Name:_____

CHEMISTRY 4021/8021
MIDTERM EXAM 3 — SPRING 2014

Q1) What physical effects contribute to the free energy of solvation, i.e., the free energy change associated with moving a solute molecule from the gas phase to a liquid solution at a constant standard-state concentration (e.g., 1 M)? How do most modern continuum solvation models incorporate those different effects into a calculation? (30 points)

use the backs of pages as needed

Q2) Consider a QM/MM calculation in which the boundary between the two regions does *not* cross any covalent bonds. Describe how computationally the QM and MM regions may be separately or jointly polarized (or not) by the other region. Full mutual polarization is most physically realistic, but why might one choose not to adopt such an approach? What "tricks" might be used to increase the accuracy of a calculation in which one or both regions are unpolarized? (30 points)

Q3) Use one or more potential energy diagrams to illustrate the following concepts in electronic spectroscopy: (i) vertical excitation energy, (ii) fluorescence, (iii) phosphorescence, (iv) Stokes shift, (v) solvatochromism. Within the context of the configuration interaction with single excitations (CIS) theory, how is an electronic excited state represented? (40 points)