3) Hybridization and Molecular Orbital Model

The following compound is added to margarine to make it taste more like butter. Identify an **incorrect** statement about this structure.

1) All carbons and oxygens lie in the same plane

2) There is one $\pi$ molecular orbital and one $\pi^*$ molecular orbital in this molecule

3) The two CH$_3$ groups have tetrahedral geometry

4) There is at least one sp$^2$ hybridized carbon in this molecule

5) There are no sp hybridized atoms in this molecule

This question was based on Practice question 14.17 but it escaped my attention that the solutions manual misleadingly states that “the six atoms are not in the same plane because of free rotation around the central C-C bond” (pg. 461 in the guide). I am aware that some of you picked answer A) either because you had done the problem or went over this discussion in CLAS. **You should get full credit if you answered 1) in this problem.**

So, are these atoms in the same plane or not? The answer depends on if you adopt a static or dynamic view on the structure of molecules. **In the static view**, which we have discussed so far, a molecule adopts the minimum energy geometry. The minimum energy geometry is determined by VSEPR rules, hybridization, MO considerations, and interactions between parts of the molecule. In this case, hybridization tells that each of the C=O carbons is planar but it does not tell us what the dihedral angle O=C–C=O is. We need to think in terms of the interactions between groups. Recall that each C=O is a dipole, and the energy is lowest if the dipoles align antiparallel. This logic tells us that the lowest energy structure is planar as shown on the right. Any structure where the six atoms are not in the plane has less favorable alignment of dipoles, and thus higher energy.

Molecules are not static. Even at absolute zero, atoms move. Bonds vibrate and bend, and groups of atoms may rotate around single bonds. **In the dynamic view**, we also consider these structures as contributing to the structure of the molecule, especially at higher temperatures. For example, the normally pyramidal trigonal NH$_3$ molecules occasionally adopt a planar trigonal geometry that lasts for a fraction of a picosecond. The bending vibration in CO$_2$ makes few structures bent, and few formaldehyde (CH$_2$=O) molecules adopt structures that are not perfectly planar. In the case of biacetyl, there is some rotation around the single C-C bond, and at any moment, few molecules adopt geometries where the six atoms are not in the same plane. However, both the experiment$^1$ and calculations$^2$ show that the barrier for the rotation in biacetyl is rather high, and it is incorrect to say that there is a free rotation around the C–C bond. A correct statement would be that the rotation around C-C bond in biacetyl is strongly hindered. You will learn more about the dynamic view in your upper-level courses.