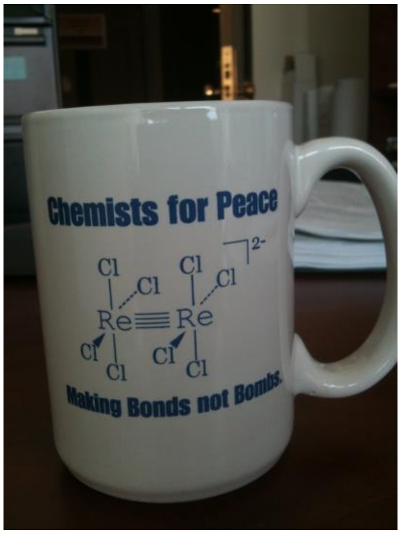
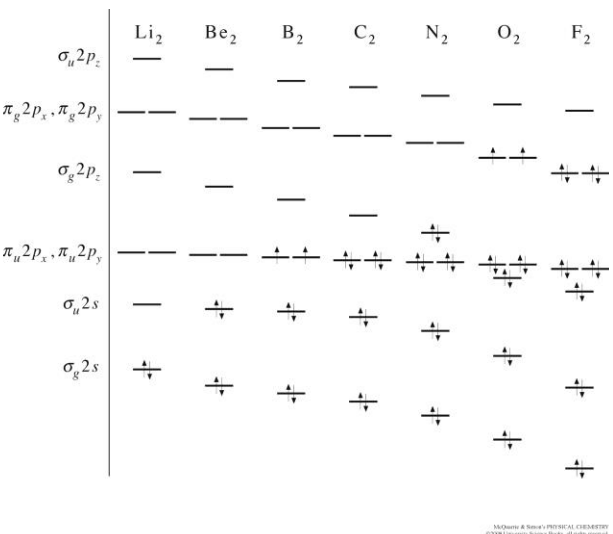
Chemical bonding and absorption of light

Part 1:



The picture of the left shows a promotional coffee mug by a UC Berkeley student group called “Chemists for Peace.” Their “logo” is the inorganic complex $Re_2Cl_4^{2-}$. Your job is to describe the chemical bonding in $Re_2Cl_4^{2-}$ and figure out what **bonding** MOs create the 4 bonds between the 2 Re atoms. The MOs are constructed from the atomic d-orbitals on the Re atoms, with the exception of the $d_{x^2-y^2}$ orbitals, which are used for bonding with the Cl atoms. For each bonding MO involved in the Re-Re quadruple bond, write down the mathematical formula (sum or difference of specific atomic orbitals), the orbital shape (σ, π, δ), inversion symmetry (g or u).

Part 2:

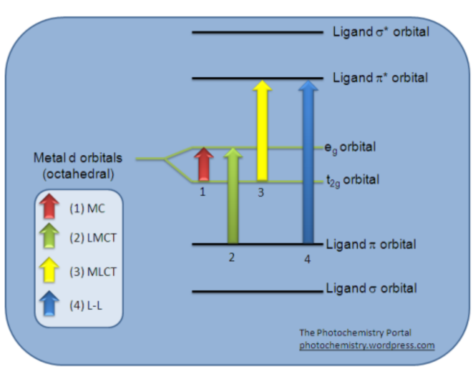


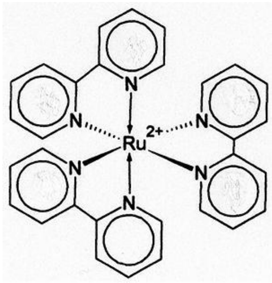
A. Which molecule has a stronger bond, N_2 or N_2^+. Explain your answer.

B. Which molecule has a stronger bond, O_2 or O_2^+. Explain your answer.

C. Which transition (from which MO to which MO) is the lowest energy **allowed** transition in N_2. Explain your answer.

Part 3:





Dye-sensitized solar cells usually use Ru(II) complexes as light absorbing molecules. A prototypical Ru(II) complex is shown on the right above. On the left is a picture showing some possibilities for transitions involved in light absorption. e_g and t_{2g} refer to the atomic d-orbitals on Ru, which have g symmetry.

(a) show that atomic d-orbitals have g symmetry

The red arrow shows a transition between the atomic d-orbitals. The yellow arrow shows a transition between metal d-orbitals and a π* MO on the ligand, which, let's assume, has the same inversion symmetry as a π* MO made of p-orbitals in a diatomic molecule. The green arrow shows a transition between a ligand π MO, which, let's assume, has the same inversion symmetry as a π MO made of p-orbitals in a diatomic molecule. And finally, the blue line shows a transition between the ligand π and π* MOs.

(b) what are the inversion symmetries of the π and π* ligand orbitals?

(c) Of the 4 transitions shown with arrows, which ones are allowed and which are forbidden?