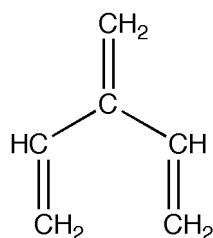


Revised exercise 10: Molecular orbital theory

Molecular orbital (MO) theory helps calculate the electron density around different atoms in a molecule, and thus allows the prediction of reactivity of various atoms within a molecule, as well as the degree of delocalization that occurs in the molecule. Moreover, MO theory calculations result in predictions of the energy levels of various molecular orbitals.

In this exercise, the molecule we will work with is 3-methylene-1,4-pentadiene.



1. How many **molecular orbitals** are possible for the π system of this molecule? What is an easy way to tell how many MOs there will be?

2. The table below shows the calculated electron densities of the different MOs (the values were obtained by using the Huckel method of electron density calculation). The various C columns represent the electron density near that particular carbon; negative values mean the “-” lobe of the wavefunction. The first five carbons (C_1 to C_5) are the pentadiene part; C_6 represents the methylene carbon.

Wavefunction number	C_1	C_2	C_3	C_4	C_5	C_6
1	0.230	0.444	0.628	0.444	0.230	0.325
2	0.500	0.500	0	-0.500	-0.500	0
3	0.444	0.230	-0.325	0.230	0.444	-0.628
4	-0.444	0.230	0.325	0.230	-0.444	-0.628
5	0.500	-0.500	0	0.500	-0.500	0
6	0.230	-0.444	0.628	-0.444	0.230	-0.325

What do the **zeroes** of electron density represent?

In wavefunction 6, what occurs between carbon 1 and carbon 2 to the wavefunction?

3. Draw **schematic views of the different molecular orbitals**, using the densities in the table above as a guide. Clearly label each drawing with the wavefunction number (use the table above) it represents.

4. Using the answer to question 2 as a guide, draw the **energy level diagram** for the MOs. Add the correct number of electrons to the diagram as needed and indicate the HOMO and LUMO levels.