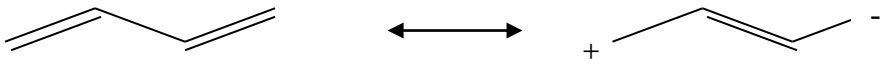
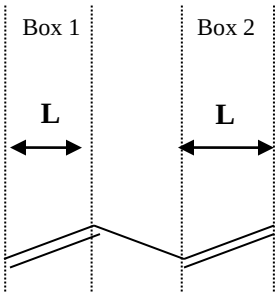
Let us try and understand the concept of resonance structures using the “particle-in-a-box”. Consider the molecule with the following Lewis dot structure. It has resonance structures as shown.



Case I: No delocalization

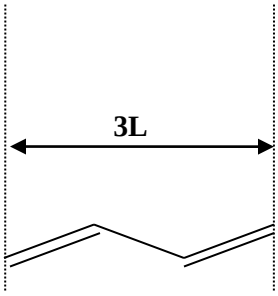
Let us now study this problem assuming that there can be no delocalization. That is no resonance. In this case the C=C and C-C will have different lengths.



In Box 1 we have two electrons and length of the box is indicated. Box 2 also contains two electrons. Using the expression for the energy in the particle in box obtain the total energy of the system of four electrons. Assume that the two electrons in Box 1 occupy the lowest energy state (n=1) and similarly for the two electrons in Box 2.

Case I: Delocalized electrons

Lets now study this problem assuming that there can be delocalization. That is the four electrons are “delocalized” along the complete molecular frame as indicated below. In this case the C=C and C-C will have the same length.



Now we have a single box and all four electrons are in that single box. The length of this larger box is three times the length of the boxes in the previous page (only approximately). Assume that the four electrons occupy the two lowest energy states in the box (n=1 and n=2), two electrons per state as before. Calculate the total energy for the system of four electrons.

Which of the two cases, Case I or Case II leads to a lower energy system?
Hence which system must be more stable?
Does this provide a rationalization for the concept of resonance and delocalization?