CHM616 - Assignment #1

Due Date: 30/1/2022

Q1. For H_2O & H_2O_2 Molecules, Construct both xyz & z-matrix form geometries and perform RHF/6-31G calculation. Report nuclear repulsion energy & RHF energy for each calculation. Verify that xyz & z-matrix calc for each molecule gives same results. The geometry for each molecule is given below.

H_2O:

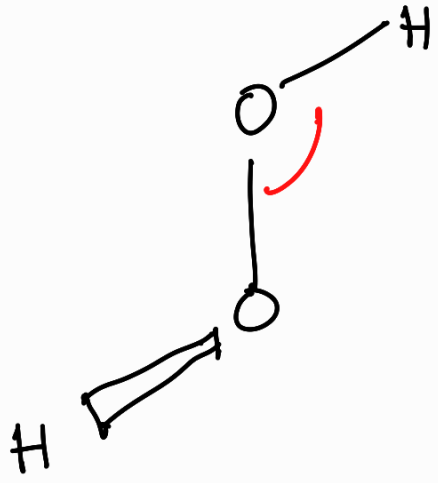
$R(OH) = 0.95A^0$

$A(HOH) = 104.5^\circ$

xyz: Molecule must be in xy plane,

with oxygen at the origin.

H_2O_2:



$R(O-O) = 1.47 A^\circ$

$R(O-H) = 0.95 A^\circ$

$A(HOO) = 95^\circ$

$D(H-O-O-H) = 90^\circ$

Xyz: One oxygen at origin, the other oxygen along +ve z-axis; One (O-O-H) must be in xz-plane & the other O-O-H must be in zy-plane.

(contd)

Q2. Setup RHF calculations on Ne atom for the following basis sets. Note that basis set is to be set using $BASIS input group.

1. MINI
2. MIDI
3. STO-3G (STO with NGAUSS=3)
4. 3-21G (N21 with NGAUSS=3)
5. 4-31G (N31 . . . . =4)
6. 6-31G (N31 . . . . =6)
7. 6-311G (N311 — . . . =6)
8. CC-pVDZ (GBASIS = CCD)
9. CC-pVTZ (— . . — = CCT)
10. CC-pVQZ (— . . = CCQ)

For each basis set, collect following info from output file.

① No of Basis functions (size)

② RHF energy

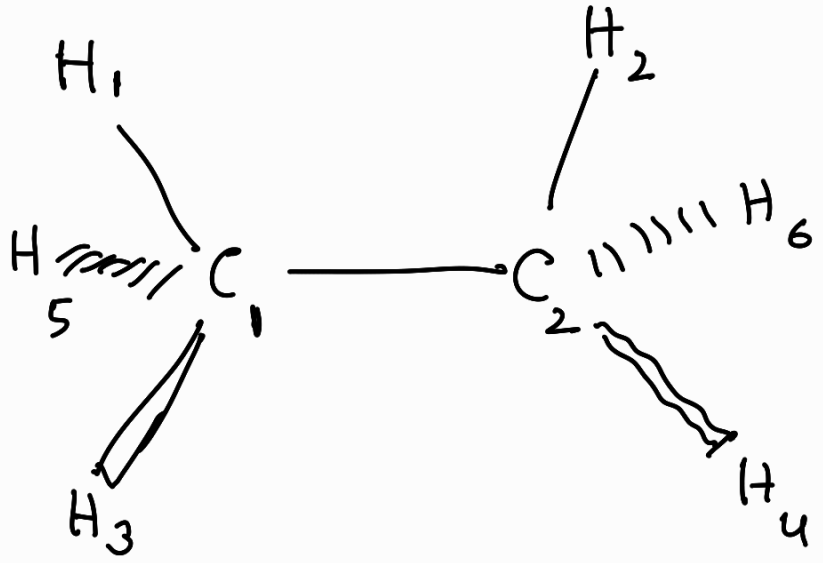
Prepare the following table sorted with increasing basis set size

Basis	# of Basis Funs	RHF Energy
.	.	.
.	.	.
.	.	.
.	.	.

Make a graph of # of Basis Funs of x-axis & RHF Energy on y-axis.

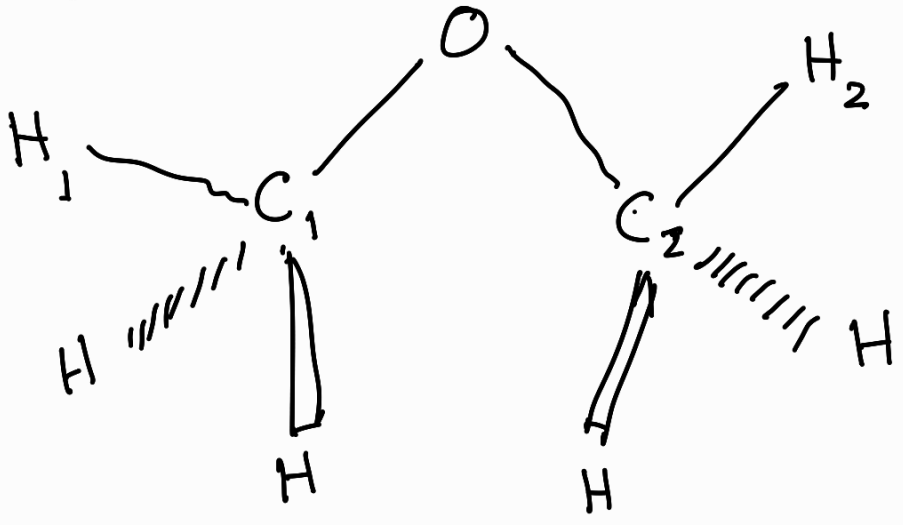
Q3. Construct Symbolic Z-matrix for the following molecules & perform RHF/6-31G calculation. Use some sensible values for C-C, C=C, C-H, C=O, C-O bonds, and angles and diherals. Rough geometry is indicated in these figures.

(a) C_2H_6



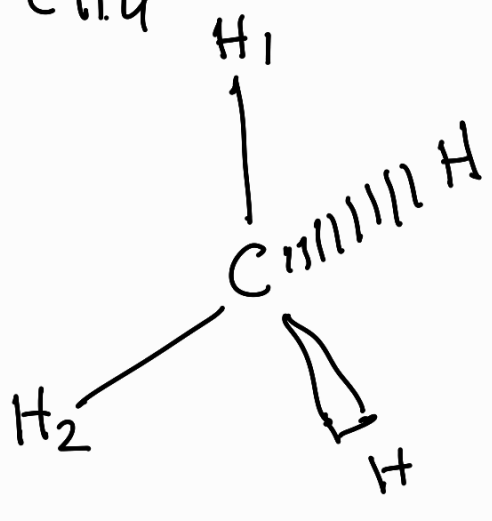
Here, H_1, C_1, C_2, H_2 are in plane H_3 & H_4 are in front & H_5 & H_6 at back.

(b) $(CH_3)_2O$



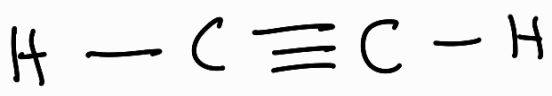
Here, H_1, H_2, C_1, C_2 & O are in a plane.

(c) CH_4

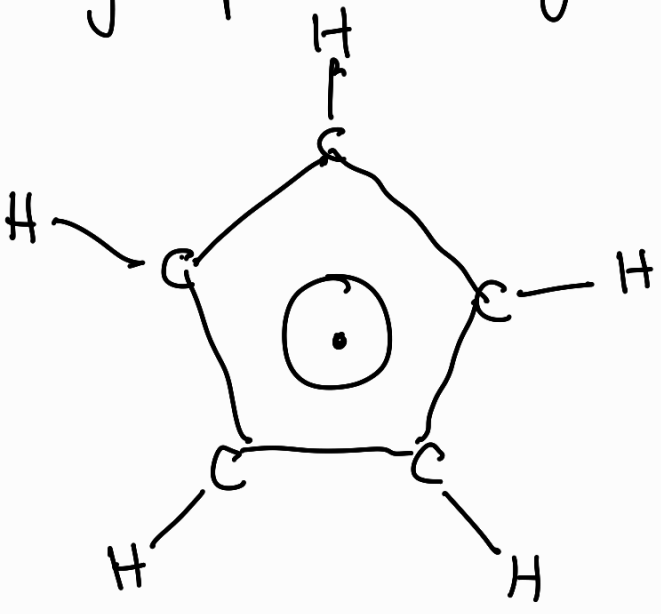


(d) C_2H_2

(Linear)



(e) Cyclopentadienyl anion $(C_5H_5)^-$



(D_{5h} Symmetry)

Use of dummy atoms is encouraged.