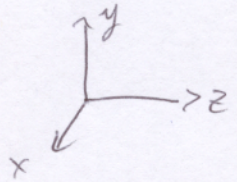
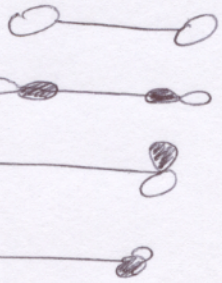
Ch.5 - Exercise 5.7 - Draw an MO Diagram for N_3^-

$:\ddot{N}=\overset{\oplus}{N}=\ddot{N}:^{\ominus}$ $\quad D_{\infty h} \xrightarrow{\text{descend in symmetry}} D_{2h}$

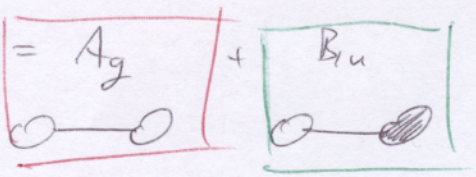


D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$
Γ_{2s}	2	2	0	0	0	0	2	2
Γ_{2p_z}	2	2	0	0	0	0	2	2
Γ_{2p_y}	2	-2	0	0	0	0	-2	2
Γ_{2p_x}	2	-2	0	0	0	0	2	-2

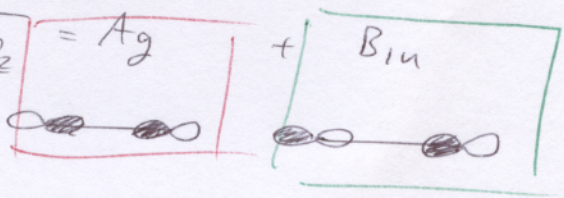


Outer Atoms => formed by reducing the reducible representations

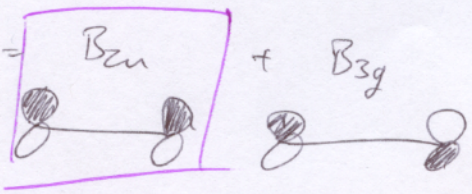
$\Gamma_{2s} = A_g + B_{1u}$



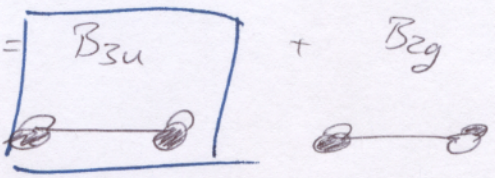
$\Gamma_{2p_z} = A_g + B_{1u}$



$\Gamma_{2p_y} = B_{2u} + B_{3g}$



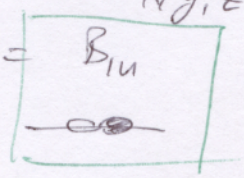
$\Gamma_{2p_x} = B_{3u} + B_{2g}$



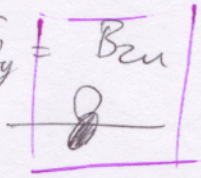
Central Atom => easy to tell symmetries of central atom by looking at the irreducible representations with x, y, z symmetries.

$\Gamma_{2s} = A_g$

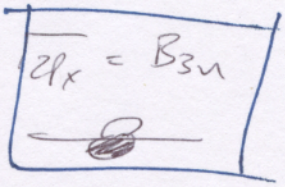
$\Gamma_{2p_z} = B_{1u}$



$\Gamma_{2p_y} = B_{2u}$



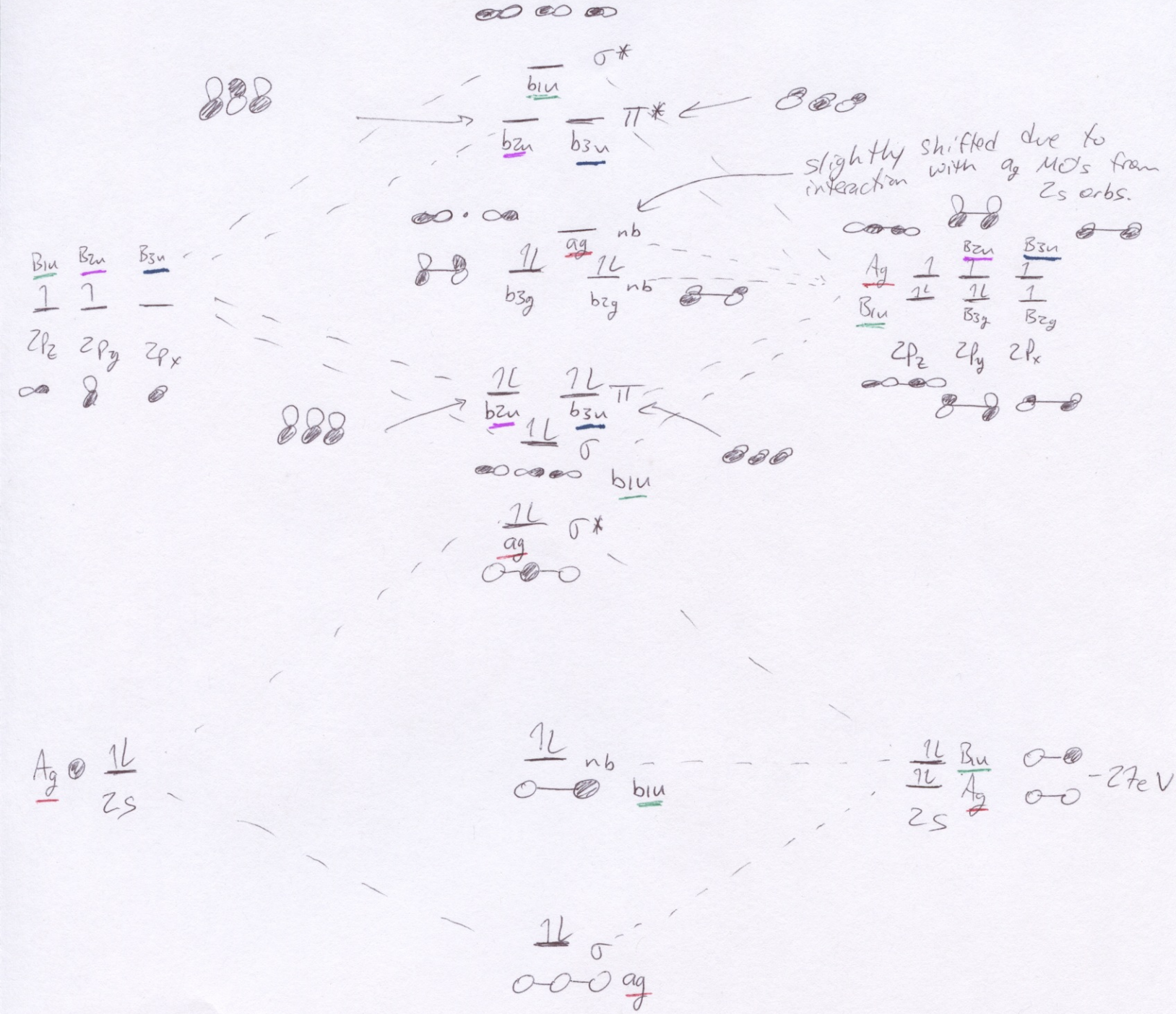
$\Gamma_{2p_x} = B_{3u}$



↳ $2p_N = -13 eV$ => 2p's will interact with each other

↳ $2s_N = -27 eV$ => 2s's will interact with each other.

↳ 2s's and 2p's will have minimal interaction.



$N^{\oplus}$ $\quad :\ddot{N}=N=\ddot{N}:^{-}$ $\quad {}^{\ominus}N\cdots N^{\ominus}$

↳ 2 σ bonds
↳ 2 π bonds
↳ 3 lone pairs

} Doesn't fully match our Lewis Dot Structure. ~~One lone pair is likely delocalized~~
One pair of electrons from our structure is probably delocalized between all 3 N's