1. In this problem, the molecular orbital model will be applied to understand the $\pi^* \leftarrow \pi$ absorption of phenylalanine. The absorption will be considered in the context of Overhead 73 with the lower energy state as the right-side, second-row from the bottom orbital and the higher energy state as the left-side, third-row from the bottom orbital. The atomic $p_z$ orbitals are denoted $|p_1\rangle, \ldots, |p_6\rangle$ with $|p_1\rangle$ on the C atom on the bottom of the ring and clockwise numbering of $|p_1\rangle, \ldots, |p_6\rangle$. Consider $\langle p_j | p_j \rangle = 1$ and $\langle p_j | p_k \rangle = 0$ for $j \neq k$. Consider the Hamiltonian $H$ with $\langle p_j | H | p_j \rangle = \alpha$, $\langle p_j | H | p_k \rangle = \beta$ if $C_j$ and $C_k$ are directly bonded, and $\langle p_j | H | p_k \rangle = 0$ if $C_j$ and $C_k$ are not directly bonded. The $\alpha$ and $\beta$ each correspond to a specific energy value and both $\alpha$ and $\beta$ are negative.

a. (30 points) Use Overhead 73 to determine the normalized molecular orbital for the initial state of the transition in terms of $|p_1\rangle, \ldots, |p_6\rangle$. Use Overhead 73 to determine the normalized molecular orbital for the final state of the transition in terms of $|p_1\rangle, \ldots, |p_6\rangle$.

b. (40 points) Evaluate the average total energy of the initial state where your answer is in terms of $\alpha$ and $\beta$. Evaluate the average total energy of the final state where your answer is in terms of $\alpha$ and $\beta$.

c. (10 points) Use the b result to determine the transition energy in terms of $\alpha$ and $\beta$.

d. (20 points) Use Overhead 35 to determine the experimental $\pi^* \leftarrow \pi$ transition energy of phenylalanine to three significant figures in units of kJ/mole.

e. (10 points) Use the c and d results to determine $\beta$ to three significant figures in units of kJ/mole.

f. (20 points) One way of understanding the $\pi^* \leftarrow \pi$ transition is conversion of a specific number of double C=C bonds in the aromatic ring to single C-C bonds. Use Overhead 73 to determine this specific number and explain your determination.

g. (20 points) Provide the literature energy of a C=C bond to three significant figures in units of kJ/mole. Provide the literature energy of a C-C bond to three significant figures in units of kJ/mole. Provide the reference(s) for these literature values. Use these values in the f model to estimate the $\pi^* \leftarrow \pi$ transition energy to three significant figures in units of kJ/mole.

h. (10 points) Are the d and g values in semi-quantitative agreement or are they not in semi-quantitative agreement? Provide a reasoned explanation for your choice.