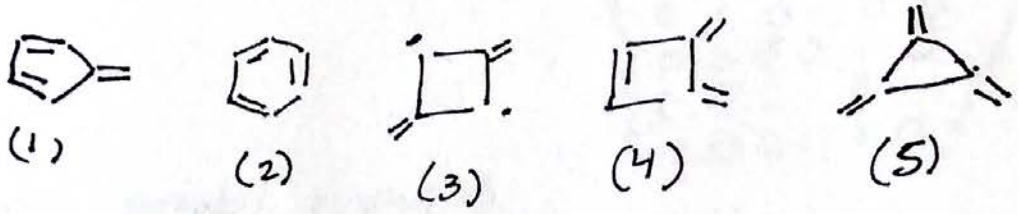
1. 

(1) $\alpha + 2.11\beta,\ \alpha+\beta,\ \alpha + 0.62\beta$

$E(I) = 2(\alpha + 2.11\beta) + 2(\alpha+\beta) + 2(\alpha + 0.62\beta)$

$E(I) = 6\alpha + 7.46\beta$

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(2) $\alpha + 2\beta,\ \alpha+\beta,\ \alpha+\beta$

$E(II) = 2(\alpha+2\beta) + 4(\alpha+\beta) = 6\alpha + 8.00\beta$

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(3) $\alpha + 2.24\beta,\ \alpha+\beta,\ \alpha$

$E(III) = 2(\alpha+2.24\beta) + 2(\alpha+\beta) + 2\alpha = 6\alpha + 6.48\beta$

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(4) $\alpha + 2.25\beta,\ \alpha+0.80\beta,\ \alpha + 0.56\beta$

$E(IV) = 2(\alpha+2.25\beta) + 2(\alpha+0.80\beta) + 2(\alpha+0.56\beta)$

$E(IV) = 6\alpha + 7.22\beta$

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(5) $\alpha + 2.41\beta,\ \alpha+0.62\beta,\ \alpha+0.62\beta$

$E(V) = 2(\alpha+2.41\beta) + 4(\alpha+0.62\beta) = 6\alpha + 7.30\beta$

$E(II) < E(I) < E(V) < E(IV) < E(III)$

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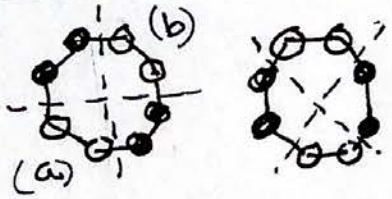
2. 

If the 4 atoms in the (a) and (b) regions are "folded" out of the plane, the orbital on the left goes down energy while that on the right goes up in energy. Placing the "last" two electrons in the orbital on the left thus favors a buckled structure.

. For Pyridine $H = \begin{pmatrix} 0.5 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$

The orbital energies are:

$\alpha + 2.11\beta$, $\alpha + 1.12\beta$, $\alpha + \beta$, $\alpha - 0.84\beta$, $\alpha - \beta$, $\alpha - 1.93\beta$

So the degeneracies present in benzene are removed.