

Physical Chemistry II
Problem Set 5—due Wednesday, March 26, 2003
Revised on 3/12/03--Note revisions in red

1. (5 points) Atkins and de Paula Exercise 14.5(b). **You should also predict the bond order for each of these molecules.**
2. (5 points) Atkins and de Paula Exercise 14.6(b). **You should also predict the bond order for each of these molecules.**
3. (5 points) Atkins and de Paula Exercise 14.7(b). **You should justify your answers by writing down the bond orders before and after the addition/removal of an electron.**
4. (5 points) Atkins and de Paula Exercise 14-9(b). Briefly justify your ordering.
5. (5 points) Consider a molecular orbital given by $\Psi = N(0.145A + 0.844B)$, where A and B are normalized and orthogonal to each other. Find a linear combination of A and B that is both normalized and orthogonal to Ψ . (Based on Atkins and de Paula Exercise 14-11(b).)
6. (15 points) Atkins and de Paula Problems 14.2 and 14.3. Use Excel (or another spreadsheet program) to plot both functions on a common set of axes. Plot enough points to make the curvature of each function clear. Also, be sure to do the qualitative sketch asked for in Problem 14.3, and justify briefly the form of your qualitative sketch.
7. (15 points) Atkins and de Paula Problems 14.8 and 14.9. Use Excel (or another spreadsheet program) to plot both potential energy curves on a common set of axes. ~~Plot enough points to make the curvature of each curve clear.~~ Be sure to use your curve in Problem 14.8 to predict H_2^+ 's bond dissociation energy and equilibrium bond length.