CH4430/CH5410
Fall Semester 2000

Instructor: Professor Dallas Bates
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Office Hours: 11-12:00 M-W, F
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Reference Texts:
Computational Chemistry, G.H. Grant and W.G. Richards (Oxford
Chemistry Primer # 29), revised 1998.

Grading: Grades will be from a combination of activities:

Group Homework
Individual Homework
In-class tests –2-(may include take home portion)
(dates: 10-2-00 and 11-8-00)
Poster session (last week of class)
Final exam

10% 10% 40% 10% 30%

Topics (chapters numbers refer to Hoffinan):

Chapter 1 (and pp 180-188 in Chapter 8) Bonding, conjugated, pi systems, HOMO’s,
LUMO’s, aromaticity, concerted reactions
Chapter 10 Mechanisms of Organic Reactions
(includes predicting physical properties and biological activity, linear
free energy relationships (Hammett and Hansch plots), using ChemPlus
to calculate partition coefficients)
Chapter 5 Stereochemistry, conformational analysis,
using molecular mechanics (HyperChem) to predict
conformational energies
Chapter 9 Planning organic synthesis (expanded
retrosynthetic analysis and synthon sections)
Chapter 6 Functional group synthesis
Chapter 7 C-C bond formation
Synthesis papers from the literature exemplifying synthesis chapters

Note: No class 9-22-0, 9-25-00, 11-15-00, and 11-19-00. These days will be compensatory class time for
the out-of-class time required to learn HyperChem and ChemPlus software. You also need to know how to
enter data, plot data and conduct multiple linear regression analysis (the TREND function) in Microsoft
EXCEL. This will be covered in class, but a working knowledge of EXCEL will be useful.