

231B: Molecules

Quiz 4, Winter 2020
(Dated: February 27, 2020)

1. What is the spin multiplicity of the ground state of H_2 and of H_2^+ ?
2. Give the electronic Hamiltonian for H_2 .
3. Which one of the following changes significantly when going from H_2 to D_2 : R_e , D_e , ω ?
4. Within the harmonic approximation, say how your answer to the previous question will change?
5. Give an expression for the matrix element H_{AA} in H_2^+ for 1s orbitals ($\gamma = 1$).
6. Sketch how the matrix element H_{AA} should depend on R , giving its value as $R \rightarrow \infty$.
7. Sketch a molecular energy curve for H_2 as a function of R , giving its value as $R \rightarrow \infty$.
8. Sketch the curve within the Hartree-Fock approximation. What qualitative error does it make?
9. For a molecule with $y_e = 0$, deduce a formula for the number of states it will bind in terms of D_e , ω , and x_e .
10. Deduce an expression for x_e in terms of D_e and ω for the Morse potential, for which

$$\epsilon_n = -V_0 \left(1 - \frac{\alpha(n + \frac{1}{2})}{\sqrt{2\mu V_0}} \right)^2$$