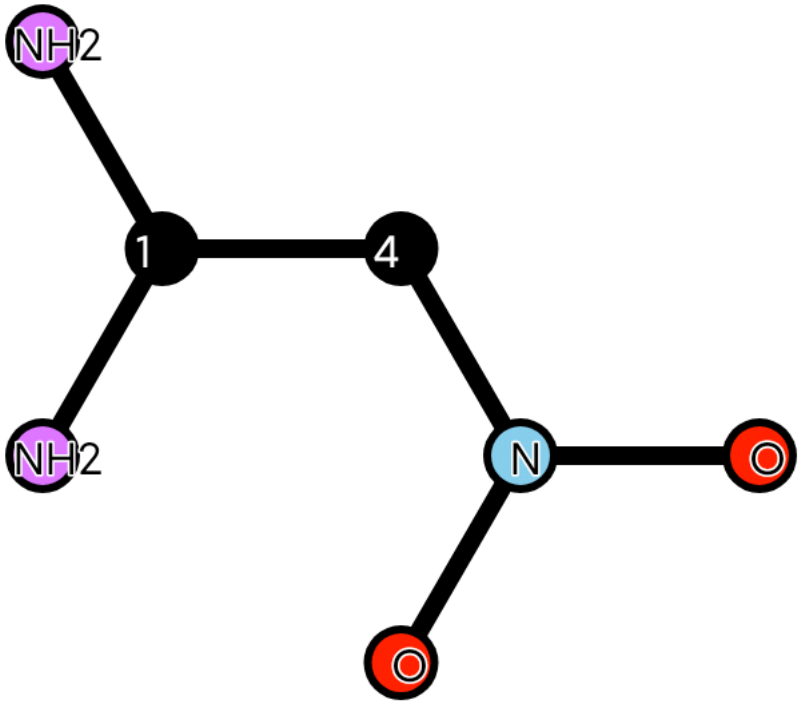
Print calculated values

Report generated by:root, 17.02.2020 - 09:58:45

The following determinant is calculated:

-x	1.3	1.3	1.0	0.0	0.0	0.0
1.3	-x+1.47	0.0	0.0	0.0	0.0	0.0
1.3	0.0	-x+1.47	0.0	0.0	0.0	0.0
1.0	0.0	0.0	-x	1.3	0.0	0.0
0.0	0.0	0.0	1.3	-x+1.47	1.95	1.95
0.0	0.0	0.0	0.0	1.95	-x+1.18	0.0
0.0	0.0	0.0	0.0	1.95	0.0	-x+1.18

It is about this molecule:

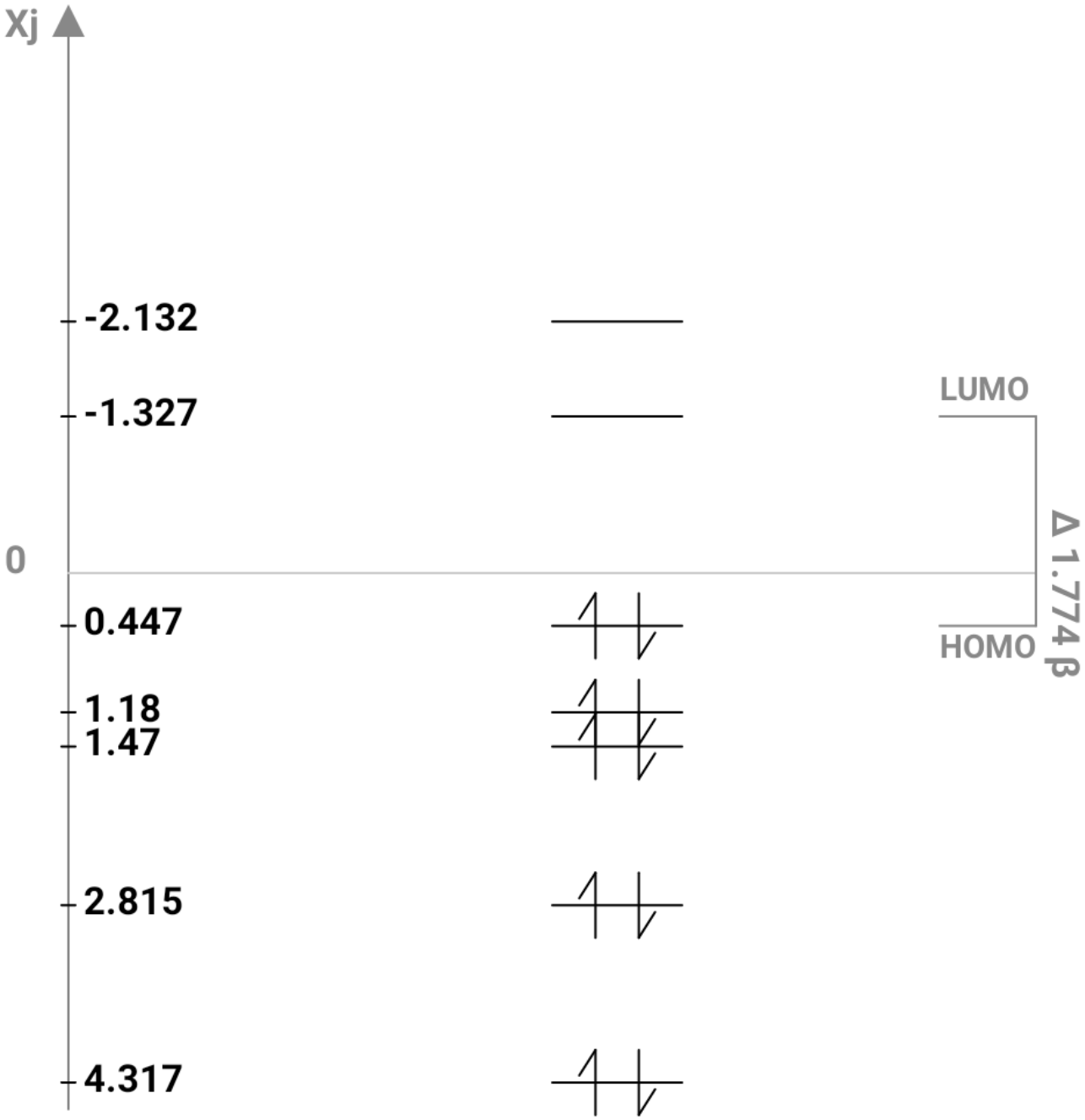


HMO-Energies

x1 = 4.317; x2 = 2.815; x3 = 1.47; x4 = 1.18; x5 = 0.447; x6 = -1.327; x7 = -2.132;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 7α + 20.458β -

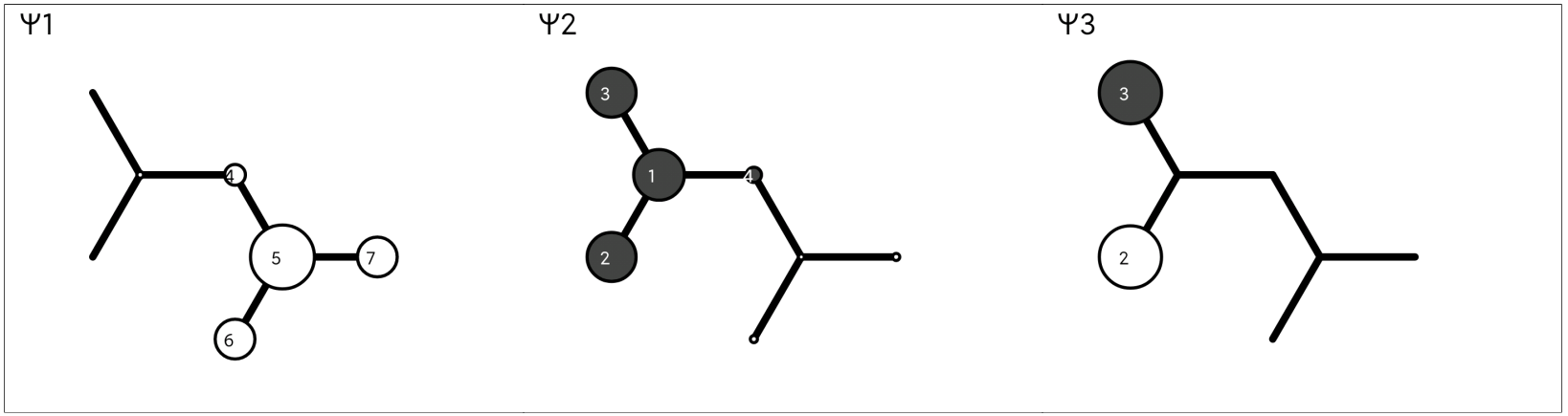
this corresponds to one πelectron: 2.046β

2. Hueckel-coefficient

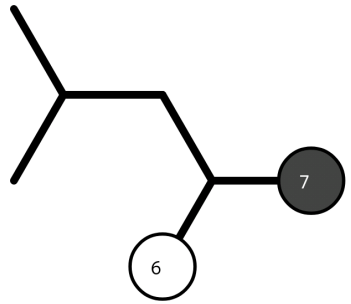
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7
	x1= 4.317	x2= 2.815	x3= 1.47	x4= 1.18	x5= 0.447	x6= -1.327	x7= -2.132
1	0.076	-0.576	0.0	0.0	0.211	-0.649	-0.444
2	0.034	-0.557	0.707	0.0	-0.268	0.302	0.16
3	0.034	-0.557	-0.707	0.0	-0.268	0.302	0.16
4	0.236	-0.173	0.0	0.0	0.792	0.077	0.53
5	0.727	0.068	0.0	0.0	0.11	0.421	-0.527
6	0.452	0.081	0.0	0.707	-0.293	-0.327	0.311
7	0.452	0.081	0.0	-0.707	-0.293	-0.327	0.311

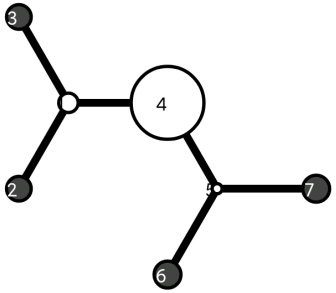
2.2. Molecule orbital presentation:



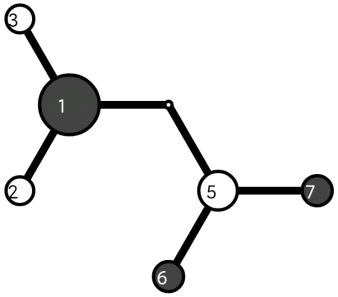
Ψ4



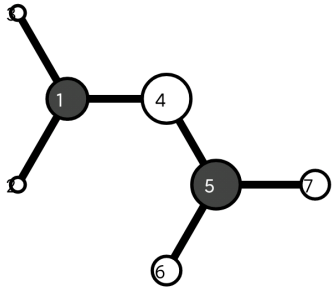
Ψ5



Ψ6



Ψ7

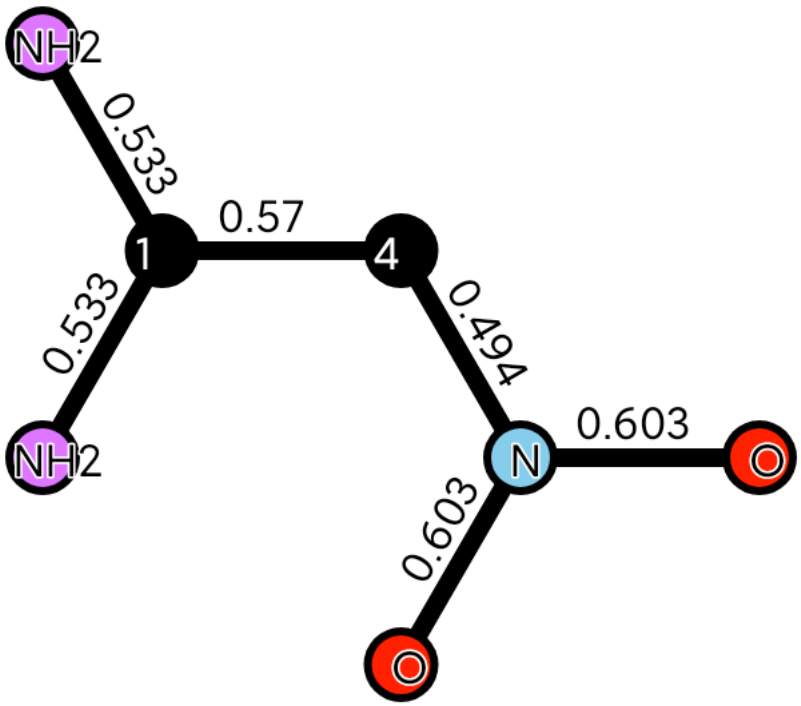


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7
1	0.764						
2	0.533	1.767					
3	0.533	-0.233	1.767				
4	0.57	-0.216	-0.216	1.427			
5	0.078	-0.085	-0.085	0.494	1.09		
6	-0.149	0.098	0.098	-0.279	0.603	1.593	
7	-0.149	0.098	0.098	-0.279	0.603	-0.407	1.593

3.2. Presentation of bond order:

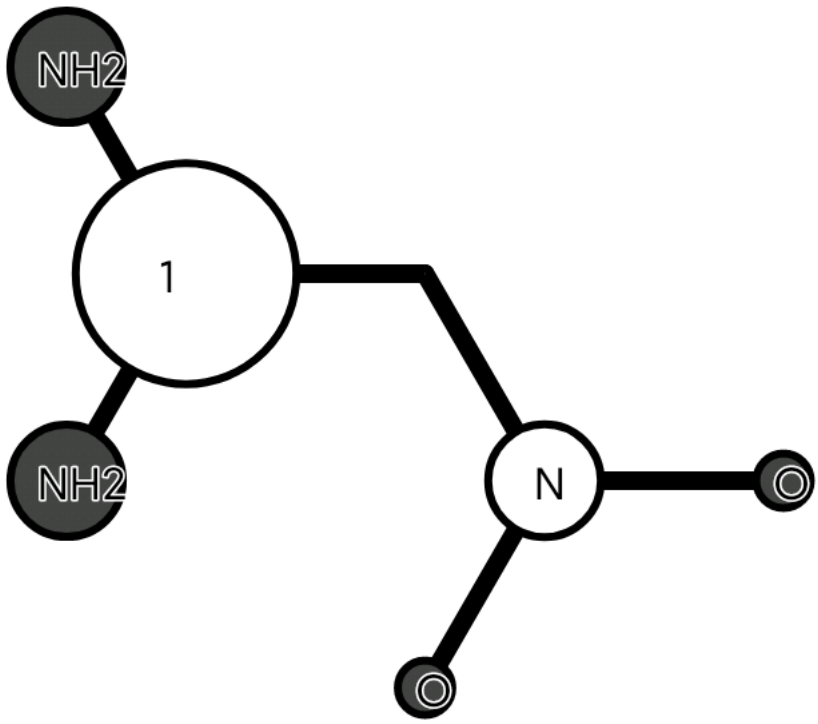


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7
1	0.664						
2		-0.338					
3			-0.338				
4				0.002			
5					0.339		
6						-0.164	
7							-0.164

4.2. Presentation of molecule:

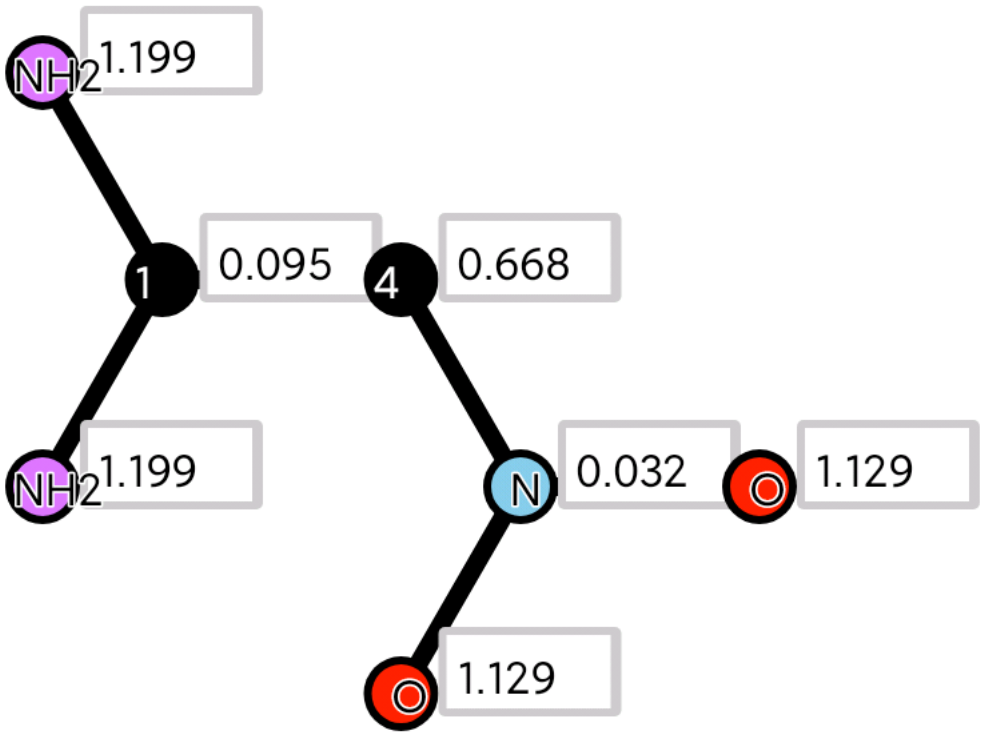


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7
0.095	1.199	1.199	0.668	0.032	1.129	1.129

5.2. Presentation of molecule:

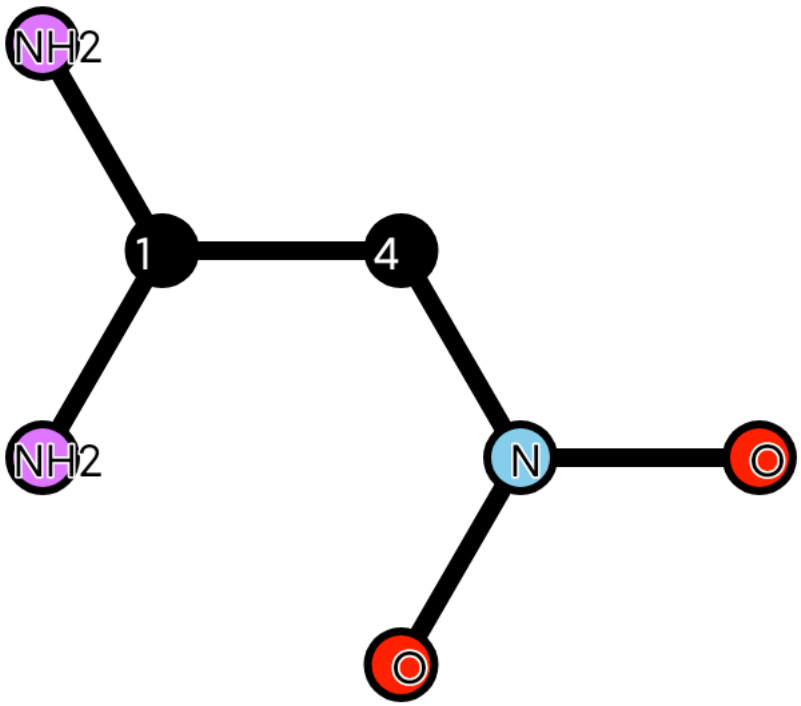


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7
1	0.246						
2	-0.048	0.131					
3	-0.048	-0.028	0.131				
4	-0.107	-0.03	-0.03	0.298			
5	-0.006	-0.006	-0.006	-0.055	0.169		
6	-0.019	-0.01	-0.01	-0.039	-0.049	0.206	
7	-0.019	-0.01	-0.01	-0.039	-0.049	-0.081	0.206

6.2. Presentation of molecule:

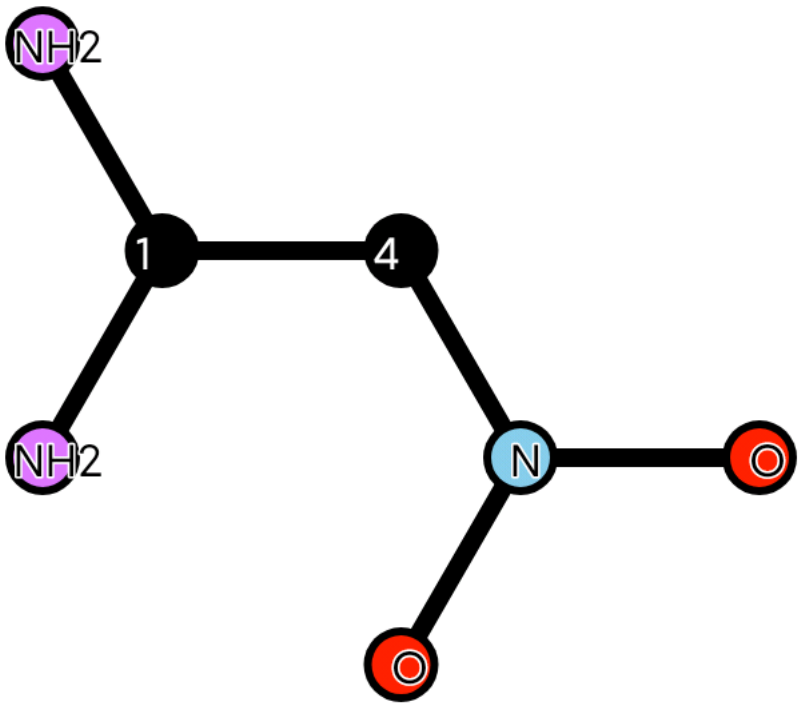


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7
1 2	0.002	-0.137	0.042	0.059	0.006	0.014	0.014
1 3	0.002	0.042	-0.137	0.059	0.006	0.014	0.014
1 4	0.086	0.055	0.055	-0.108	-0.019	-0.035	-0.035
4 5	-0.031	-0.017	-0.017	-0.087	0.017	0.068	0.068
5 6	0.012	0.008	0.008	0.05	-0.02	-0.133	0.075
5 7	0.012	0.008	0.008	0.05	-0.02	0.075	-0.133

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3	1 4	4 5	5 6	5 7
1 2	0.314					
1 3	-0.097	0.314				
1 4	-0.17	-0.17	0.356			
4 5	0.051	0.051	-0.152	0.27		
5 6	-0.021	-0.021	0.059	-0.119	0.212	
5 7	-0.021	-0.021	0.059	-0.119	-0.097	0.212

8.2. Presentation of molecule: