

## Nitration of Methyl Benzoate. Modeling with the SPARTAN computer program.

This document will help you run the calculations in the handout "Nitration of Methyl Benzoate".

Additional instructions and corrections (numbers refer to the steps given in the Rotello handout):

- 1) Logging onto and running SPARTAN on the SGI Indy in the Organic Lab. The Silicon Graphics Indy computer is always left on. Do not touch any buttons on the blue computer box to the right of the 20" monitor. If the machine has been idle for awhile, the screen will be dark. Simply press the space bar on the keyboard and wait about 15 seconds. Using the left mouse button (use the left mouse button for all operations unless otherwise noted), double click on the Chem 268 icon, enter the password (same as last semester) then double click on the SPARTAN icon. (You do not have to type SPARTAN as described in the Rotello handout.)
- 4) Add the underlined: "pull down the menu bar, which is beneath and to the right of the Groups and Rings buttons".
- 5) If necessary, to view the ester group better, rotate the molecule by holding down the middle mouse button and moving the mouse. The entire molecule can be moved around the screen with the right mouse button. Try holding down the shift key while doing these operations.
- 11) Electrostatic potential should read electrostatic charge.
- 12) Whenever a confirmation comes up, click on "OK". Also, when finished working in some windows it is necessary to click on "Done" before going on to the next step.
- 13) The calculation will take a few minutes.
- 14) Display -> Properties -> Energy.
- 15) Do not quit if you plan to do the "extra-neat stuff".

Extra-neat Stuff: play around with this. Try "Transparent" and other settings. Positively-charged parts of the molecule are shown as blue and negatively-charged parts as red. The charges are not different enough on the o-, m-, and p- carbons to show up easily as different colors, but you can observe the different charges on the electronegative oxygens compared to carbon and hydrogen, and get a feel for some of what the SPARTAN program can do.

Logging off: after quitting spartan, click on "desktop" in the upper left of the screen, then on "log out".

(p samal, 1/02)