Points:  
1 / 11 /  
2 / 12 /  
3 / 10 /  
4 / 10 /  
5 / 15 /  
6 / 10 /  
7 / 12 /  
8 / 10 /  
9 / 10 /  
Total: 100 points /
1) Why is naphtalene colourless but its isomer, azulene, blue? Also, why are tomatoes red? (Use frontier orbitals for your argument)
2) Determine the point group symmetries for each molecule:

a) \( S_{12} \)

b) trans-butadiene

c) 

d) 

3) Consult the literature to find discussions of the aromaticity or antiaromaticity of the following structures: tropylium ion, cyclopentadienyl cation, COT dianion. What do these articles indicate about our generalizations of aromatic character?

4) Cyclopropanone has a higher dipole moment than would be expected on the basis of the carbonyl group alone. Rationalize this higher dipole moment. How does resonance theory explain the polarity?
The six coordinate ions IF$_6^-$ and XeOF$_5^-$ are isoelectronic, but they adopt two very different structures. Each structure may be thought of as derived from seven-coordinated geometries. The two most common seven-coordinated geometries are the capped octahedron and the pentagonal bipyramid, shown below:

a) The structure of IF$_6^-$ is derived from the capped octahedron, with a lone pair occupying the face-capping position. What is the point group symmetry of IF$_6^-$?

b) The structure of XeOF$_5^-$, on the other hand, adopts the geometry having the highest possible symmetry derived from the pentagonal bipyramid. Draw this ion and assign its point group symmetry.

c) Why might XeOF$_5^-$ have a different structure than the fluorine containing anion IF$_6^-$?
6) Both experimental and theoretical studies indicate that the C1-C2 bond length (l) and the C1-C2-C3 bond angle (α) in molecules having the following general structure:

![Diagram of molecule structure with C1, C2, C3, and C3' connected by bonds](image)

are strongly correlated. One study found that they could be related by the equation:

\[ l = 2.0822 - 0.0049 \alpha \]

where distances are in Angstrom and angles are in degrees.

a) What does this equation indicate about the change in bond length expected when the adjacent angle changes to a value greater or less than 109.5 degree?

b) Rationalize the form of the equation in terms of the concept of variable hybridization and in terms of the VESPR theory.
7) Draw a CLEAR Three-dimensional representation of the following compounds:

a) 2E,4E,6R,10R-4,6,10,12-tetramethyl-2,4-tridecadien-7-one

b) S-3-butene-1,2-diol

c) 3R,4S-3-bromo-4-chloro-3-methylhexane

d) Z,Z-deca-3,7-diene-1,5,9-triyne

e) R-(\text{-})(4-methylcyclohexylidene)acetic acid

f) (2S,3S)octane-2,3-diol (a pheromone of the grape borer (Xylotrechus pyrrhoderus))
8) Construct a qualitative orbital model for twisted ethylene, in which the two CH₂ groups lie in mutually perpendicular planes. Why does the molecule prefer coplanarity?

9) cis-3,7-Dimethyl-1,5-cyclooctanedione underwent two successive Baeyer-Villager rearrangements to give two products, both with the molecular formula C₁₀H₁₆O₄. When one of these products was reduced with LiAlH₄, two achiral diols were obtained. When the other was reduced, the single product was a chiral diol (obtained as racemic mixture). What are the structures of the final products?