

Name: _____

CHEMISTRY 4021/8021
MIDTERM EXAM 3 – SPRING 2013

Q1) Compare and contrast continuum and explicit solvent models. What strengths and weaknesses are associated with each? Give an example of a study where one model would clearly be more appropriate than the other. (30 points)

use the backs of pages or p. 4 as needed

Q2) Write down a Hamiltonian operator for a QM/MM calculation in which the boundary between the two regions does not cut any covalent bonds. Define all symbols. If you were to use your operator in a Monte Carlo simulation of a quantum solute in a periodic box of classical chloroform molecules, explain what would be involved in a single Monte Carlo step. What would change if you were interested in modeling an excited electronic state of the solute? (40 points)

Q3) What is a primary kinetic isotope effect? Computationally, what is required to compute the primary kinetic isotope effect for a given reaction? Does quantum mechanical tunneling *increase* or *decrease* a primary isotope effect? For a reaction where tunneling plays no role, would you expect a primary kinetic isotope effect computed at the *ab initio* Hartree-Fock level to be too large or too small (justify your answer)? (30 points)

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4

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