Chemistry 412, Fall Semester 1999, Dr. Glaser
Quiz 1: "Basis Sets," Monday, October 18, 1999, 25 minutes.

Your Name:

Question 1. Basis Sets. (24 points)

(a) Explain the difference between a **minimal** and an **extended** basis set for carbon. Provide an example for each type of basis set as part of your answer. (8 points)

Minimal basis set: One basis function for every AO in the core and the valence shell.
Extended basis set: More than one BF per AO in the core and the valence shell.
Examples: Minimal basis: STO-KG. Extended basis set: 3-21G, 6-31G, DZ

(b) Explain the difference between a **double-ζ** and a **split-valence** basis set. Provide an example of your choice to illustrate the point. (8 points)

DZ: Two basis functions for every AO in core and valence.
Split-valence: One BF per core-AO and two (or more) BFs per valence AO.

(c) State what H-atom **polarization functions** are and explain how they work. Briefly discuss whether these functions are more important in hydridic or acidic molecules. (8 points)

p-functions
they allow for a reduction of the symmetry and more directional bonding
more important for hydridic systems (much more density at H)

Points for Question 1:	/24		
Points for Question 2:	/14		
Points for Question 3:	/12	Total Points:	/50

Question 2. Calibrated Pople Basis Sets. (14 points)

Consider silaacetylene, H-C≡Si-H	**H-C≡Si-H**
Number of valence AOs on the C-atom?	4 (2s and 2p set)
Number of core AOs on the heteroatom?	5 (1s, 2s, 2p)
Number of BFs to describe the C-atom at STO-3G?	5 (1s, 2s, 2p)
Number of BFs to describe the heteroatom at 3-21G?	13 (5 core + 8 val.)
Number of BFs to describe the heteroatom at 6-311+G*? (5d)	26 (5 core,16 val., 5d)
Number of BFs to describe the H-atom at 6-311+G*? (5d)	3 (3s, 311 has 3 digits)
Total number of BFs at 6-311G** (5d)	52 (6/H, 18/C, 22/Si)

Question 3. Numerical Example. (12 points)

Attached is the basis set section of an output of an *ab initio* calculation of silene SiH_2 (the Si analog of carbene).

(a) Describe the H and Si basis sets in the "( ) & [ ]" nomenclature. (4 points)

H (5s) [3s] Si (13s, 9p, 2d,1f) [6s, 5p, 2d, 1f]

(b) Write down the H's inner s-basis function as an expansion of the primitives. Write down the Si's inner p-basis function as an expansion of the primitives. No need for normalization. Just write down the expansions using the numbers you find in the attachement. (8)

The inner s-functioon for H

Norm. $0.0254 \cdot \exp(-33.86 \cdot r^2) + 0.1903 \cdot \exp(-5.095 \cdot r^2) + 0.8521 \cdot \exp(-1.1588 \cdot r^2)$

The inner p-function of Si (note the r-factor before each exponential term)

Norm. $0.00887 \cdot r \cdot \exp(-335.5 \cdot r^2) + 0.06083 \cdot r \cdot \exp(-78.90 \cdot r^2) + 0.2910 \cdot r \cdot \exp(-24.99 \cdot r^2)$
$+ 0.7321 \cdot r \cdot \exp(-9.220 \cdot r^2)$