

**CHEMISTRY 4021/8021**  
**MIDTERM EXAM 1 – SPRING 2013**

Q1) In molecular mechanics, what are the advantages and disadvantages of having multiple atom types for a single element? Use at least one example in the context of your answer. (15 points)

Q2) What is a "polarizable" force field? What are the advantages and disadvantages of using a polarizable force field. (15 points)

*use the backs of pages as needed*

Q3) You have an output file containing one million snapshots from a 298 K Monte Carlo simulation of a box of liquid water containing 512 flexible molecules under periodic boundary conditions and constant pressure. Explain how you would compute the expectation value of the H–O–H bond angle (you may use words or equations). If the bending potential is harmonic, what shape would you expect for the continuous angle distribution function? (10 points)

Q4) What is a four-index integral, often abbreviated  $(\mu\nu | \lambda\sigma)$ ? Why do semiempirical theories approximate these integrals, and what approximations do they employ? (15 points)

Q5) How many contracted basis functions are required for a calculation on H<sub>2</sub>O with the 6-311G(d) basis set (which by default uses a set of 6 cartesian d functions)? (5 points)

Q6) If instead of 6-311G(d) we were to use 6-311+G(2df,2pd), which energy would you expect to go down by more, the HF energy, or the CCSD(T) energy? Why? (5 points)

Q7) An atomic orbital basis function is to a \_\_\_\_\_ as a Slater determinant is to a configuration interaction wave function. (5 points)

Q8) What does a hyperfine coupling constant indicate and what kind of spectroscopy is involved in its measurement? (10 points)

Q9) What is the ideal gas molecular partition function and what approximations are involved in computing it for a given molecule? For what is the partition function useful? (20 points)