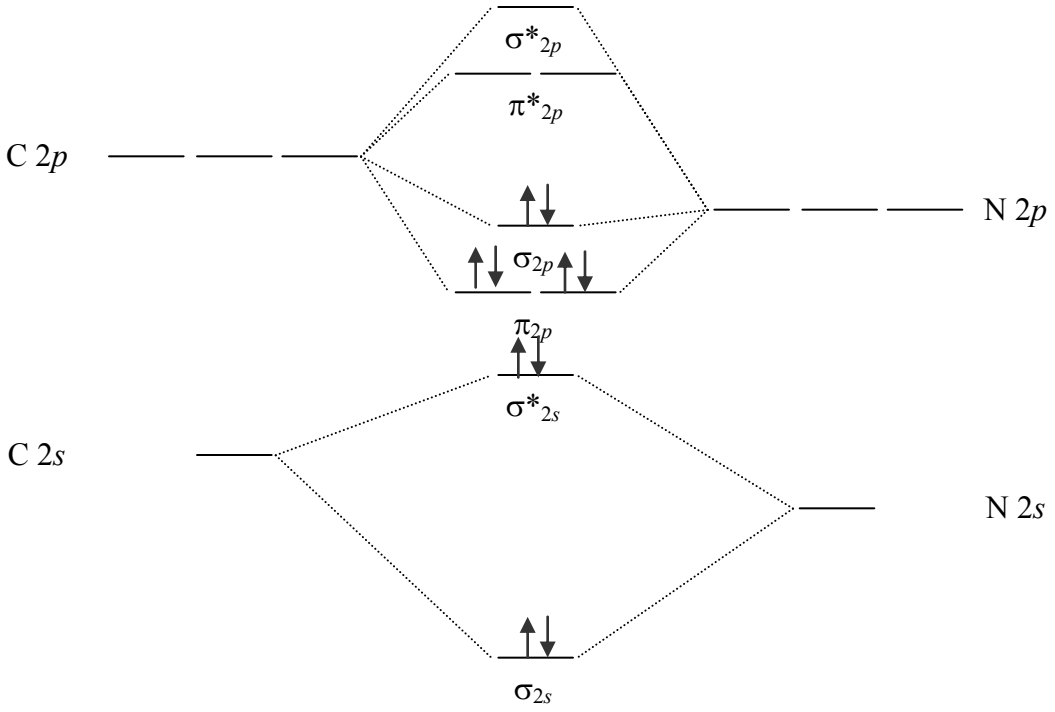
**Discussion – 12/13/10**
**MOs and Hybridization**

1. a.

[:C≡ N:]$^-$ Bond order = (8 – 2) / 2 = 3




CN-

b. Comparison of Lewis and MO models of CN-

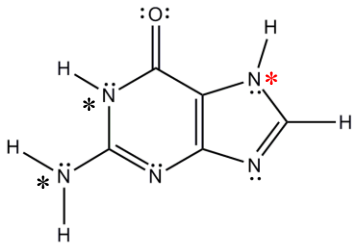
CN- Consistent: Both have triple bond (B.O. = 3)

Inconsistent: - Lewis structure shows lone pairs on each atom rather than all e- being shared (MO)

- Lewis structure indicates a negative formal charge on C, whereas MO suggests more electron density on N, which is consistent with EN considerations

c. Both molecules exhibit sp mixing, and the MOs should reflect this. In $N_2$, the molecular orbitals would be distributed equally between the two N atoms, whereas in CN-, the bonding orbitals have greater electron density on the more electronegative atom (N). The antibonding orbitals have more electron density on the less electronegative atom (C).

2. a. Completed structure of guanine (carbons at each intersection are implied):

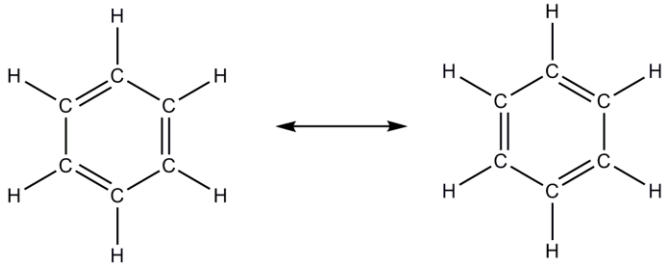


b. 17 sigma bonds; 4 pi bonds.

c. All carbons are $sp^2$ hybridized; trigonal planar; with 120˚ bond angles.

d. We predict that the three N's marked with * are $sp^3$ hybridized, with 109.5˚ bond angles. The remaining N atoms are $sp^2$ hybridized, with 120˚ bond angles.

e. i. Benzene:



ii. For the structure drawn in (a), the bond angles in the six membered ring would be expected to be 120˚ for each atom except for the N§, which is predicted to have bond angles of 109.5˚. However, it is not possible to form a planar six-membered ring unless ALL the angles are 120˚. But, if the bond angles really are 109.5˚, we would not expect the H bonded to the N§ to lie in the plane of the ring.

iii. The observation that that all the bond angles in the ring are 120° and the six atoms in the ring and the H bonded to the N§ ARE in a plane implies all the atoms in the ring are sp2 hybridized (trigonal planar). The resonance structures below are consistent with this geometry. The implication of this result is that the lone pair on the N§ in guanine occupies an unhybridized p orbital so that it can participate in delocalized π bonding with other atoms in the ring, thereby lowering the energy of the molecule.