Quiz #11 10/23/2006 (Mon) Chapters 7-8 Name: _____

1. (a) Explain the difference between the two basis sets, 6-31G* and 6-31G**.

   (b) How many basis functions would they have for methane (CH_4)? Explain.

   _____ with 6-31G*

   _____ with 6-31G**

2. Explain the difference between the two types of stationary points, minima and transition state, especially how we check if we have minima or transition state after geometry optimization.

3. List at least three reasons why we need to calculate vibrational frequencies on optimized structures.

4. List at least two **experimental** methods we can use to confirm the following calculated properties.
   (a) Structure (geometry) _____
   (b) Vibrational frequency _____

5. Pick one of the following exchange-correlation density functionals (E_{XC}) and describe it briefly: SVWN or BP86 or B3LYP.

6. Draw the following chemical structures.
   (a) acetaldehyde (b) vinyl alcohol (c) benzene (d) methylamine