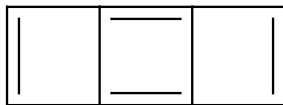
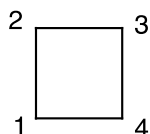


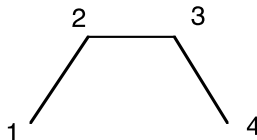
- (1) Determine the molecular orbital energies, the delocalization energy and the  $\pi$ -bond order for:



- (2) There are two limiting cases for the  $C_4$  carbocyclic system, cyclobutadiene (I) and butadiene (II).



I



II

For each structure

- Construct the SALC-MO expressions for the wavefunctions.
  - Calculate the energies of the molecular orbitals
  - Construct the molecular orbital diagram and calculate the delocalization energy.
  - Determine the  $\pi$  bond orders.
- (3) Consider the  $C_8H_8$  molecule in a hypothetical planar form with a point group of  $D_{8h}$ .

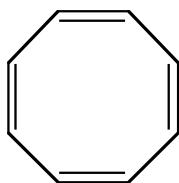


Table 7.1 on page 146 in Cotton summarizes the SALC-MO wavefunctions and the energies obtained from solutions of the secular determinant. Derive these results.