Name:_____

CHEMISTRY 5021/8021
MIDTERM EXAM — SPRING 2004

1. Molecular Mechanics (50 points)

Write two different functional forms that might be used to describe the potential energy associated with bond stretching. Carefully define all terms in the equations. Now, contrast the two: what are the relative merits of one compared to the other? Why might a given force field adopt one and not the other? Note that there are many possible answers here—I am not looking for any *specific* two forms.

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2. Semiempirical Theory (50 points)

An AM1 calculation on benzene provides a 298 K heat of formation of 23.5 kcal mol^{-1}. Explain in a detailed fashion exactly how this heat of formation value was arrived at. You need *not* explain anything about geometry optimization.

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3. Ab Initio MO Theory

a) How many basis functions are required for a HF calculation on glycine ($C_2H_5NO_2$) using the 6-31G(d) basis set? (25 points)

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b) Select by letter from the list at the bottom of the page the proper answer to the following questions. There is only one correct answer to each question. (5 points each)

(1) This post-Hartree-Fock level employs second-order perturbation theory to estimate the energy associated with electron correlation and formally scales as N^5.

(2) This correlated level of theory expresses the complete wavefunction as a linear combination of configuration state functions but fails to be size-consistent.

(3) This is a potential problem with unrestricted Hartree-Fock wave functions that is not a problem for restricted open-shell Hartree-Fock wave functions.

(4) This is a multilevel model that attempts to correct for incompleteness in basis set size and accounting for electron correlation by additive means.

(5) This single level of theory scales less favorably than MP3 but more favorably than MP5.

A: MP3	B: spin contamination	C: nondynamical correlation
D: G2	E: CCSD(T)	F: MP2
G: CISD	H: ROHF	I: hyperconjugation

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