Molecular Modeling For Process Engineering AY 2023-24

Luigi Pagani

June 19, 2024

0.1 Ethane Molecule

The optimized energy is −79.8416414 Hartrees, which is found near the end of the output under "SCF Done". The optimization successfully converged in 8 steps, as indicated by "Optimization completed" and "Stationary point found". The optimized C-C bond length is 1.532119 angstroms, and the optimized C-H bond lengths are 1.095627 angstroms. The optimized H-C-H angles are 107.5275°, and the optimized C-C-H angles are 111.3513°. The molecule has D3D symmetry in the optimized geometry, which is a staggered conformation. The dipole moment is 0, as expected for the nonpolar ethane molecule, and the quadrupole moments reflect the symmetry of the charge distribution. A frequency calculation was not done, so we cannot say for sure this is a true minimum. However, the very small forces and displacements suggest that it is likely a minimum. In summary, a geometry optimization was performed at the B3LYP/6-31+G(d,p) level of theory, producing a reasonable, symmetric minimum energy structure for ethane with geometric parameters consistent with expectations.

0.1.1 Final Z-Matrix

```
C
C,1,d1
H,1,d2,2,a1
H,1,d3,2,a2,3,b1,0
H,1,d4,2,a3,3,b2,0
H,2,d5,1,a4,3,b3,0
H,2,d6,1,a5,6,b4,0
H,2,d7,1,a6,6,b5,0
```

0.1.2 Variables

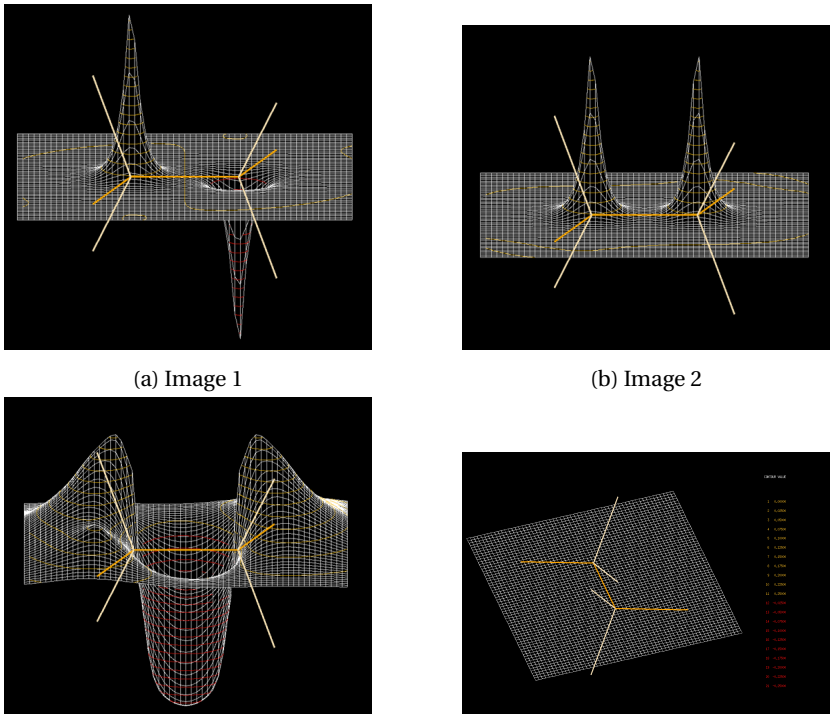
```
d1 = 1.53211939
d2 = 1.09562688
d3 = 1.09562688
d4 = 1.09562688
d5 = 1.09562688
d6 = 1.09562688
d7 = 1.09562688
a1 = 111.3512645
a2 = 111.3512645
a3 = 111.3512645
a4 = 111.3512645
a5 = 111.3512645
a6 = 111.3512645
b1 = 120.0
b2 = -120.0
b3 = 60.0
```

b4 = 120.0
b5 = -120.0

$$E(RB3LYP) = -79.8416414283 A.U.$$

0.2 Orbitals

Here are displayed the 4 orbitals, from the total of 9, calculated via Gaussian09 and displayed via the Molden software program.



(a) Image 1

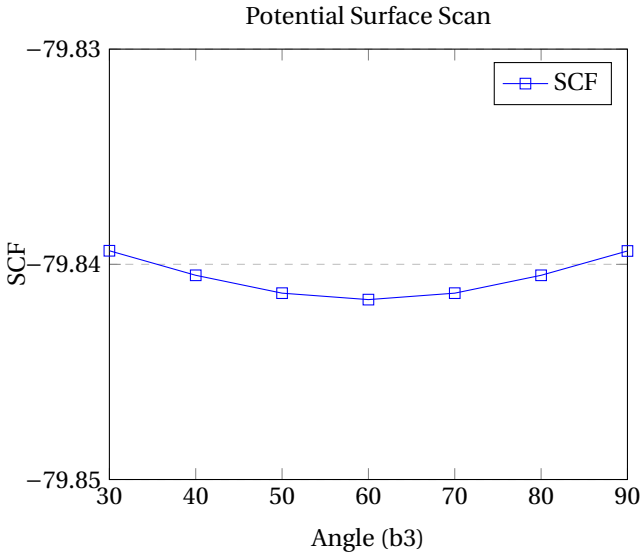
(b) Image 2

(c) Image 3

(d) Image 4

Figure 1: Four images

0.3 Variation of the Energy based on the angle between the two Methyl Groups



Note that the energy values are symmetric with respect to the lowest energy configuration, where the methyl angle $b3 = 60.0$.

0.4 Propane Molecule

Final structure in terms of initial Z-matrix:

C
C,1,d1
C,2,d2,1,a1
H,1,d3,2,a2,3,b1,0
H,1,d4,2,a3,3,b2,0
H,1,d5,2,a4,3,b3,0
H,2,d6,1,a5,3,b4,0
H,2,d7,1,a6,3,b5,0
H,2,d8,1,a7,3,b6,0
H,3,d9,1,a8,2,b7,0
H,3,d10,1,a9,2,b8,0
H,3,d11,1,a10,2,b9,0

Variables:

d1=1.53313003
d2=1.53312457

d3=1.09563276
d4=1.09672507
d5=1.09671929
d6=1.098051
d7=1.09805085
d8=1.09671891
d9=1.09563323
d10=1.09672476
a1=112.97671198
a2=111.56258778
a3=111.10249548
a4=111.10159423
a5=109.38517973
a6=109.3832623
a7=111.10144737
a8=111.56272137
a9=111.10244664
b1=179.99801495
b2=-59.81015185
b3=59.80563621
b4=122.09578854
b5=-122.09692187
b6=59.80497849
b7=179.99749566
b8=-59.81056764

E(RB3LYP) = -119.159151909 A.U. after 11 cycles

Chapter 1

Claude 3 Reformatting

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H,2,d7,1,a6,6,b5,0
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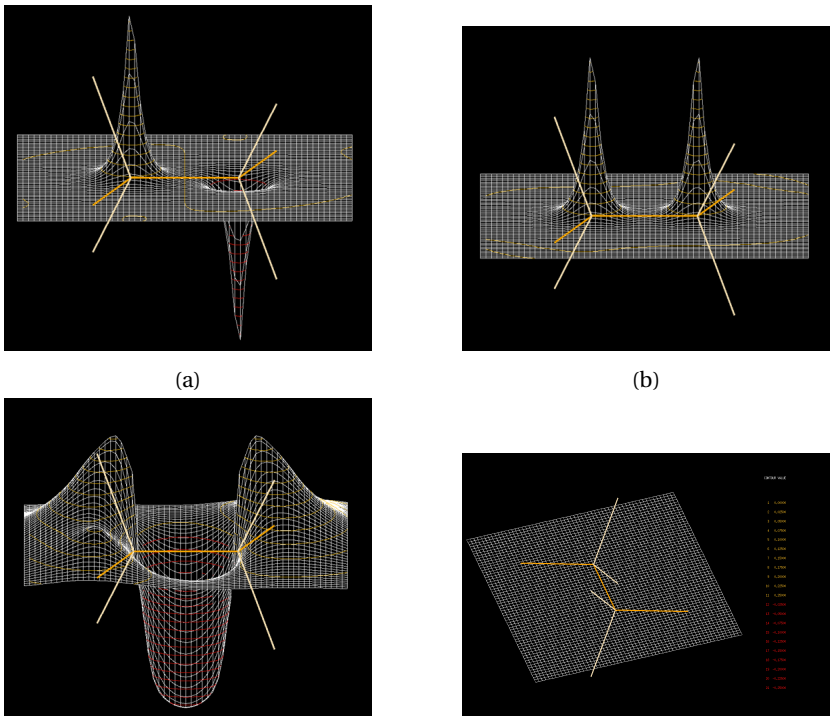
Here are displayed 4 orbitals, chosen randomly from the total of 9, calculated via Gaussian09 and displayed via the Molden software program.

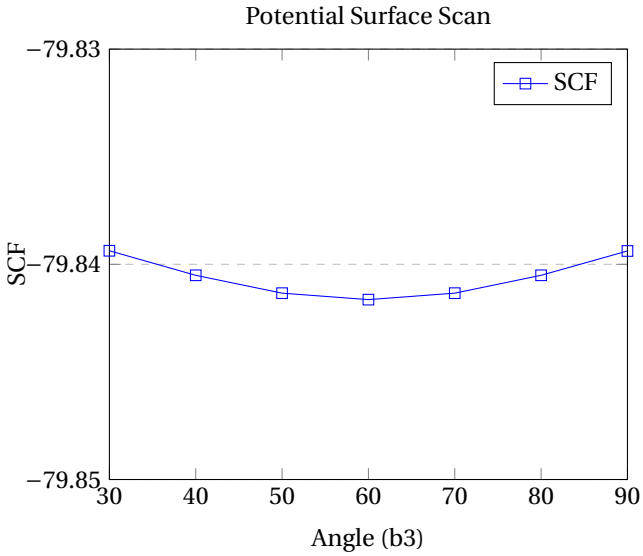


(a) (b)

(c) (d)

Figure 1.1: Four images

1.3 Variation of the Energy based on the angle between the two Methyl Groups



Note that the energy values are symmetric with respect to the lowest energy configuration, where the methyl angle $b3 = 60.0$.

1.4 Propane Molecule

The optimized structure of propane in terms of the initial Z-matrix is:
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C,2,d2,1,a1
H,1,d3,2,a2,3,b1,0
H,1,d4,2,a3,3,b2,0
H,1,d5,2,a4,3,b3,0
H,2,d6,1,a5,3,b4,0
H,2,d7,1,a6,3,b5,0
H,2,d8,1,a7,3,b6,0
H,3,d9,1,a8,2,b7,0
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H,3,d11,1,a10,2,b9,0

The optimized variables are:

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d2 = 1.53312457
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b5 = -122.09692187
b6 = 59.80497849
b7 = 179.99749566
b8 = -59.81056764

The optimized energy at the RB3LYP level of theory is $E = -119.159151909$ A.U. after 11 optimization cycles.