Solutions week 10

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- Q13.5 While the Lewis structure highlights the presence of lone pairs and suggests that bonding arises from increased electron density between atoms, we must remember that molecular orbitals (MOs) are generally delocalized, and electrons are indistinguishable. This means that bonding and lone pair electrons don't occupy distinct, localized spaces as the Lewis model suggests, and the sigma bond may well be delocalized. Thus, while the Lewis structure provides a helpful approximation of electron arrangement, it overlooks electron delocalization and indistinguishability, limiting its accuracy in quantum mechanical terms.

- Q13.10 Localized orbitals can't be represented in a molecular orbital (MO) energy diagram because MO theory inherently describes electrons as delocalized over the entire molecule, not confined to specific atoms or bonds. In MO theory, molecular orbitals are formed by linear combinations of atomic orbitals from all atoms in the molecule, resulting in orbitals that are spread across the molecule rather than restricted to individual bonds or lone pairs. An MO energy diagram displays these delocalized orbitals ranked by energy levels, but localized orbitals (like lone pairs in a Lewis structure) don't fit this framework, as they imply a certain degree of localization that MO theory does not inherently support. To describe localized orbitals, one would typically use Valence Bond (VB) theory or hybridization models, which focus on individual bonds and lone pairs, in contrast to the delocalized perspective of MO theory.

- Q13.8 Localized and delocalized models are equally valid because they yield the same wave function for closed-shell molecules, which determines all observable properties, such as energy and electron density. Since the wave function remains unchanged, experiments can't differentiate between the two models.

- Q13.15 No, the MO energy levels of a nonplanar cyclic polyene are not well described by the Hückel model. The Hückel model assumes a planar structure where p-orbitals overlap maximally to create delocalized π-bonding. In a nonplanar molecule, this overlap is reduced, disrupting the π-system's delocalization. Therefore, the Hückel model, which relies on idealized planar geometry for accurate π-orbital interaction, cannot accurately describe the MO energy levels in this case.