Q1: Considering the Born - Oppenheimer approximation for a 1D H₂⁺ show that the Schrodinger equation can be written as:

\[ T_N \psi_N + E \psi_N = E \psi_N \]  (1)

Hints:
First use the trial solution of:

\[ \psi(z, Z_1, Z_2) = \psi(z, Z_1, Z_2) \psi_N(Z_1, Z_2) \]  (2)

and,

\[ H = T_e + T_N + V \]  (3)

where \( z \) is the coordinate of the electron and \( Z_1, Z_2 \) are the coordinates of the nuclei.

Second an approximation needs to be made when we reach:

\[ H \psi_N = \psi_N T_e \psi + \psi T_N \psi_N + V \psi_N + W = E \psi_N \]  (4)

where:

\[ W = - \sum_{l=1}^{1} \frac{\hbar^2}{2m_I} \left( \frac{\partial^2 \psi}{\partial Z_I^2} + \frac{\partial \psi}{\partial Z_I} \right) \]  (5)

Q2: Consider H₂:
(a) Write down a secular determinant for the two 1s orbitals in the case when the overlap integral between them is zero. This should be accompanied by a molecular orbital diagram. What is the bond order for this molecule?
(b) The overlap term S is non-zero, reintroduce this into the above equation to show that antibonding orbitals are more antibonding then bonding orbitals are bonding. Again a molecular orbital diagram should be drawn.
(c) Use these arguments above to describe why H₂⁺ is not a stable molecule.

Q3: Prove that the bonding and antibonding functions for H₂⁺ are orthogonal with respect to each other.

Q4: Considering a diatomic molecule with 2 different atomic species (element A and element B) with the secular determinant:

\[ \begin{vmatrix} \alpha_A - \beta - ES & \beta - ES \\ \beta - ES & \alpha_B - \beta \end{vmatrix} = 0 \]  (7)

by solving the roots for energy( we can take S=0) and sketching the molecular orbital energy levels show that bonds between atomic orbitals with similar energy dominate bonding.

Hint: As \( \alpha_A = \langle A | H | A \rangle \), \( \alpha_B = \langle B | H | B \rangle \) and \( \beta = \langle A | H | B \rangle \) one can say that:

\[ |\alpha_A - \alpha_B| >> \beta \]  (8)

and use the approximation:

\[ (1 + x)^{1/2} = 1 + \frac{1}{2} x \]  (9)

Q5: Apply the condition of the \( \frac{dx}{dc_k} = 0 \) to the Rayleigh-Ritz method, and derive the secular determinant.