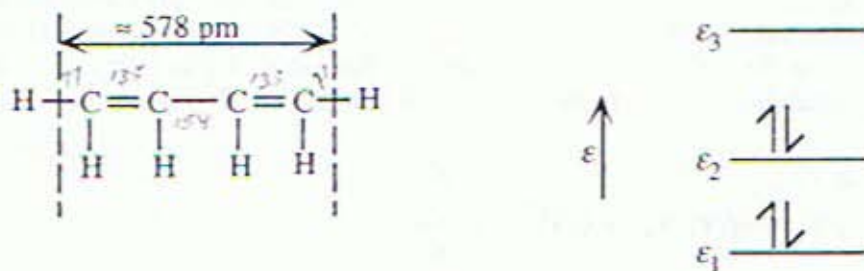


Problems

use equation 8; $\epsilon = \frac{n^2 h^2}{8 \cdot m \cdot a^2}$

1. The particle-on-a-line problem is often used as a model for the π -electrons in conjugated molecules. Assume that the π -electrons of 1,3 butadiene move along a straight line of 578 pm (two C=C bond lengths of 135 pm, one C-C bond length of 154 pm, plus an addition one-half of a C-C bond length at the two terminal carbon atoms: $77 + 135 + 154 + 135 + 77 = 578$ pm). The energy level diagram is shown below.



- a) Why are there four electrons in the energy level diagram?
 b) Why are only two electrons placed in ϵ_1 ? π molecular orbital can hold max of 2 e⁻
 c) What is the energy of an electron in ϵ_2 (in joules)?
 d) At what energy (in joules) is the ϵ_3 level?
 e) What energy is required to promote an electron from ϵ_2 to ϵ_3 (in joules)?
 f) If this energy is supplied by a photon, what is the wavelength of the photon?
 g) Compare this wavelength to the experimentally observed wavelength of 217 nm.

- a) Four electrons, two double bonds \rightarrow four π electrons
 b) Pauli Exclusion Principle (a wave function that describes an electron can hold only 2 electrons each with opposite spin)
 c)
$$\epsilon = \frac{n^2 h^2}{8 \cdot m \cdot a^2} = \frac{2^2 \times (6.6 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (5.7 \times 10^{-10})^2}$$

$$= 7.21 \times 10^{-19} \text{ J}$$

 d) Apply for $\epsilon_3 \rightarrow \epsilon_3 = 1.62 \times 10^{-18} \text{ J}$
 e) The energy required to promote an electron is the difference in energy levels: $\Delta \epsilon = 8.99 \times 10^{-19} \text{ J}$
 f) $\lambda = hc/E = 221 \text{ nm}$
 g) This is very close to the observed value 217 nm.