Free electron calculation of the energy levels of benzene

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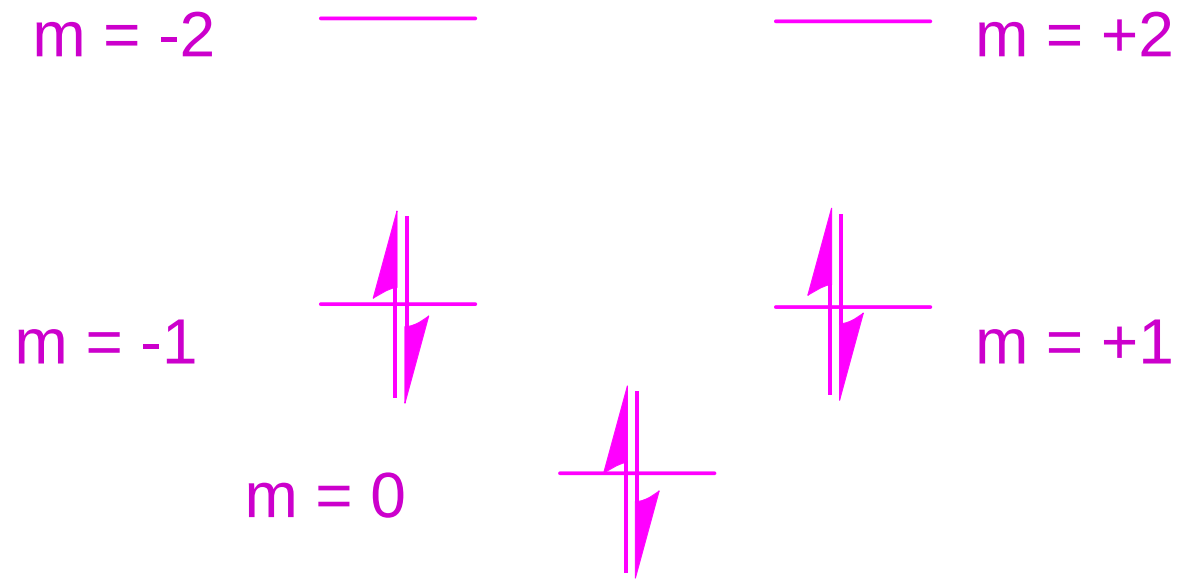
Solution: The energy level diagram in the free electron model is:



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Solution: The energy difference between the ground (g) and excited (e) states is given by:

$$\Delta E = \frac{h^2}{8\pi^2 m R^2}\left({m_e}^2 - {m_g}^2\right)$$

where $m_g = 1$ and $m_e = 2$.

$$\Delta\tilde{\nu} = \frac{\Delta E}{hc} = \frac{h}{8\pi^2 c m R^2}\left({m_e}^2 - {m_g}^2\right)$$

Free electron calculation of the energy levels of benzene

Use the free electron model to obtain the transition energies of benzene with a radius of 1.5 Å and 6 π electrons.

Solution: The energy factor in the particle on a circle model is

$$\frac{6.626\ x\ 10^{-34}}{8\pi^2(2.99\ x\ 10^{10})(9.11\ x\ 10^{-31})(1.5\ x\ 10^{-10})^2} = 13{,}700\ cm^{-1}$$

Therefore:

$$\Delta\tilde{\nu} = (13{,}700\ cm^{-1})(2^2 - 1^2)$$

and the wave number is:

$$\Delta\tilde{\nu} = 41{,}100\ cm^{-1}$$