CHEM/421 2011

Computational Lab #1

Gaussian Viewer 03

I. Build the structures (exactly as shown), save the images and insert them in your lab report (Word file). Fill the table below:

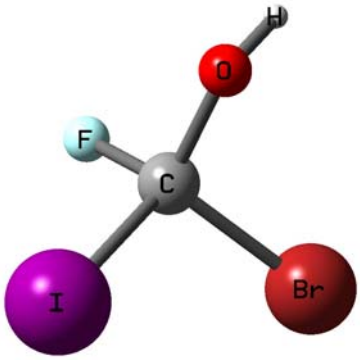
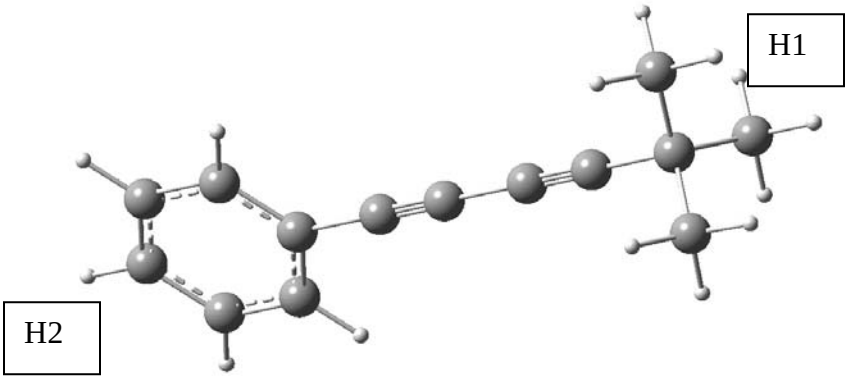


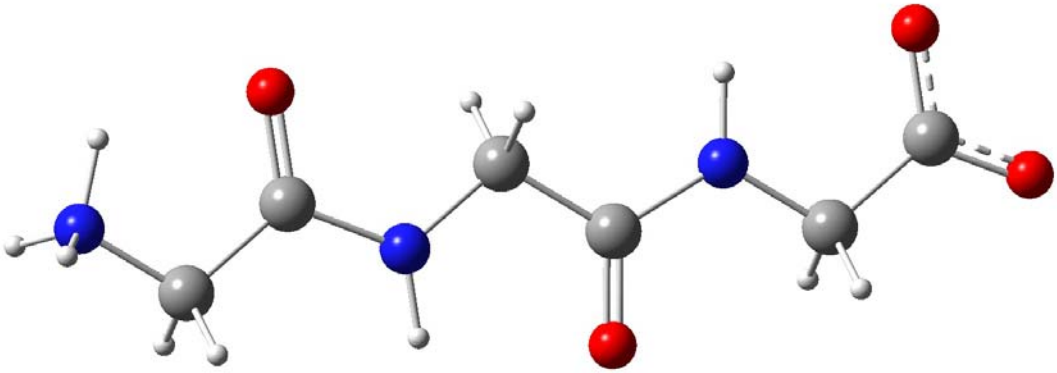
Table #1. Bond lengths and distances between atoms, in Å, bond angles and dihedral angles, in deg, predicted by Gaussian Viewer

	Distance	Angle
C-O		
C-Br		
C-I		
C-F		
O-H		
I-C-Br		
H-O-C		
I-C-O-H		
F-C-I-Br		

II. Build the structure as shown below. Report the H1-H2 distance?



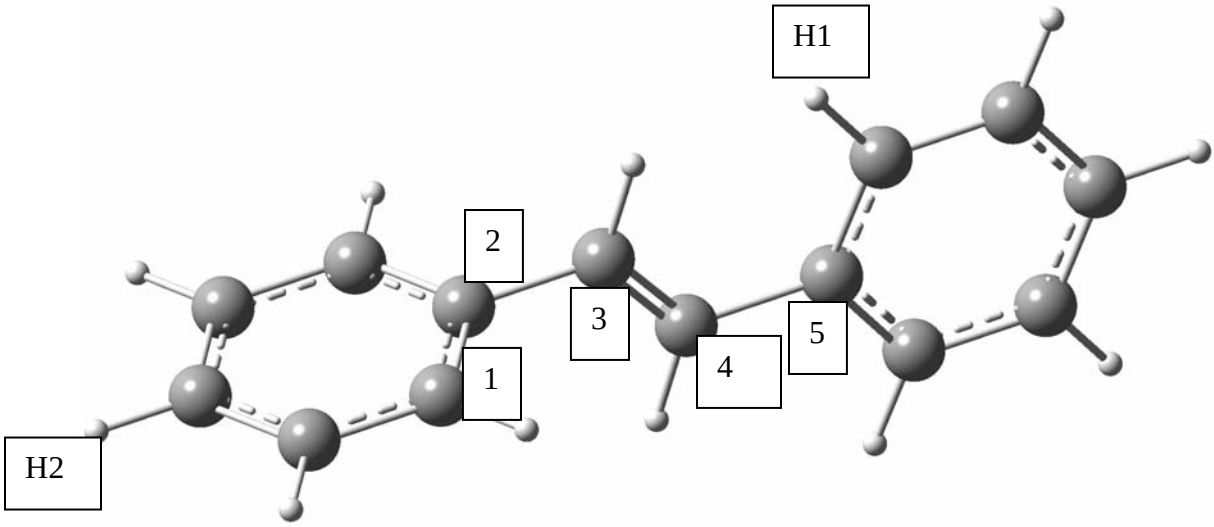
III. Build the polypeptide as shown below (use the template).



Report the distance between the two most remote atoms.

Report the N-C-C bond angle for the N-terminus.

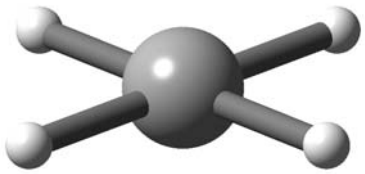
IV. Build the structure shown below.



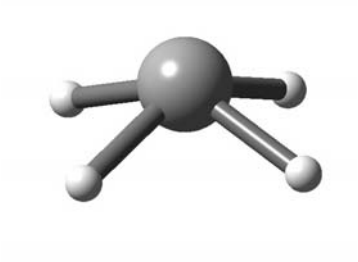
Set the 1234 dihedral angle to zero
Set the C4-C5 distance to 1.48 Å

What is the distance between H1 and H2?

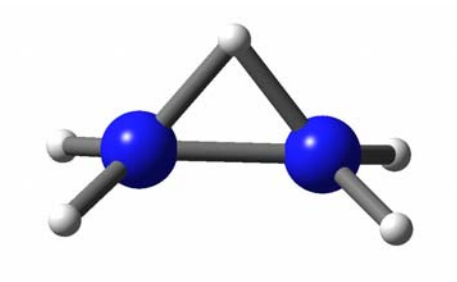
V. Symmetry.
Build the following structures. Be sure that you have a proper symmetry group.



D_{4h} (square planar methane)



C_{4v} (square pyramidal methane)



Transition state structure (C_2v) for the !,2 proton shift for protonated hydrazine ($NH_2NH_2H^+$)