

**Chemistry 433, Winter Semester 1998, Dr. Glaser**

**Quiz II: “Basis Sets”, Monday, April 20, 1998, 25 minutes.**

Your Name:

**Question 1. Split-Valence Basis Sets and Basis Set Augmentation.** (24 points)

(a) Explain what a **split-valence basis set** is by comparison of the STO-3G and 3-21G basis sets of oxygen. (8 points)

(b) Using an illustration, explain what **polarization functions** are. Give an example of an oxygen-containing molecule that would require polarization functions in the basis set. (8 points)

(c) Using an illustration, explain what **diffuse functions** are. Give an example of an oxygen-containing molecule that would require diffuse functions in the basis set. (8 points)

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 formaldehyde,  $\text{H}_2\text{C}=\text{O}$ ,  
and its sulfur analog,  $\text{H}_2\text{C}=\text{S}$ .

	$\text{H}_2\text{C}=\text{O}$	$\text{H}_2\text{C}=\text{S}$
Number of valence AOs on the heteroatom?		
Number of BFs to describe the heteroatom at STO-3G?		
Number of BFs to describe the heteroatom at 3-21G?		
Number of BFs to describe the heteroatom at 6-31G*?		
Total number of BFs at 6-31G* (1.5 p.)		
Total number of BFs at 6-311G** (1.5 p.)		

**Question 3. Numerical Example.** (12 points)

Attached is the basis set section of an output of an ab initio calculation of water.

(a) Describe the basis set shown in the attachment in the “() & []” nomenclature. (4 points)

(b) Write down the H-1s inner basis function as an expansion of the primitives. No need for normalization. Just write down the expansion using the numbers you find in the attachment. (4)

(c) For the calculation of the electrical dipole moment of water, would you rather use this basis set or the basis set 6-31G\*\*? Explain in a few words. (4 points)