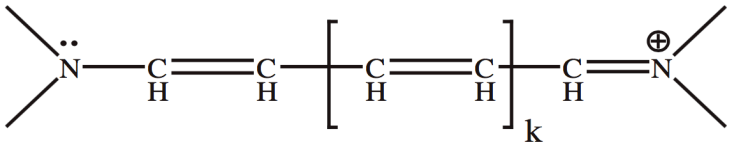
I. Considering the molecule given below



where $k = 0,1,2,3,4,...$ and a total of $m = 2k + 5$ atoms in the conjugated chain including the nitrogen atoms, whereas the hydrogen atoms are excluded, because they are not part of the conjugated network of bonds. Treat this molecular system as linear molecule. Answer the following questions by the application of quantum mechanical particle in a box (PIB) model.

1. How many electron pairs participate in the π-system of the molecule (when k=0)?

2. Is the number of π-electrons equals to the quantum number of the ground state HOMO? Provide your rationale.

3. Identify n_{HOMO} and HOMO – LUMO gap with increase of k. Show that ΔE is inversely proportional to length (L) of the molecule. Provide a schematic diagram (a graph) for this inverse relation between ΔE and L.

4. Would there be a value of k for which the molecule loses its HOMO-LUMO gap (aka the band gap)? Would that be metallic?

5. Can a metallic state be achieved for larger values of k? Provide your rationale.

6. Do you see a transition from molecule to a crystal for larger values of k? How would you justify that?

II. Construct molecular orbital energy level diagram for H_2O in its ground state using fragment molecular orbitals.

III. 3. Construct molecular orbital energy level diagrams for NH_3 when it is trigonal planar and pyramidal molecular arrangements. Notice the differences in the HOMO and LUMO levels in each case.

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