. Thus, 10 electrons will fill the first 5 levels and the first transition will be from level 5 \rightarrow 6. The ground state quantum number will be $n_g = 5$ and the excited state quantum number will be $n_e = 6$.

$$\Delta E = \frac{h^2}{8ma^2}(n_e^2 - n_g^2) = \frac{(6.626 \times 10^{-34} \text{ Js})^2}{8 \times 9.1 \times 10^{-31} \text{ kg} \times (15.1 \times 10^{-10} \text{ m})^2} (6^2 - 5^2) = 2.9 \times 10^{-19} \text{ J} = 14,670 \text{ cm}^{-1}.$$

The wavelength can be obtained from

$$\Delta E = hc/\lambda \text{ or } \lambda = hc/\Delta E = \frac{(6.626 \times 10^{-34} \text{ Js})(2.99 \times 10^8 \text{ m/s})}{(2.9 \times 10^{-19} \text{ J})} = 681 \text{ nm}.$$

$$\text{Transition energy} = \underline{14,670 \text{ cm}^{-1}}.$$

$$\text{Transition wavelength} = \underline{681 \text{ nm}}.$$

Transition energy = _____.

Transition wavelength = _____.