

Laude's CH301 Worksheet 7: VB and MO

1. Use valence-bond theory to predict the hybridization and other properties of these compounds

Cmpd	Lewis structure	Hybridization of central atom	# of σ bonds	# of π bonds	Atomic orbits that form the σ and π bonds: Example: σ_{sp^2-1s}
CH ₄	H : C : H H	sp ³	4	0	σ_{sp^3-1s}
N ₂	: N : : N : :	sp	1	2	σ_{sp-sp} π_{2p-2p}
CO ₂	: O : : C : : O :	sp	2	2	σ_{sp-2p} π_{2p-2p}
NH ₃	H : : N : H H	sp ³	3	0	σ_{sp^3-1s}
C ₂ H ₂	H : C : : C : H	sp	3	1	σ_{sp-1s} σ_{sp-sp} π_{2p-2p}
SF ₆	: F : : S : : F :	sp ³ d ²	6	0	$\sigma_{sp^3d^2-2p}$
NH ₂ ⁻	: : N : H	sp ³	2	0	σ_{sp^3-1s}

2. Build these compound using molecular orbital theory and predict

Compound	MO building			Bond order	Para or dia-magnetic?
Li ₂	Li 2s ² 1		Li 2s ² 1	1	dia
N ₂	N 2p ³ 1 1 1		N 2p ³ 1 1 1	3	dia

O_2	<p>Detailed description: This diagram shows the atomic orbitals (AOs) of two oxygen atoms (O) forming a molecule. Each oxygen atom has a 2s orbital containing a pair of electrons ($\uparrow\downarrow$) and two 2p orbitals. The 2p orbitals each contain four electrons: one pair in a bonding orbital above the molecular plane ($\uparrow\uparrow$), one pair in a bonding orbital below the plane ($\downarrow\downarrow$), and one pair in a non-bonding orbital above the plane ($\uparrow\downarrow$). The overlap of the bonding AOs results in a bonding molecular orbital ($\uparrow\uparrow$) and a antibonding molecular orbital ($\downarrow\downarrow$). The overlap of the non-bonding AOs results in two non-bonding molecular orbitals, one above the plane ($\uparrow\downarrow$) and one below the plane ($\uparrow\downarrow$).</p>	2	para
O_2^{2-}	<p>Detailed description: This diagram shows the atomic orbitals (AOs) of two oxygen atoms (O-) forming a molecule. Each oxygen atom has a 2s orbital containing a pair of electrons ($\uparrow\downarrow$) and two 2p orbitals. The 2p orbitals each contain four electrons: one pair in a bonding orbital above the plane ($\uparrow\uparrow$), one pair in a bonding orbital below the plane ($\downarrow\downarrow$), and one pair in a non-bonding orbital above the plane ($\uparrow\downarrow$). The overlap of the bonding AOs results in a bonding molecular orbital ($\uparrow\uparrow$) and a antibonding molecular orbital ($\downarrow\downarrow$). The overlap of the non-bonding AOs results in two non-bonding molecular orbitals, one above the plane ($\uparrow\downarrow$) and one below the plane ($\uparrow\downarrow$).</p>	1	dia
F_2	<p>Detailed description: This diagram shows the atomic orbitals (AOs) of two fluorine atoms (F) forming a molecule. Each fluorine atom has a 2s orbital containing a pair of electrons ($\uparrow\downarrow$) and two 2p orbitals. The 2p orbitals each contain four electrons: one pair in a bonding orbital above the plane ($\uparrow\uparrow$), one pair in a bonding orbital below the plane ($\downarrow\downarrow$), and one pair in a non-bonding orbital above the plane ($\uparrow\downarrow$). The overlap of the bonding AOs results in a bonding molecular orbital ($\uparrow\uparrow$) and a antibonding molecular orbital ($\downarrow\downarrow$). The overlap of the non-bonding AOs results in two non-bonding molecular orbitals, one above the plane ($\uparrow\downarrow$) and one below the plane ($\uparrow\downarrow$).</p>	1	dia
CN^-	<p>Detailed description: This diagram shows the atomic orbitals (AOs) of a carbon atom (C) and a nitrogen atom (N-) forming a molecule. The carbon atom has a 2s orbital containing a pair of electrons ($\uparrow\downarrow$) and two 2p orbitals. The 2p orbitals each contain four electrons: one pair in a bonding orbital above the plane ($\uparrow\uparrow$), one pair in a bonding orbital below the plane ($\downarrow\downarrow$), and one pair in a non-bonding orbital above the plane ($\uparrow\downarrow$). The overlap of the bonding AOs results in a bonding molecular orbital ($\uparrow\uparrow$) and a antibonding molecular orbital ($\downarrow\downarrow$). The overlap of the non-bonding AOs results in two non-bonding molecular orbitals, one above the plane ($\uparrow\downarrow$) and one below the plane ($\uparrow\downarrow$).</p>	3	dia

note: *S-orbitals filled, not shown*

3. Rank the bond energy and bond length for the 6 compounds in problem 2 based on bond order

Increasing bond length: $N_2 = CN^- < O_2 < Li_2 = O_2^{2-} = F_2$

Increasing bond energy: $Li_2 = O_2^{2-} = F_2 < O_2 < N_2 = CN^-$