CHEMISTRY 3BB3 1999/2000

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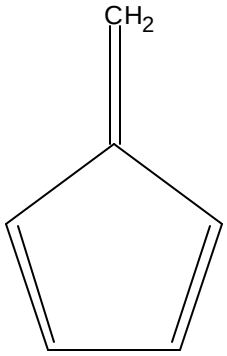
ASSIGNMENT 4

DUE: February 17, 2000



1. The structure is of the molecule fulvene. Construct the determinant for a Hückel calculation for this molecule.

2. The determinant reduces to the secular equation

$$x^6 - 6x^4 + 8x^2 + 2x - 1 = 0$$

where $x = (\alpha - E)/\beta$. Calculate the six roots of this equation to 3 decimal places. One way to do this is to plot the function on a spreadsheet, and look for the x values at which the function is zero.

3. The coefficients for the molecular orbitals are given below. Carbon 6 is the CH_2 carbon, and it is attached to carbon 5.

	C1	C2	C3	C4	C5	C6
a	-0.439	0.153	0.153	-0.439	0.664	-0.356
b	0.601	0.372	-0.372	-0.601	0	0
c	0.429	0.385	0.385	0.429	0.523	0.247
d	-0.350	0.279	0.279	-0.350	-0.190	0.749
e	0	0.5	0.5	0	-0.5	-0.5
f	-0.372	0.601	-0.601	0.372	0	0

Associate each of these MO's with an energy from question 2, and explain your reasoning.

4. Calculate the bond order for each bond, if there are two electrons in each of the three lowest energy MO's.