The particle-in-a-box or free electron model predicts that the transition energy of ethene is 109,060 cm^{-1}. Fill in the table below with the energies for butadiene and hexatriene. One easy way to do this is to determine the ratio of the transition energies of both butadiene and hexatriene relative to ethene. Use those ratios to calculate the transition energies.

Molecule	L (Å)	Ratio	ΔE (cm^{-1})
Ethene	2.89	1	109,060
Butadiene	5.78	0.416	45,370
Hexatriene	8.67	0.259	28,250

Solution: For ethene the transition is from 1 → 2, butadiene 2 → 3 and hexatriene 3 → 4.
The ground state quantum number is n_g and the excited state quantum number is n_e.
The general formula is:
Ethene

$$\Delta E_e = \frac{h^2}{8mL_e^2}(n_{e,e}^2 - n_{g,e}^2)$$

Butadiene

$$\Delta E_b = \frac{h^2}{8mL_b^2}(n_{e,b}^2 - n_{g,b}^2)$$

Hextriene

$$\Delta E_h = \frac{h^2}{8mL_h^2}(n_{e,h}^2 - n_{g,h}^2)$$

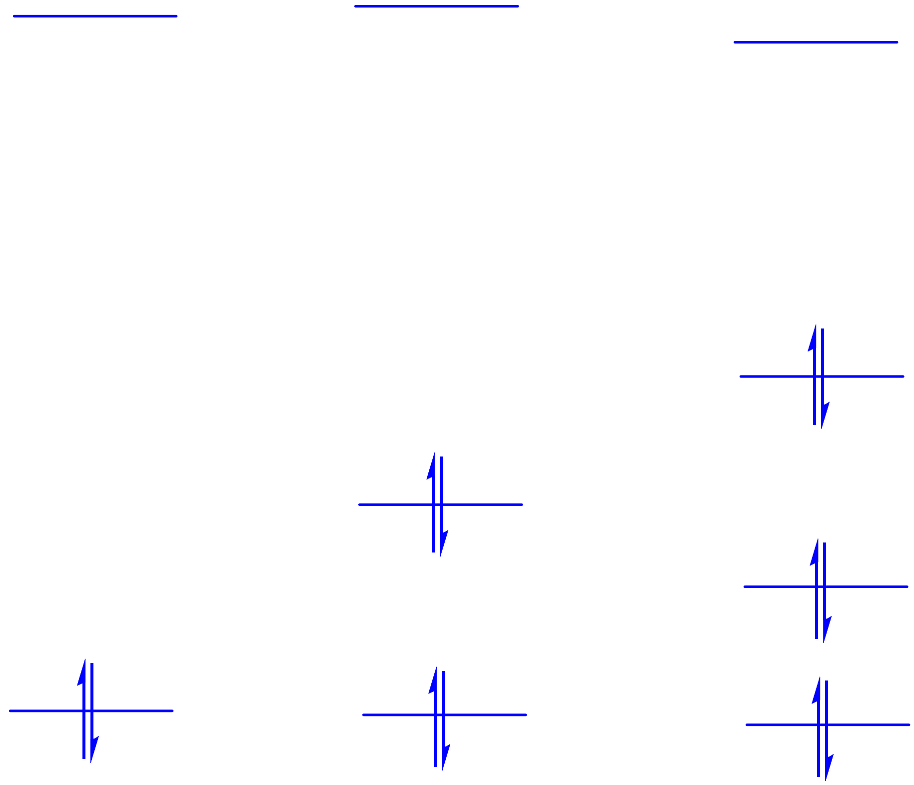
$$\frac{\Delta E_h}{\Delta E_e} = \frac{L_e^2(n_{e,h}^2 - n_{g,h}^2)}{L_h^2(n_{e,e}^2 - n_{g,e}^2)}$$

The ratio

$$\frac{\Delta E_b}{\Delta E_e} = \frac{L_e^2(n_{e,b}^2 - n_{g,b}^2)}{L_b^2(n_{e,e}^2 - n_{g,e}^2)} = \frac{2.89^2(3^2 - 2^2)}{5.78^2(2^2 - 1^2)} = 0.416$$

The $h^2/8m$ cancels. And likewise the ratio

$$\frac{\Delta E_h}{\Delta E_e} = \frac{L_e^2(n_{e,h}^2 - n_{g,h}^2)}{L_h^2(n_{e,e}^2 - n_{g,e}^2)} = \frac{2.89^2(4^2 - 3^2)}{8.67^2(2^2 - 1^2)} = 0.259$$



Ethene Butadiene Hexatriene