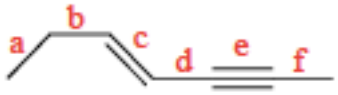
CHE 2060: Homework set 2 – KEY

Note: In questions involving drawing resonance contributors, assume that all second-row atoms should have a complete octet in all structures with the exception of positively charged carbons.

2.1: Covalent bonding in organic molecules

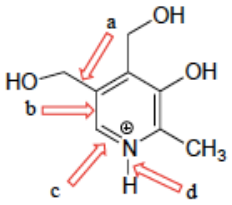
1. Rank the bonds a-f below according to increasing bond length.



Longest: a > b > d, f > c > e

2. For each of the bonds indicated by arrows b-f in the figures below, describe the bonding picture. An example is given for bond 'c'.
Note that for a double bond (bond 'c'), you will need to describe two bonds.
Note: you are being asked to describe the bonding picture for one specific resonance contributor.

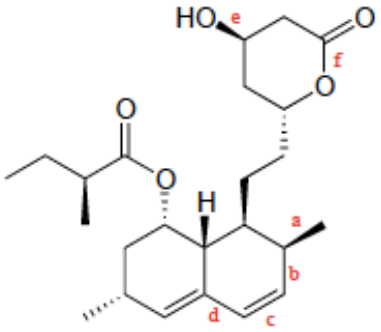
bond a: "this is a π bond formed by the overlap of an sp^3 orbital on one carbon and an sp^2 orbital on another carbon."



pyridoxine
(vitamin B_6)

(a) this is a σ bond formed by the overlap of an sp3 orbital on one carbon and an sp2 orbital on another carbon.
(b) this is a σ bond formed by the overlap of an sp2 orbital on one carbon and an sp2 orbital on another carbon.
(c) this is a σ bond formed by the overlap of an sp2 orbital on a carbon and an sp2 orbital on a nitrogen, combined with a π bond formed by the overlap of a 2p orbital on a carbon and a 2p orbital on a nitrogen.
(d) This is a σ bond formed by the overlap of an sp2 orbital on a nitrogen and a 1s orbital on a hydrogen.

3. Below is the structure of the cholesterol-lowering drug Lovastatin. For bonds a, b, c, and d: (1) Describe hybridization of the atoms in the bond; and (2) predict the trend in bond length.



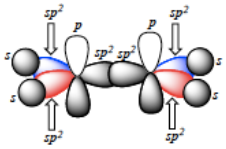
Lovastatin

Bond	atoms	hybridization	Length (pm)	ranking
a	C - C	σ, sp3 – sp3	154	longest
b	C – C	σ, sp2 – sp3	< 154	
d	C – C	o, sp2 – sp2	<< 154	
e	O – C	σ, sp3 – sp3	143	
f	C - O	σ, sp2 – sp3	< 143	
c	C = C	π, p - p	134	shortest

4. Draw a 3D-accurate picture showing the orbitals involved in bonding for dimethyl ether (CH_3OCH_3).

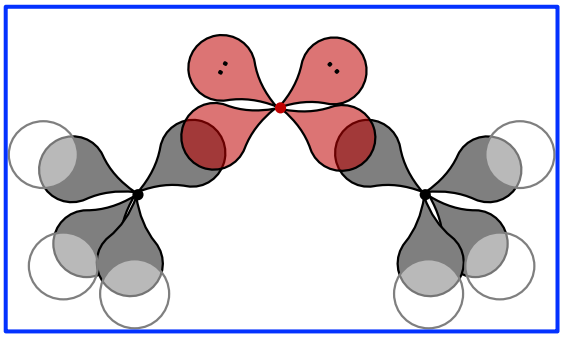
- Draw all bonds, both σ and π, as overlapping orbitals.
- Indicate whether each orbital is s, p, sp, sp^2, or sp^3, and indicate (with words or a color scheme) orbitals that are pointed into or out of the plane of the page.
- Locate all lone pairs in their appropriate orbitals.

An example is provided for ethene, CH_2CH_2:

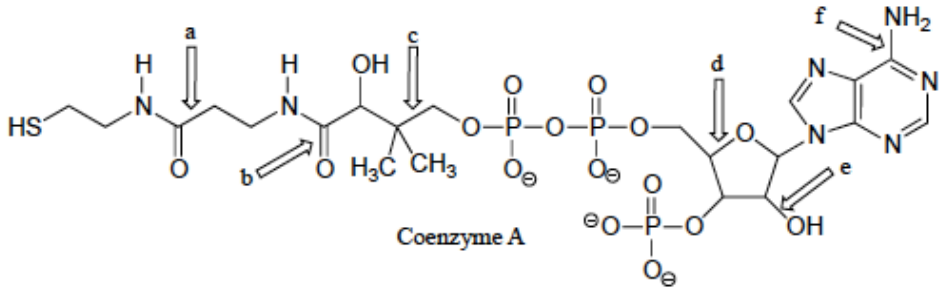


blue orbitals pointing into page
red orbitals pointing out of page

orbital overlap in ethene



5. For the bonds labeled a-f below, describe the orbitals involved in the bonds indicated by the arrows.



(a) This is a σ bond formed by the overlap of an sp2 orbital on one carbon and an sp3 orbital on another carbon.
(b) This is a σ bond formed by the overlap of an sp2 orbital on a carbon and an sp2 orbital on an oxygen, combined with a π bond formed by the overlap of a 2p orbital on a carbon and a 2p orbital on an oxygen.
(c) This is a σ bond formed by the overlap of an sp3 orbital on a carbon and an sp3 orbital on another carbon.
(d) This is a σ bond formed by the overlap of an sp3 orbital on a carbon and an sp3 orbital on an oxygen.
(e) This is a σ bond formed by the overlap of an sp3 orbital on a carbon and an sp3 orbital on an oxygen.
(f) This is a σ bond formed by the overlap of an sp2 orbital on a carbon and an sp3 orbital on a nitrogen.