

Computer Special Project

The computer special project is worth 15% of the marks in this class, and is due in my mailbox by 5:00 PM on 18 October 2002. The basics of the project are described below.

- (1) Each student will get his/her own project for investigation. Students may feel free to discuss the projects with one another, but must individually produce the final results and reports.
- (2) Each report should be word-processed or type-written. If I cannot easily read the report, marks will be deducted for illegibility. Microsoft Word and ChemDraw are excellent word processing and drawing programs with good online help facilities, and both are available through the Chemistry Resource Center. You are strongly advised to learn how to use them or alternatives (ChemWindows, WordPerfect, Chemintosh, etc.) as soon as possible for use in preparing your reports.
- (3) Each report should follow the same basic format:
 - (a) Cover page with title, your name, course name, date of submission, brief abstract (<250 words describing the problem and general outcome).
 - (b) Introduction – briefly describes the problem that was set
 - (c) Methodology – briefly describes programs used and methodology used, with appropriate referencing (e.g., “MacSpartan version 2.1, Wavefunction Inc., Irvine CA, 1998”).
 - (d) Results – this should include descriptions of optimized molecular geometries, electronic properties, molecular orbitals, or molecular vibrations for any molecules computed, with clear indication of the methods used to get them. Often, figures with molecular bond lengths and angles, and tables of charges or spin densities, are useful summaries for a molecule.
 - (e) Discussion – here, you give the best answers that you can to your problem. Wherever possible, literature references should be given for parameters such as molecular geometries, enthalpies of formation, dipole moments, and other measurable quantities. Use Beilstein Online and Chemical Abstracts as tertiary sources, but you must give primary references unless they are missing from the UMass library system and you cannot find them online.
 - (f) Conclusion – comment on the ability of the tools available to you to solve the problem that was set for you.
- (4) Mr. Joseph Simard (13th floor LGRT) is available for consultation on these projects, as am I.
- (5) The clarity and precision with which you present your results are crucial for getting a good grade. This is the heart of scientific reporting – the ability to transmit your results and conclusions in a terse but complete fashion. Thus, you should get your results as soon as possible, so you can maximize time spent upon analyzing them. It is best to keep a folder with printouts of important final results (e.g., Mulliken charge distributions, geometric coordinates, heats of formation, dipole moments). Keep all your output files on your own Chemistry Resource Center (Macintosh login or other) accounts until the end of the course, in case it is useful to look back at any computations for more information.