Chemistry 581: Quantum & Computational Chemistry

Assignment 1: Molecular Mechanics

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1. Draw a potential energy surface (PES) for a diatomic molecule (e.g., H_2). Label the horizontal and vertical axes. (2 pts)

   Solution

   Here we draw the Hartree-Fock (3-21) potential energy surface for H_2 as it depends on the diatomic separation.

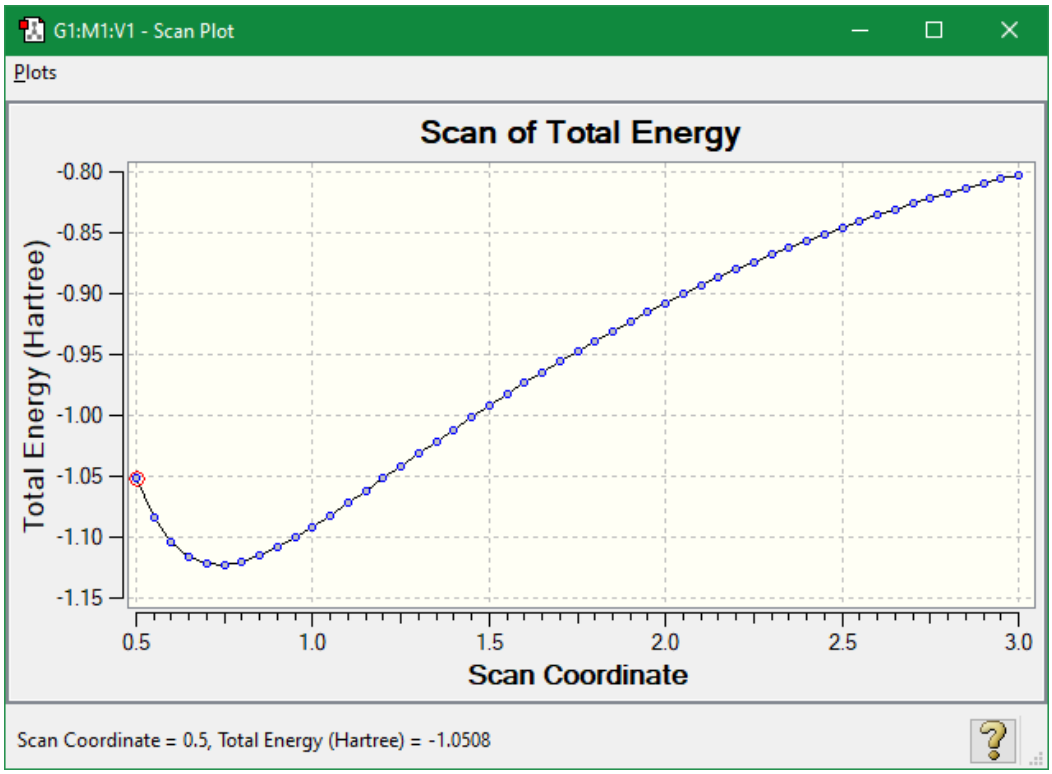

Figure 1: H_2 potential energy surface as a function of bond distance.

2. Given $k = 400\text{N/m}$ and $r_{\text{eq}} = 1\text{Å}$ for a diatomic molecule, estimate its relative energy when the bond distance is stretched to 1.2Å. (2 pts)

   Solution

   The energy in a diatomic bond can be modeled as that of a simple harmonic oscillator. Therefore the energy $V(r)$ as a function of the bond distance r takes the form $V(r) = \frac{1}{2}k(r - r_{\text{eq}})^2$, where k is the force constant and r_{eq} is the equilibrium bond distance. Then if $k = 400\text{N/m}$, $r_{\text{eq}} = 1\text{Å}$, $r = 1.2\text{Å}$, the energy in the diatomic bond is $\boxed{V(r) = 0.8\text{ÅnN}}$ (ÅnN is "Angstrom nano-Newtons").

3. To do a molecular mechanics calculation for a water molecule, we need the force constant and equilibrium bond distance of OH. What other information do we also need? (2 pts)
   Hint: the H-O-H bond angle may change.

   Solution

   In addition to the force constant and equilibrium distances of the OH bonds, **we also need the force constant and equilibrium of the H-O-H *angle*** in order to fully describe the energy of the water molecule via molecular mechanics. Note these are not equivalent to the equilibrium distance in the OH bonds because the Hydrogen atoms are not bonded and therefore the energy between them does not follow a harmonic oscillator form.

4. Draw a Newman projection for butane. Label the C-C-C-C torsional angle (τ). Draw a PES for the torsion of butane to show how the potent energy changes with τ. The torsional angle should be between 0 and 2π. (2 pts)
   Hint: The PES can be found on page 25 of the textbook.

   Solution

   Figures on next page.

5. Use the HF/3-21G method to calculate the energy of a H atom, the energy of a H_2 molecule with a bond distance that's difference from the equilibrium distance, and the energy of optimized H_2. Report your results in the shared Google Spreadsheet. (2 pts)

   Solution

   Done in class.

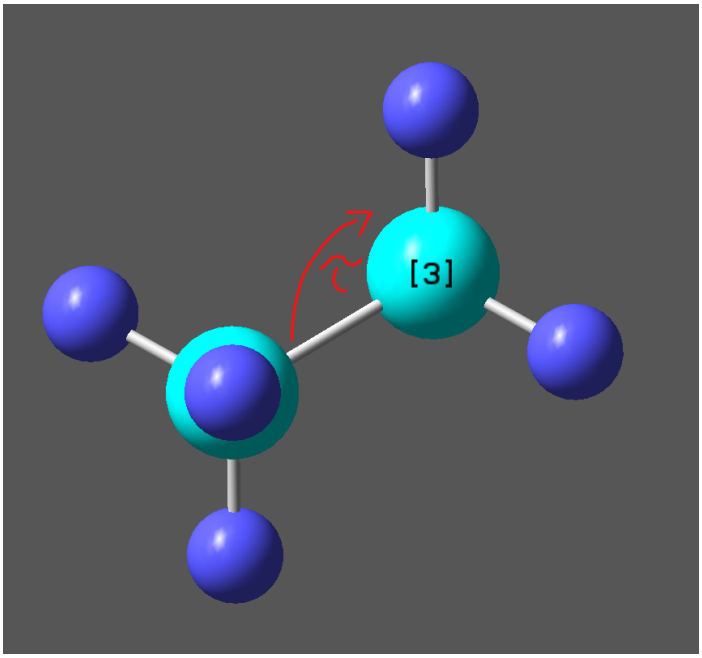

Figure 2: Newman projection of Butane with dihedral/torsion angle τ.

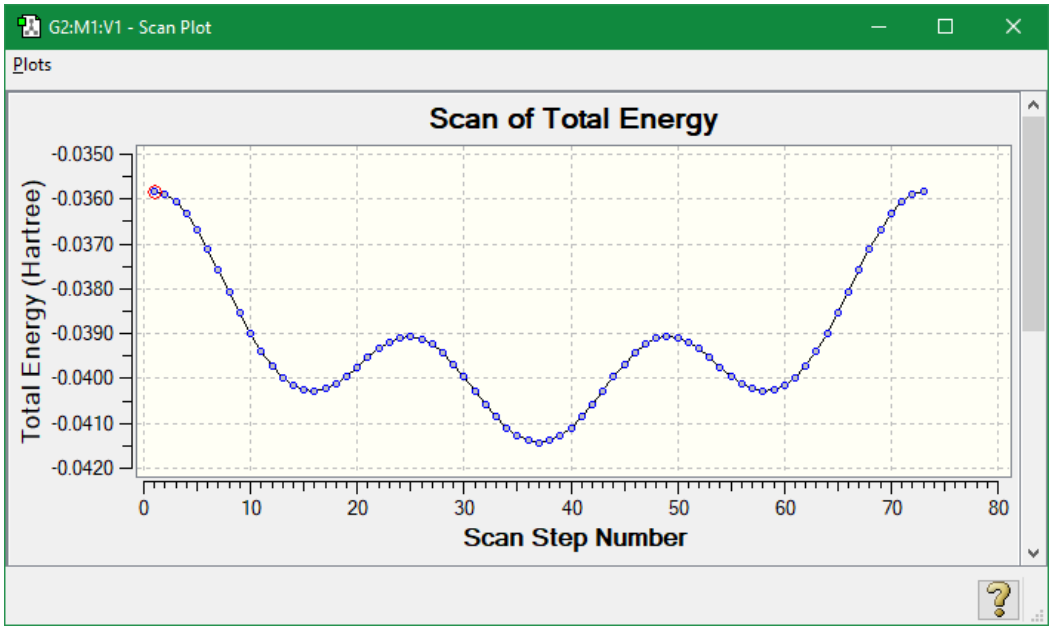

Figure 3: Potential energy surface of butane as a function of the C-C-C-C dihedral angle τ.