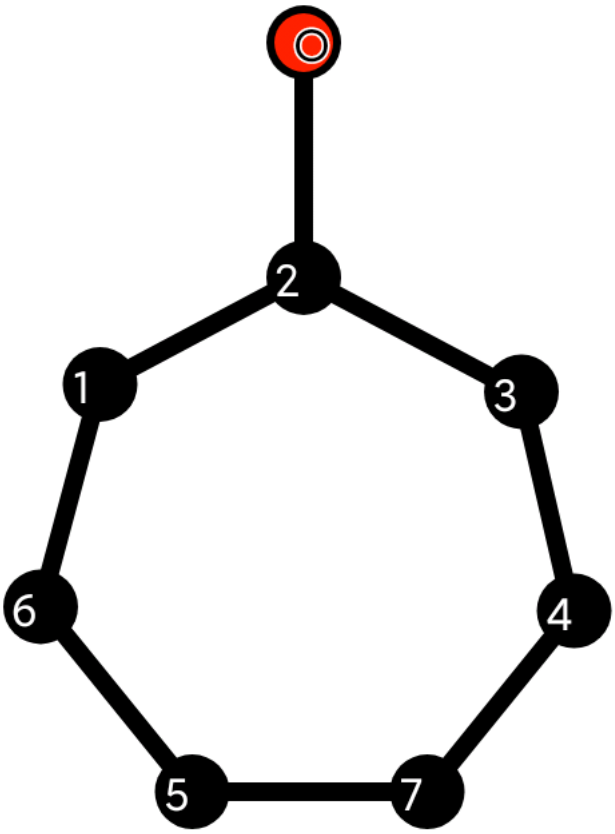
Print calculated values

Report generated by:root, 01.02.2020 - 15:56:42

The following determinant is calculated:

-x	1.0	0.0	0.0	0.0	1.0	0.0	0.0
1.0	-x	1.0	0.0	0.0	0.0	0.0	1.93
0.0	1.0	-x	1.0	0.0	0.0	0.0	0.0
0.0	0.0	1.0	-x	0.0	0.0	1.0	0.0
0.0	0.0	0.0	0.0	-x	1.0	1.0	0.0
1.0	0.0	0.0	0.0	1.0	-x	0.0	0.0
0.0	0.0	0.0	1.0	1.0	0.0	-x	0.0
0.0	1.93	0.0	0.0	0.0	0.0	0.0	-x+1.18

It is about this molecule:

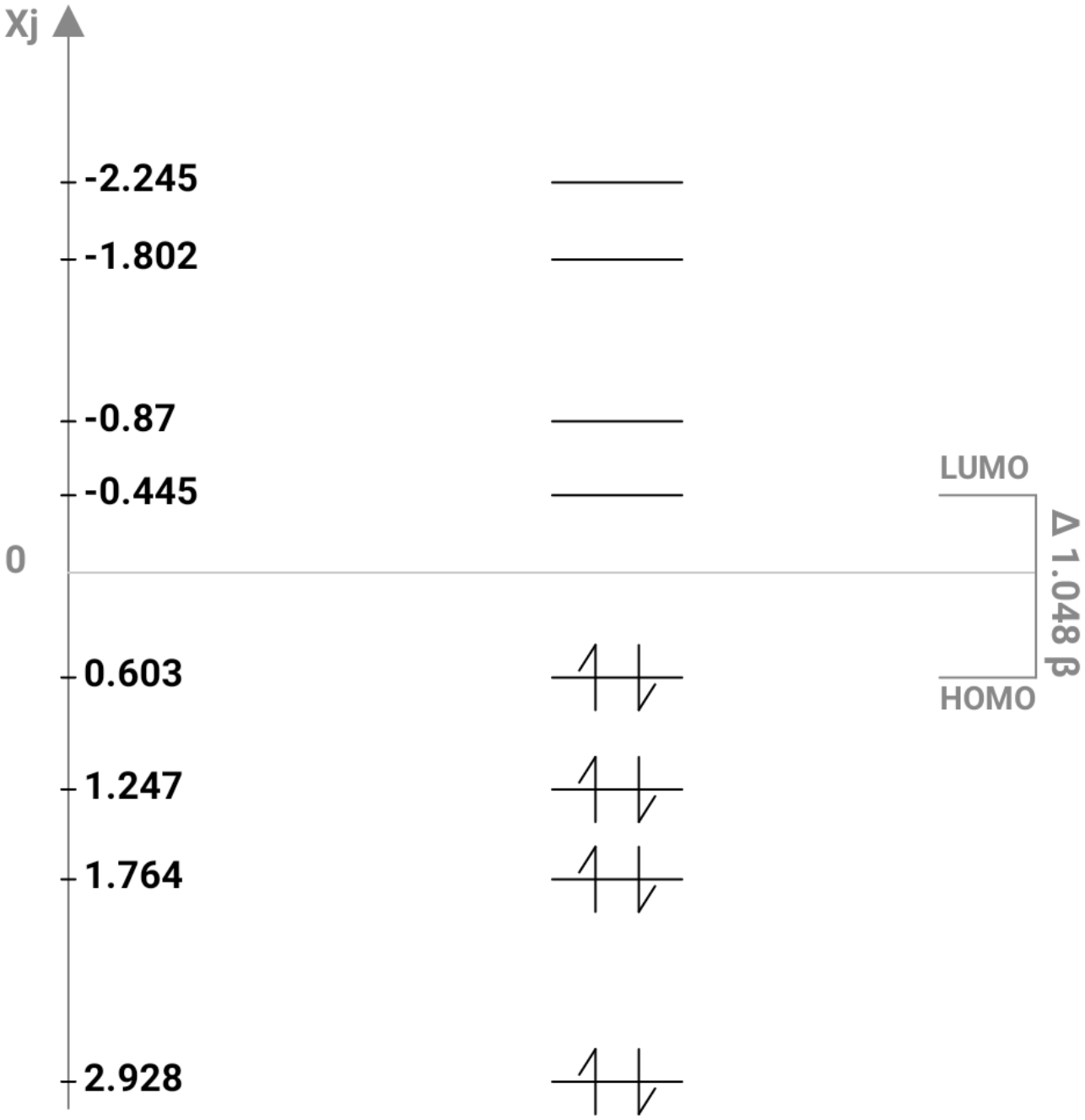


HMO-Energies

x1 = 2.928; x2 = 1.764; x3 = 1.247; x4 = 0.603; x5 = -0.445; x6 = -0.87; x7 = -1.802; x8 = -2.245;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 8α + 13.084β -

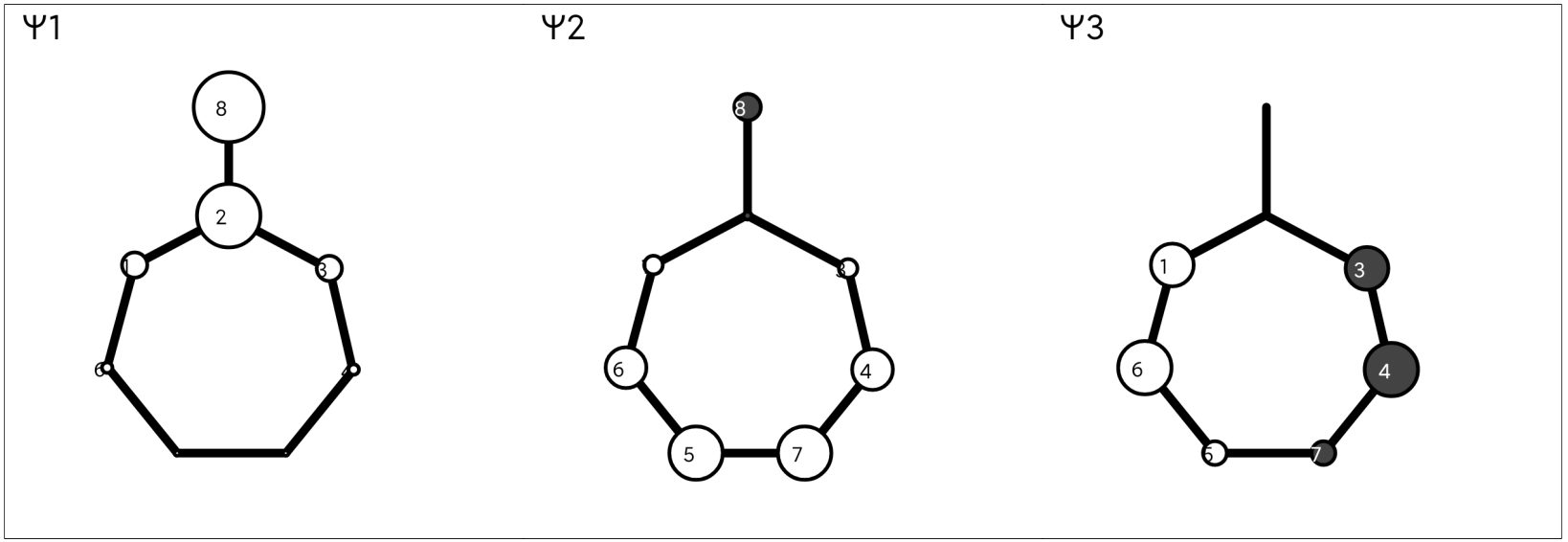
this corresponds to one πelectron: 1.636β

2. Hueckel-coefficient

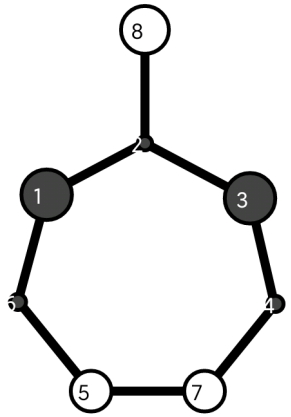
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8
	x1= 2.928	x2= 1.764	x3= 1.247	x4= 0.603	x5= -0.445	x6= -0.87	x7= -1.802	x8= -2.245
1	0.247	0.181	0.418	-0.472	0.521	-0.173	-0.232	-0.392
2	0.619	-0.079	0.0	-0.134	0.0	-0.366	0.0	0.677
3	0.247	0.181	-0.418	-0.472	-0.521	-0.173	0.232	-0.392
4	0.102	0.398	-0.521	-0.151	0.232	0.517	-0.418	0.202
5	0.053	0.521	0.232	0.381	-0.418	-0.276	-0.521	-0.062
6	0.102	0.398	0.521	-0.151	-0.232	0.517	0.418	0.202
7	0.053	0.521	-0.232	0.381	0.418	-0.276	0.521	-0.062
8	0.684	-0.26	0.0	0.447	0.0	0.345	0.0	-0.381

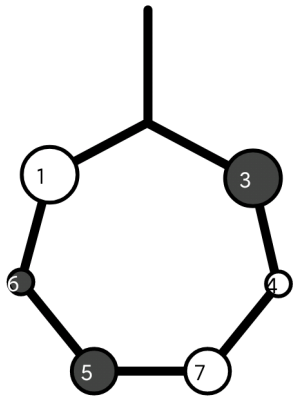
2.2. Molecule orbital presentation:



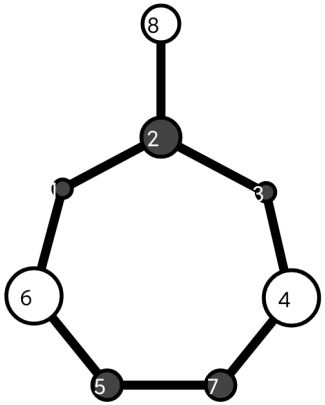
Ψ4



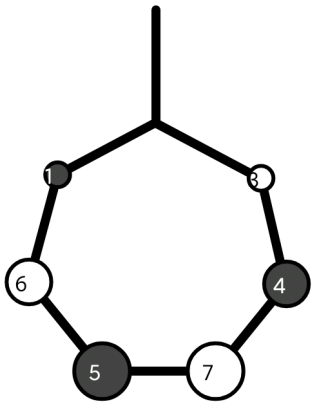
Ψ5



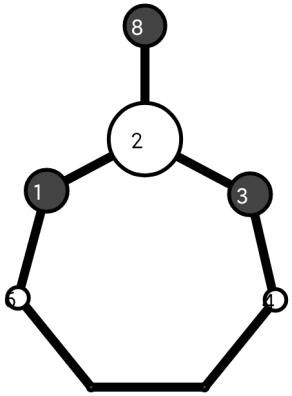
Ψ6



Ψ7



Ψ8

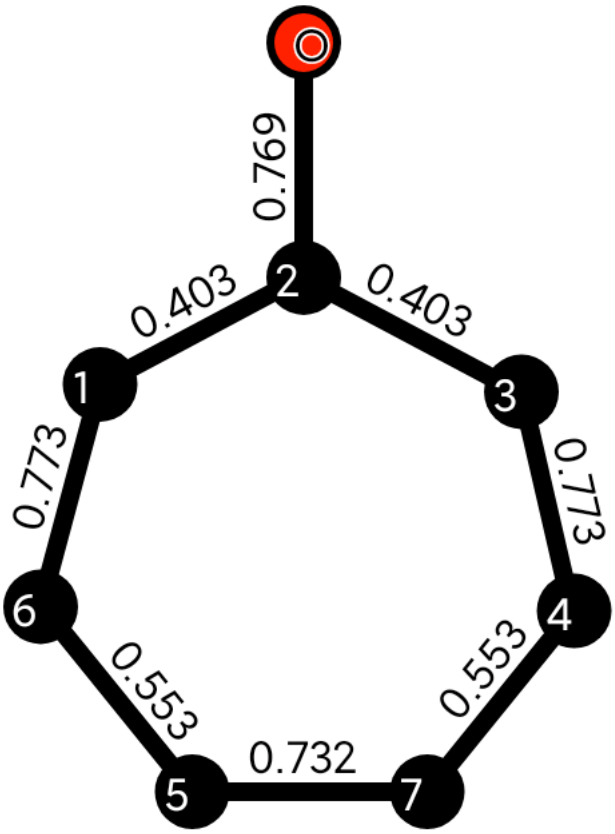


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8
1	0.982							
2	0.403	0.816						
3	0.284	0.403	0.982					
4	-0.098	0.105	0.773	0.927				
5	0.049	-0.118	-0.338	0.069	0.947			
6	0.773	0.105	-0.098	-0.159	0.553	0.927		
7	-0.338	-0.118	0.049	0.553	0.732	0.069	0.947	
8	-0.179	0.769	-0.179	-0.202	0.143	-0.202	0.143	1.471

3.2. Presentation of bond order:

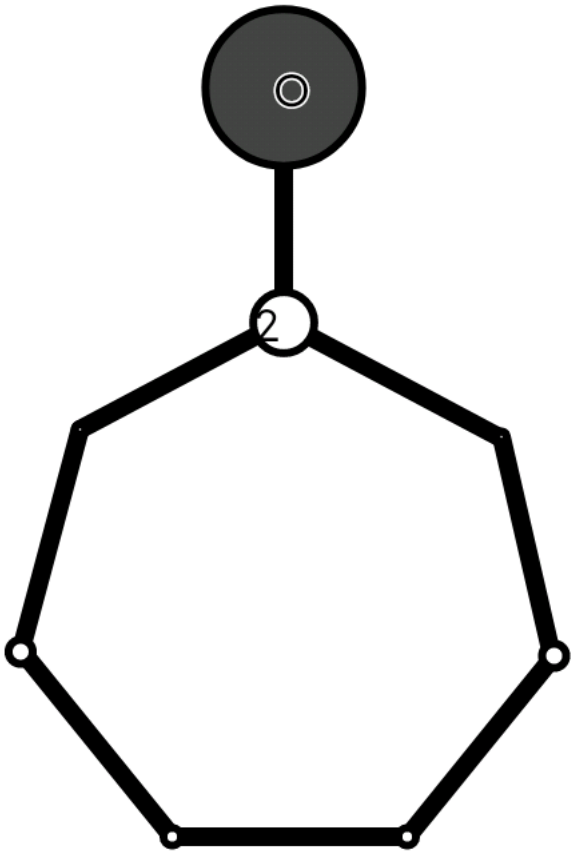


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8
1	0.018							
2		0.184						
3			0.018					
4				0.073				
5					0.053			
6						0.073		
7							0.053	
8								-0.471

4.2. Presentation of molecule:

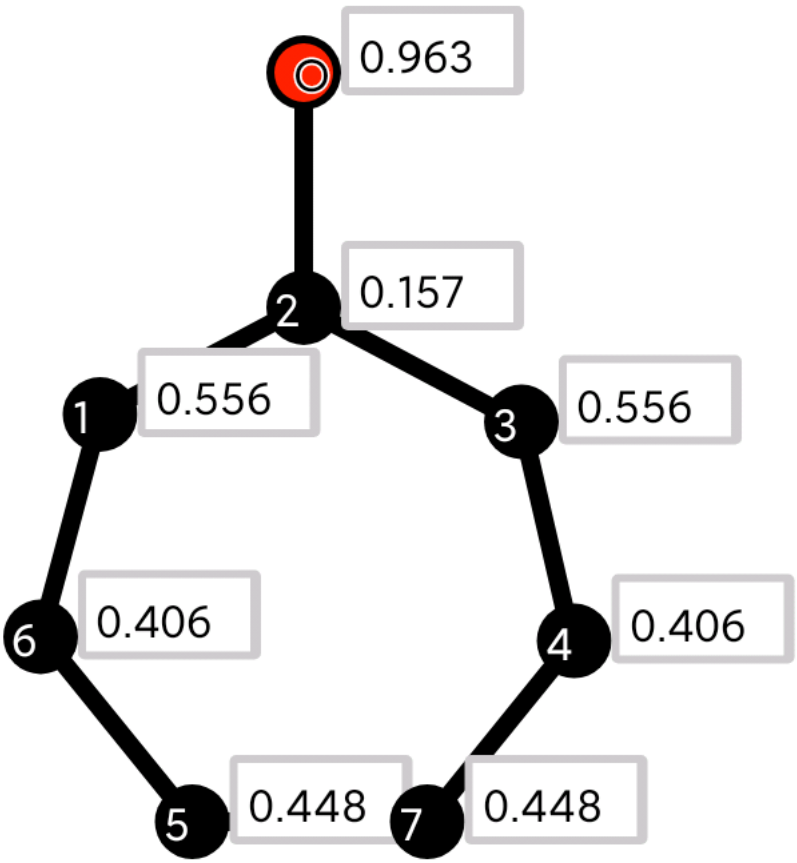


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8
0.556	0.157	0.556	0.406	0.448	0.406	0.448	0.963

5.2. Presentation of molecule:

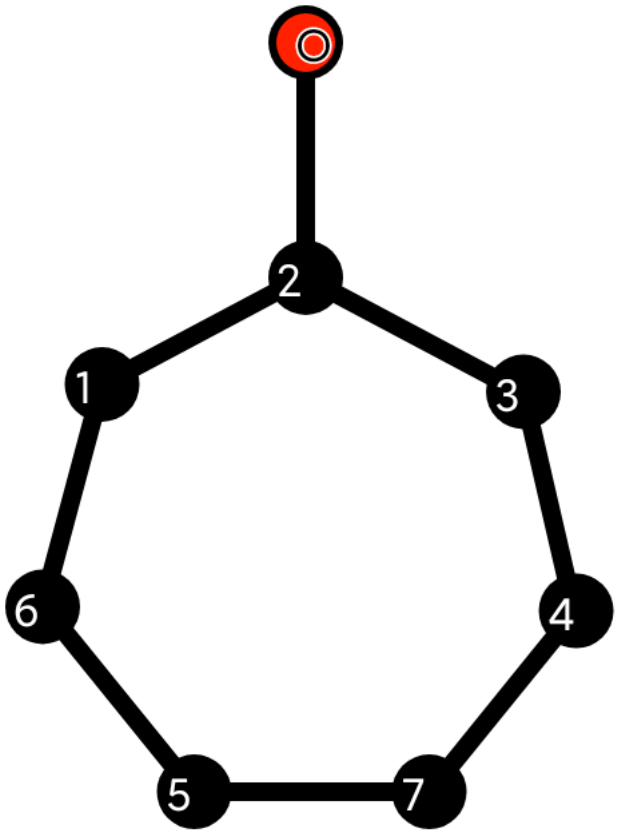


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8
1	0.538							
2	-0.031	0.212						
3	-0.126	-0.031	0.538					
4	-0.004	-0.008	-0.265	0.399				
5	0.044	-0.013	-0.152	0.017	0.445			
6	-0.265	-0.008	-0.004	-0.021	-0.081	0.399		
7	-0.152	-0.013	0.044	-0.081	-0.235	0.017	0.445	
8	-0.004	-0.108	-0.004	-0.036	-0.025	-0.036	-0.025	0.239

6.2. Presentation of molecule:

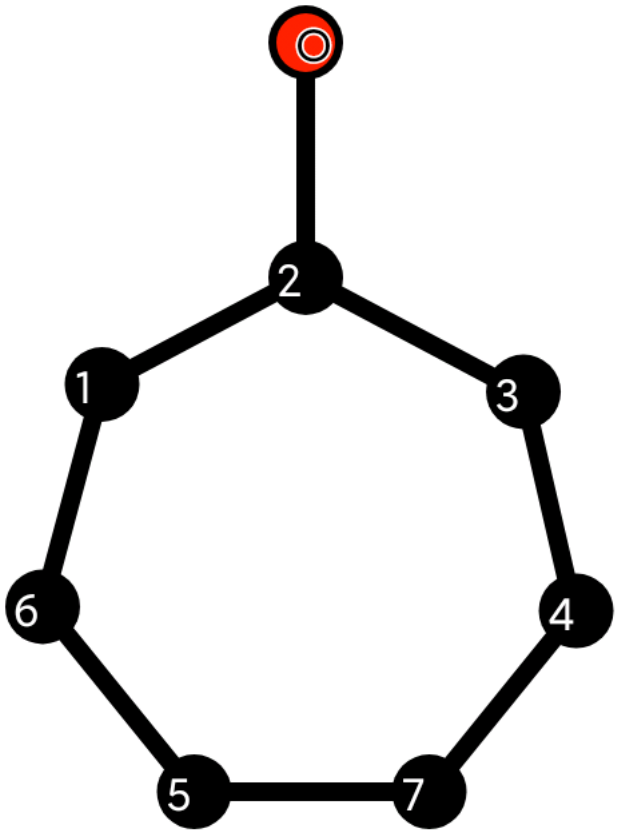


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8
1 2	0.034	0.036	-0.053	0.007	0.007	-0.053	-0.044	0.067
1 6	-0.001	-0.02	0.028	-0.013	-0.014	0.03	0.026	-0.036
2 3	-0.053	0.036	0.034	-0.053	-0.044	0.007	0.007	0.067
2 8	0.019	0.01	0.019	0.02	0.019	0.02	0.019	-0.126
3 4	0.028	-0.02	-0.001	0.03	0.026	-0.013	-0.014	-0.036
4 7	-0.033	0.013	-0.022	0.021	-0.035	0.009	0.017	0.032
5 6	-0.022	0.013	-0.033	0.009	0.017	0.021	-0.035	0.032
5 7	0.015	-0.013	0.015	-0.018	0.022	-0.018	0.022	-0.025

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	2 3	2 8	3 4	4 7	5 6	5 7
1 2	0.289							
1 6	-0.131	0.192						
2 3	-0.011	-0.015	0.289					
2 8	-0.139	0.062	-0.139	0.182				
3 4	-0.015	0.043	-0.131	0.062	0.192			
4 7	0.03	-0.055	0.064	-0.044	-0.218	0.338		
5 6	0.064	-0.218	0.03	-0.044	-0.055	0.086	0.338	
5 7	-0.037	0.109	-0.037	0.038	0.109	-0.199	-0.199	0.21

8.2. Presentation of molecule: