

MCC Summer School Laboratory Exercise
August 7, 2006
Systematic Improvement of Basis Sets

Exercise 1

In this exercise we will do Hartree-Fock calculations on CO of increasing accuracy with the Polarization Consistent basis sets of Jensen. See: F. Jensen, J. Chem. Phys. 115, 9113 (2001)

- 1) Log into copper.ncsa.uiuc.edu via ssh.
- 2) Copy the 5 GAMESS input decks (.inp files) from ~train18/dunning2/exercise1/CO/ into your directory.
- 3) Run them. To do so use the submission script ~train18/dunning2/qgms. For example, to run CO-pc-0.inp type:

```
~train18/dunning2/qgms CO-pc-0.inp
```

once you submit the jobs you will have to wait for them to finish.

- 4) Examine the output. Using gnuplot (or the plotting program of your choice) plot the Hartree-Fock energy as a function of the basis set. Also plot the dipole moment as a function of the basis set. Notice the convergence of both the energy and dipole moment as the basis set is improved.
- 5) Open the Jensen paper, which is in ~train18/dunning2/exercise1/jensen.pdf. Compare your results for the contracted polarization consistent basis with that of the uncontracted basis (Table XIII). You will need to do another set of calculations, this time at infinite separation, in order to calculate E_b , the binding energy.

Exercise 2

In this exercise we will do MP2 calculations of N₂ of increasing accuracy with the Correlation Consistent basis sets of Dunning. See: T. H. Dunning, Jr., J. Chem. Phys. 90, 1007 (1989)

- 1) Copy the 4 GAMESS input decks from ~train18/dunning2/exercise2/N2/ into your directory.
- 2) Run them. Use the qgms script as above.
- 3) Examine the output. Plot the Hartree-Fock and MP2 energies as a function of the basis set. Notice that both energies decrease as the basis set increases in size, but notice that the MP2 energy decreases more dramatically.