

Instructions for Chemistry 273 Huckel Calculation

login to hydrogen; one way to do this is using the instructions for PBSci WebSSH:
http://www.chemistry.ucsc.edu/teaching/switkes/CHEM273/HANDOUTS/SSH_CHEM273_Progs.pdf

once logged in:

hydrogen> set path = (\$path /home/hydrogen/faculty/gene/CHEM273)
#sets directory for programs must be done FIRST, must be done with caps and lower case as indicated; hydrogen> represents the 'prompt' provided when hydrogen is awaiting keyboard input; your prompt may be different

hydrogen> run_huckel azulene
runs the Huckel program in class directory looking first for azulene input file (azulene.in) in directory in which you are currently in and second in class directory; output goes to azulene.out in directory which you are currently in (should be your home directory; if you are not in your home directory, a message about no permission to save output will appear) be sure to enter the underscore (_) characters as indicated

hydrogen> display_huckel azulene

or

hydrogen> more azulene.out

output from calc is listed on screen one page at a time for those of you who know various UNIX editors, the file azulene.out could be inspected using UNIX editors

if you are using a PC or MAC to access PBSci WebSSH , the best way to get printed output is to

- open a window using a MAC or PC text editor (I use wordpad on PC)
- copy an paste calculation output from the hydrogen ("MindTerm") window
- print from your text editor in the usual way

some other molecules for which input decks are available are:

hydrogen> run_huckel bi_prop_pent

hydrogen> display_huckel bi_prop_pent

hydrogen> run_huckel naphthalene

hydrogen> display_huckel naphthalene

#by changing directories to /home/hydrogen/faculty/gene/CHEM273

hydrogen> cd /home/hydrogen/faculty/gene/CHEM273

#you can read about creating input decks for the huckel program by

hydrogen> more huckel.doc

and you can inspect various input files by

hydrogen> more azulene.in

(if you have cd'ed to CHEM273, be sure to go back to your 'home directory' , cd ~, before running more calculations)