**Names:**

# CHEMISTRY 4021/8021
# MIDTERM EXAM — SPRING 2012

*Answer in detail any 3 of the below 4 questions, working in whatever fashion you, as a collective, decide most productive. You may use any textual or electronic resource (including the internet) to assist you. You are only restricted from asking for assistance from other* people, *either in the classroom or outside of it. You may write your answers on paper (one written document per table, please) or compose them electronically and send them to me (as a pdf, please) by email date stamped before 10 a.m. (cramer@umn.edu). I'm willing to accept a combination of the two from a given table, but please make a point in both the hard and electronic copies to note the existence of the other.*

Q1) What is dispersion? Describe the physics underlying dispersion in a qualitative way and discuss the means by which dispersion is accounted for (or not) in the various theories that we have discussed in class to date.

Q2) Consider the unpleasant little molecule HOF. Discuss the two-electron integrals that would enter into a calculation of HOF at the CNDO, INDO, PM3, HF/6-31G(d), and MP2/6-31G(d) levels of theory. More specifically, what integrals are required for the construction of the Fock matrix and how are their various values determined?

Q3) When sampling phase space, what are the relative advantages and disadvantages of molecular dynamics vs. Monte Carlo algorithms? What considerations might go into choosing one over the other?

Q4) Discuss how one might go about computing the 298 K heat of formation ($\Delta H^{\circ}_{f,298}$) of gaseous 2-methylmorpholine, focusing, obviously, on approaches covered in class (or the reading) so far. Assign a level of confidence to the various protocols that you suggest, if not necessarily in quantitative terms, at least in a "best to worst" characterization. Note how computational constraints might play a role in limiting your range of choices, if at all.