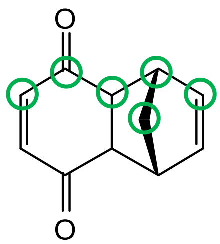
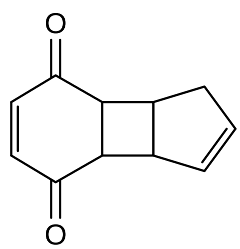
Chemistry 4361/8361 Monday, October 8

In-Class Exercise Solutions:
DEPT-90 and DEPT-135

a. Right off the bat, you know that neither of the molecules I've drawn can be the right product based on the number of equivalent carbons each has, compared to the 5 peaks in the ^{13}C NMR.

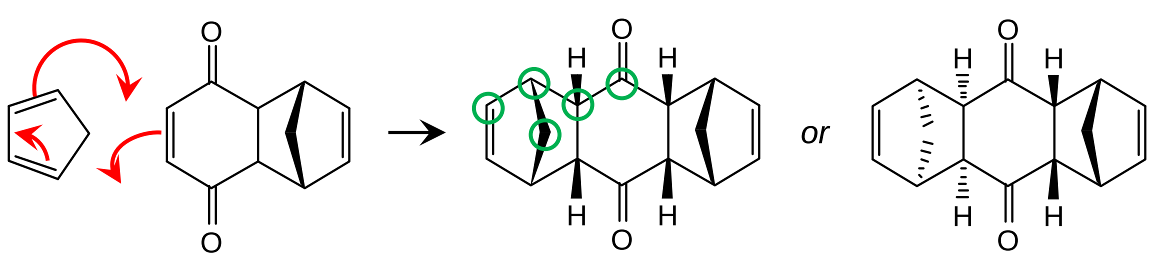


6 inequivalent carbons



molecule is asymmetric, so all 11 carbons are inequivalent

That means our product must come from subsequent reaction of one of these molecules. The [4+2] (Diels-Alder) reaction works well because the quinone double bond—the "dienophile"—is activated by the electron-withdrawing carbonyls. The other half of the quinone molecule is still activated after the first reaction, and can undergo a second Diels-Alder:



Of the two products above, the second one seems more likely based on sterics; if the first diene approached quinone from the bottom face, that would leave more room on the top face for the second diene to add. But we can't distinguish these molecules with the NMR information we have.

Both do have the right number of carbons though, and the right types—one carbonyl, one alkene, and three alkyl. We can also use the DEPT spectra to confirm this. The carbonyl peak doesn't appear in either DEPT-135 or DEPT-90, so it has no attached H's, which makes sense. The alkene carbon and two of the alkyl carbons appear in both DEPT-135 and DEPT-90, so they must be CH. And one of the alkyl carbons appears as a negative peak in DEPT-135, so it must be a CH_2. All of these make sense in terms of the products above.

b.