423 Molecular Orbital Theory Assignment

Set: 13th March 2026. Due: **25th March 5pm**

Hand-in as a PDF file on Nuku (the Assignment in the 423 folder). Diagrams and text need to be legible to me and photographs/scans clear please!

Q1. Draw a MO diagram for C_{2v} $ClBH_2$. Use the BH_2 fragment orbitals given in **Figure 1**. The Cl pAOs will have an energy between the $1b_1$ and $2a_1$ FOs and the Cl sAO will interact with the $1a_1$ FO. Explicitly demonstrate MO mixing by drawing out and combining the relevant MOs, discuss MO mixing with respect to these MOs. Depict the mixed MOs on your MO diagram.

15 marks

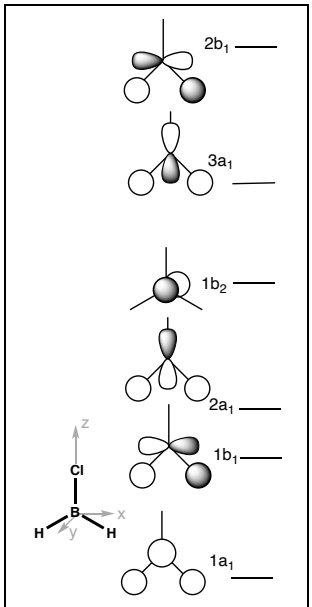

Figure 1 $ClBH_2$ fragment orbitals

Q2 Consider three oxygen atoms arranged in an equilateral triangle, that belong to the D_{3h} point group, **Figure 2**. In the following show your working at all stages.

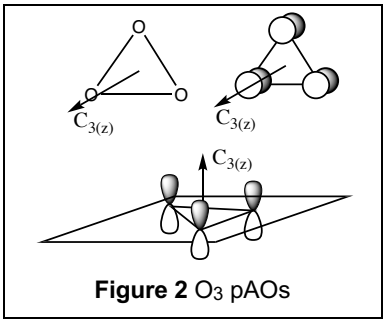

Figure 2 O_3 pAOs

i) Determine the reducible representation for the three p_π orbitals
ii) Write down the reduction and projection formulae. Briefly explain the terms in both formulae.
iii) Use the reduction formula to determine the symmetry of the p_π based symmetry adapted fragment orbitals.
iv) Use the projection formula to determine the wave function of the p_π based symmetry adapted fragment orbitals.
v) Draw an energy level diagram for the p_π based symmetry adapted fragment orbitals. Draw the fragment orbitals and write the associated equation beside each energy level. Label the symmetry of each orbital.

10 marks

Q3 Draw LCAOs for the computed MOs of borazine shown in **Figure 3**. On your diagrams annotate features important for evaluating the MO bonding character.

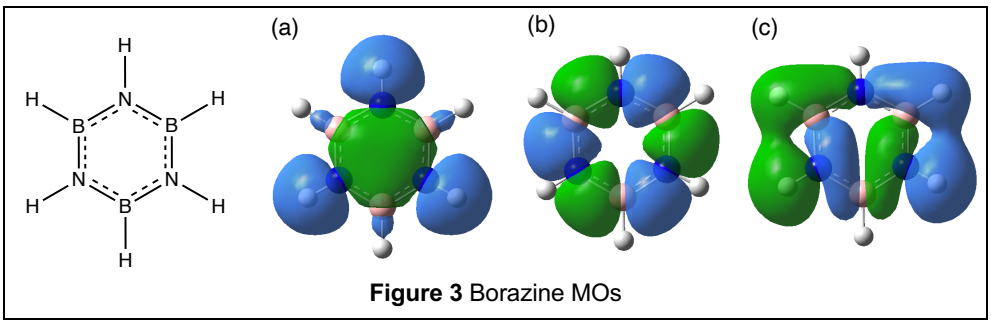

Figure 3 Borazine MOs

10 marks