Phy 491 - Hw 4

Oxygen - the homework assignment

4.1.1 Find the electron configuration of atomic oxygen in its ground state. (2 Points)

O: $1s^2 2s^2 2p^4$

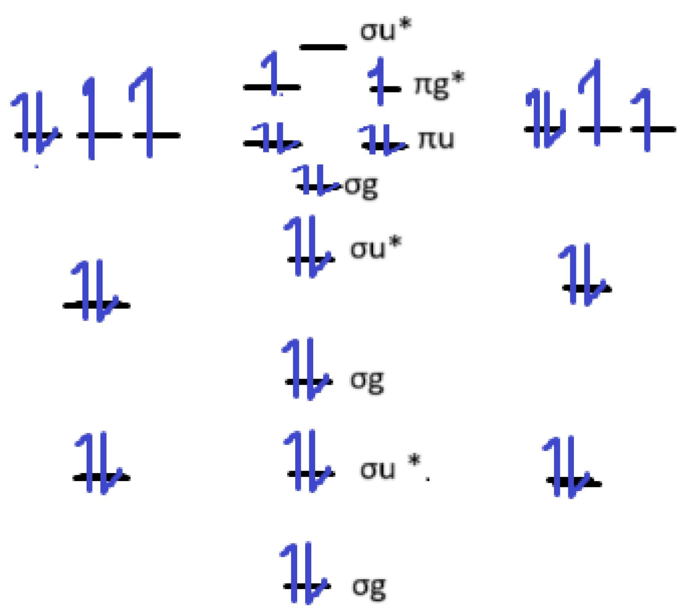
4.1.2 Write down the corresponding spectroscopic notation of the atomic oxygen ground state. (1 Points)

Spectroscopic notation: ${}^{2s+1}L_J$. Not to be confused with Molecular term symbols ${}^{2S+1}\Lambda_{g,u}$

$\sum s = 1/2 + 1/2 = 1 \to 2s + 1 = 3$
$\sum l = 1 \to S$ - hund's rule #2
More than half full: $J = L + S = 2$

Result: ${}^3S_2$

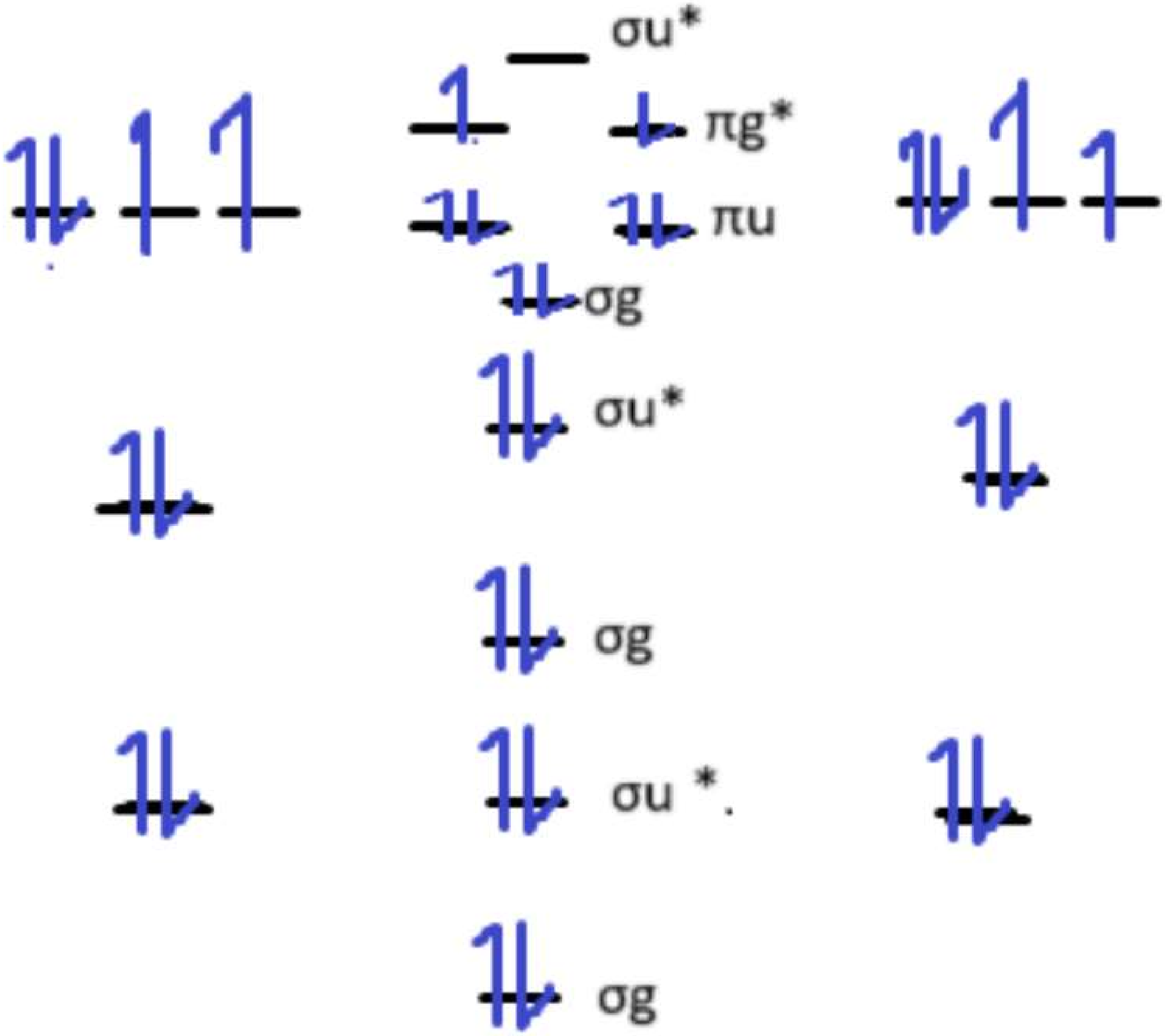
4.1.3 Oxygen in our atmosphere is commonly found in the form of O_2 gas, a dioxygen molecule. Using the LCAO approach, sketch its molecular orbital diagram and argue why it is a stable molecule. (5 Points)

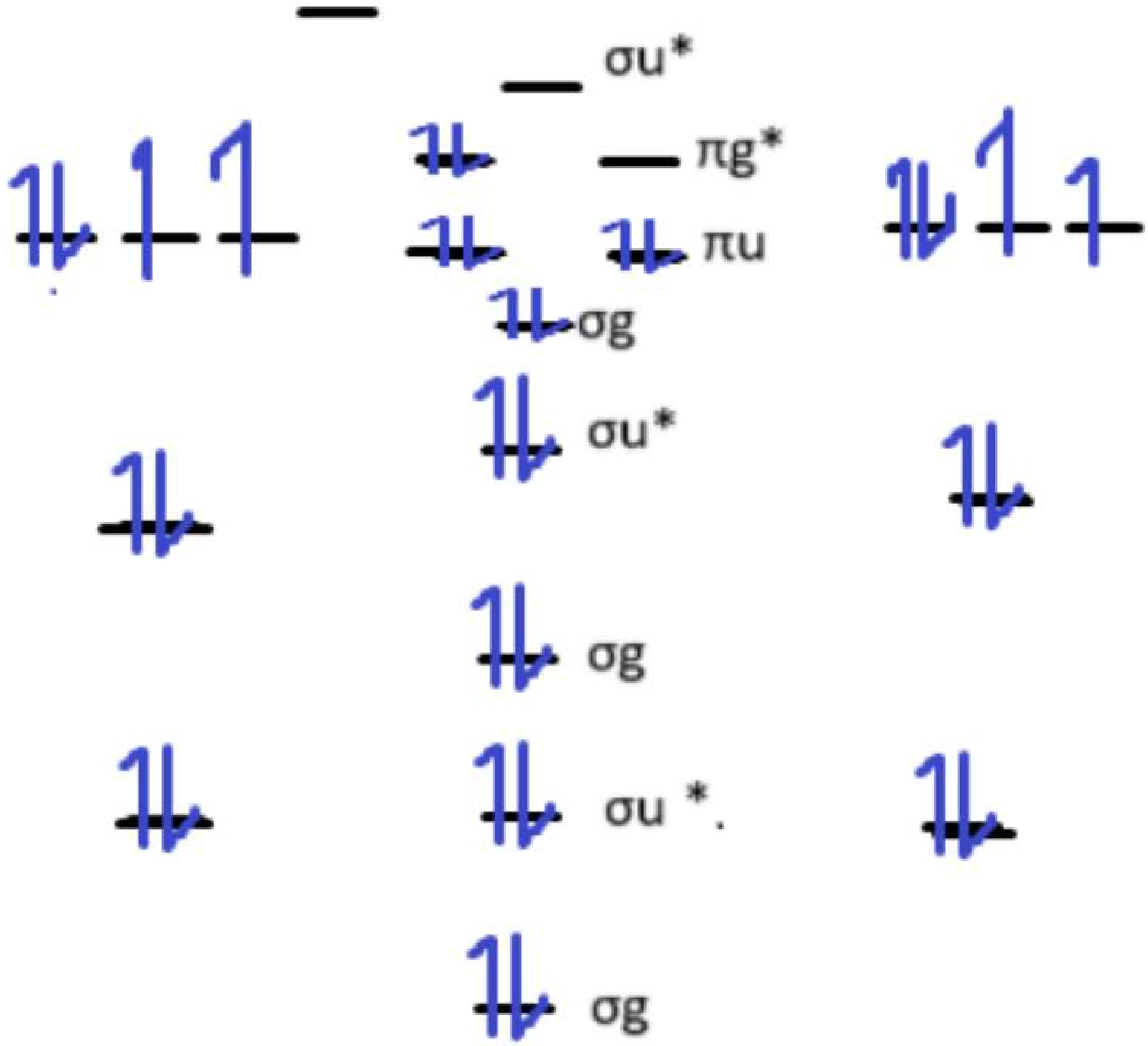


Bonding: 10
Antibonding: 8
Stability: $B = \frac{10-8}{2} = 1$

Since $B > 0$, the molecule is stable

4.1.4 Interestingly, the dioxygen molecule has two excited states with the same number of electrons in all σ, σ^*, π, and π^* molecular orbitals. Using your knowledge of electron configurations, sketch the MO diagrams for both. (5 Points)


σu*
πg*
πu
σg
σu*
σg
σu *.
σg



4.1.5 Find the molecular term symbols for all three states (3 points)

Note: see Laporte's rules for g/u

Unexcited:
$S = 2 * 1/2 = 1 \rightarrow 2S + 1 = 3$
$L = 0 \rightarrow$ \Epsilon. $g * g = g$

$$^3\Sigma_g$$

Excited (1): $S = 0$, $L = 0$

$$^1\Sigma_g$$

Excited (2): $S = 0, L = 2$

$$^1\Delta_g$$

4.1.6 What type of magnetism is expected for atomic oxygen and the three configurations of molecular oxygen discussed above? (4 Points)

Ground state: $|J| = 1$ yields weakly paramagnetic.

Excited states (1): Diamagnetic as spin momentum cancels

Excited states (2): Strongly paramagnetic. While spin still sums to zero, the combined electrons in a single orbital yields $L = 2 \rightarrow J = 2$