Print calculated values

Report generated by:root, 23.02.2020 - 09:28:10

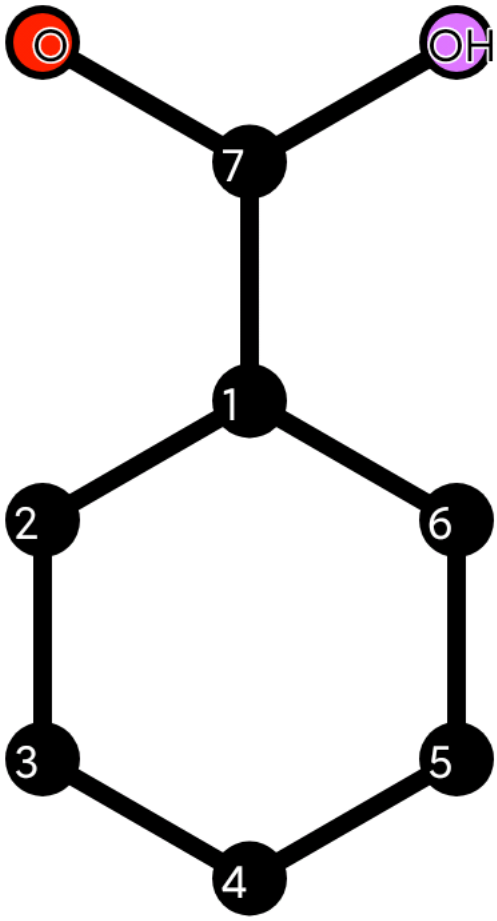
The following determinant is calculated:

-x	1.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0
1.0	-x	1.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	1.0	-x	1.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	1.0	-x	1.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	1.0	-x	1.0	0.0	0.0	0.0
1.0	0.0	0.0	0.0	1.0	-x	0.0	0.0	0.0
1.0	0.0	0.0	0.0	0.0	0.0	-x	1.93	0.9
0.0	0.0	0.0	0.0	0.0	0.0	1.93	-x+1.18	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.9	0.0	-x+2.0

It is about this molecule:

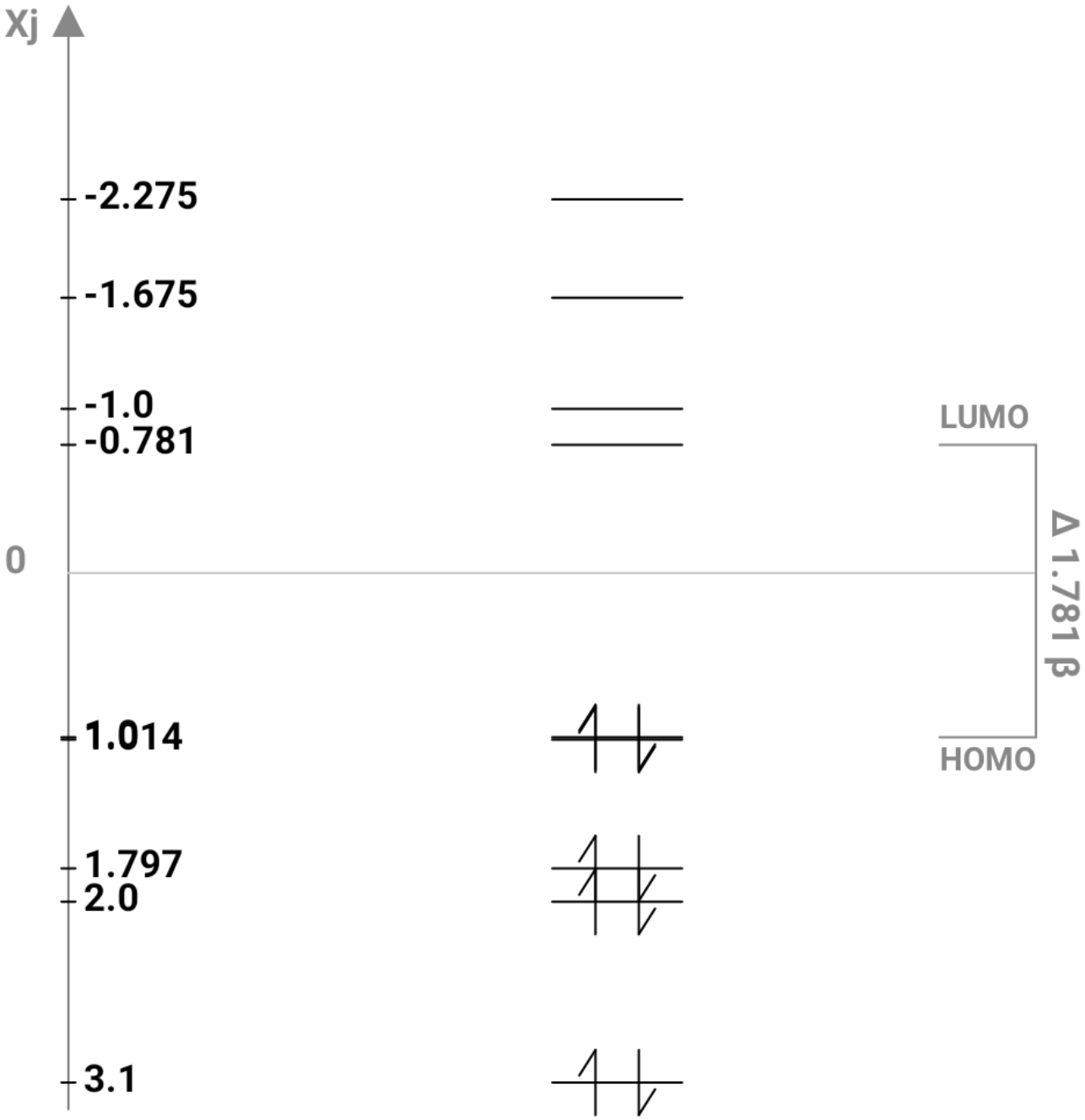
HMO-Energies

x1 = 3.1; x2 = 2.0; x3 = 1.797; x4 = 1.014; x5 = 1.0; x6 = -0.781; x7 = -1.0; x8 = -1.675; x9 = -2.275;


O
OH
7
1
2
6
3
5
4

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 9α + 17.822β -

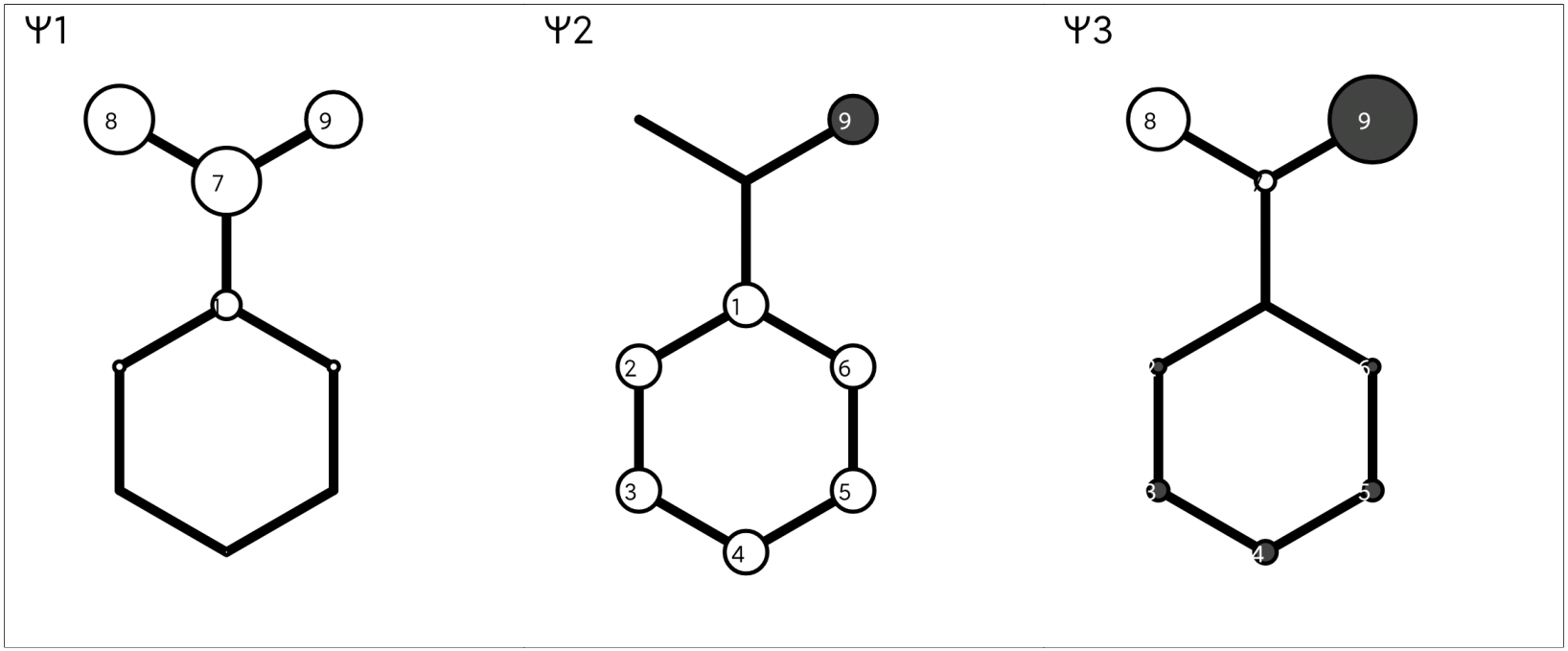
this corresponds to one πelectron: 1.782β

2. Hueckel-coefficient

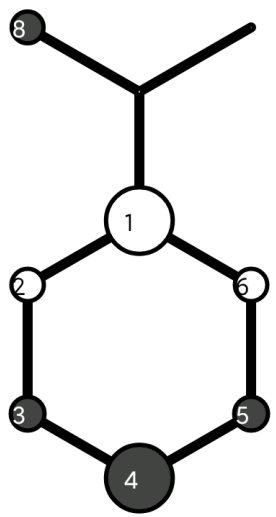
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9
	x1= 3.1	x2= 2.0	x3= 1.797	x4= 1.014	x5= 1.0	x6= -0.781	x7= -1.0	x8= -1.675	x9= -2.275
1	0.248	0.372	-0.041	0.557	0.0	0.464	0.0	0.076	0.517
2	0.092	0.372	-0.121	0.271	-0.5	-0.345	0.5	0.19	-0.332
3	0.038	0.372	-0.177	-0.283	-0.5	-0.194	-0.5	-0.394	0.237
4	0.024	0.372	-0.197	-0.557	0.0	0.497	0.0	0.47	-0.209
5	0.038	0.372	-0.177	-0.283	0.5	-0.194	0.5	-0.394	0.237
6	0.092	0.372	-0.121	0.271	0.5	-0.345	-0.5	0.19	-0.332
7	0.585	0.0	0.169	0.023	0.0	0.329	0.0	-0.507	-0.513
8	0.588	0.0	0.528	-0.267	0.0	-0.324	0.0	0.343	0.286
9	0.479	-0.413	-0.749	-0.021	0.0	-0.106	0.0	0.124	0.108

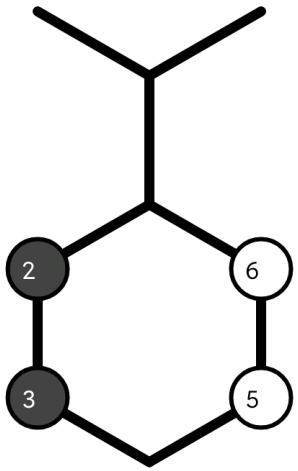
2.2. Molecule orbital presentation:



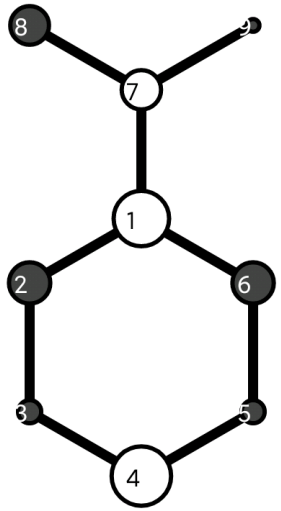
Ψ4



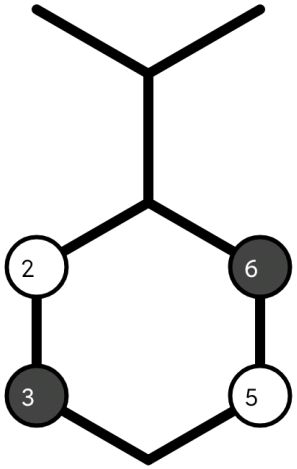
Ψ5



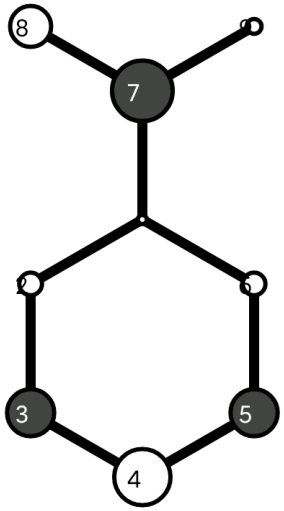
Ψ6



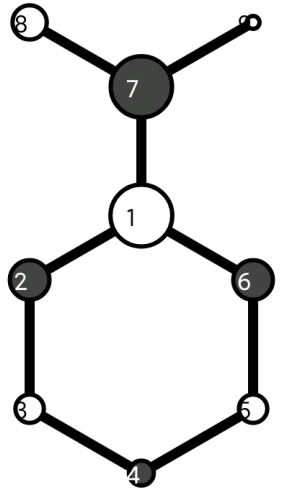
Ψ7



Ψ8



Ψ9

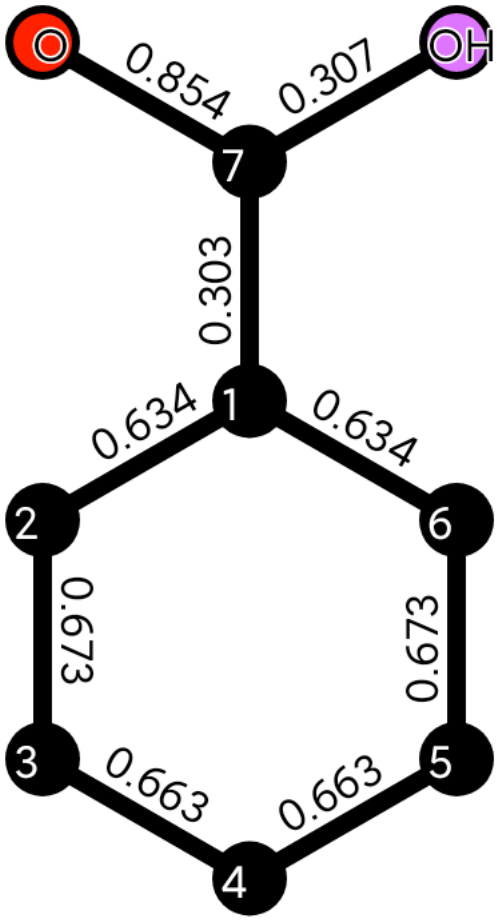


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9
1	1.024								
2	0.634	0.97							
3	-0.005	0.673	1.001						
4	-0.317	0.026	0.663	0.976					
5	-0.005	-0.327	0.001	0.663	1.001				
6	0.634	-0.03	-0.327	0.026	0.673	0.97			
7	0.303	0.08	-0.029	-0.064	-0.029	0.08	0.743		
8	-0.048	-0.164	0.009	0.119	0.009	-0.164	0.854	1.391	
9	-0.032	-0.049	0.005	0.034	0.005	-0.049	0.307	-0.216	1.923

3.2. Presentation of bond order:

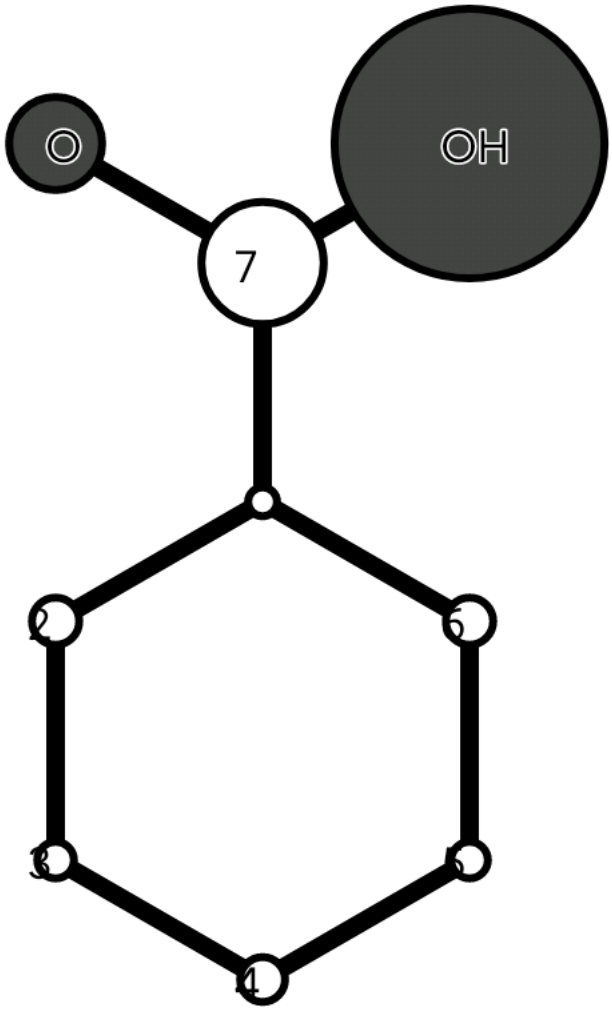


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9
1	0.087								
2		0.142							
3			0.11						
4				0.135					
5					0.11				
6						0.142			
7							0.368		
8								-0.28	
9									-0.812

4.2. Presentation of molecule:

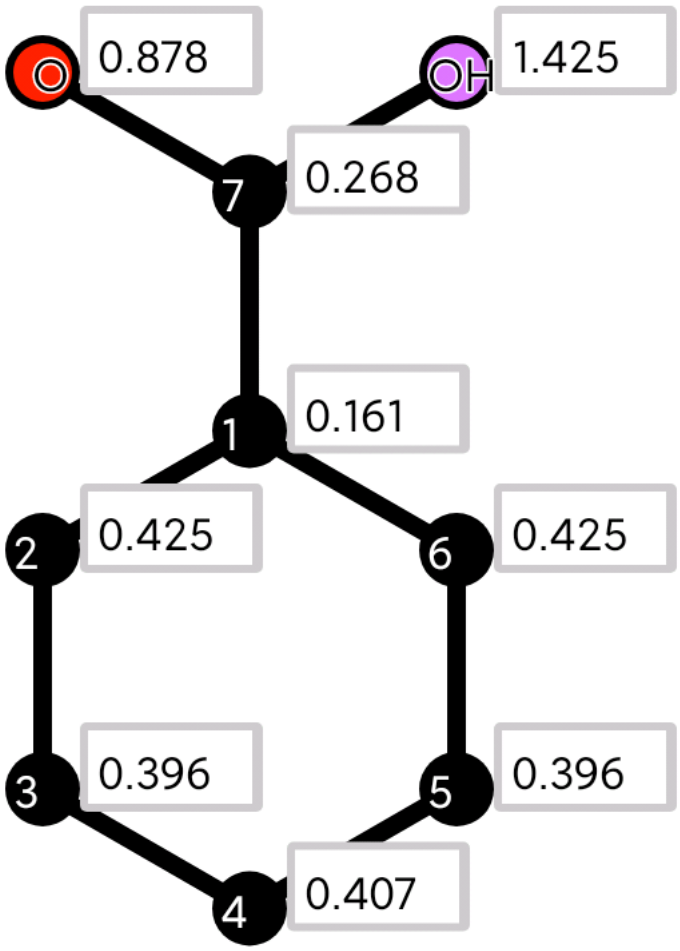


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9
0.161	0.425	0.396	0.407	0.396	0.425	0.268	0.878	1.425

5.2. Presentation of molecule:

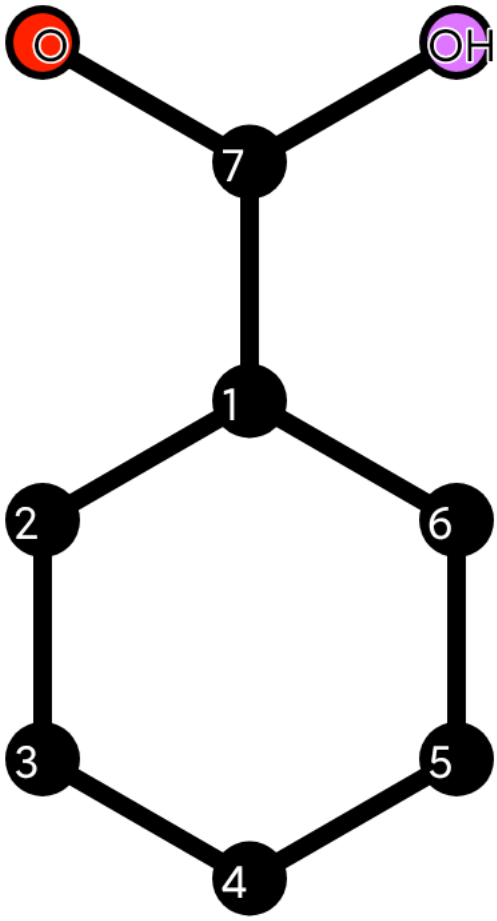


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9
1	0.358								
2	-0.142	0.412							
3	0.008	-0.161	0.397						
4	-0.095	0.011	-0.155	0.404					
5	0.008	-0.099	0.01	-0.155	0.397				
6	-0.142	0.005	-0.099	0.011	-0.161	0.412			
7	-0.011	-0.003	0.0	-0.004	0.0	-0.003	0.2		
8	0.015	-0.021	0.001	-0.017	0.001	-0.021	-0.167	0.234	
9	0.001	-0.002	0.0	-0.001	0.0	-0.002	-0.013	-0.025	0.041

6.2. Presentation of molecule:

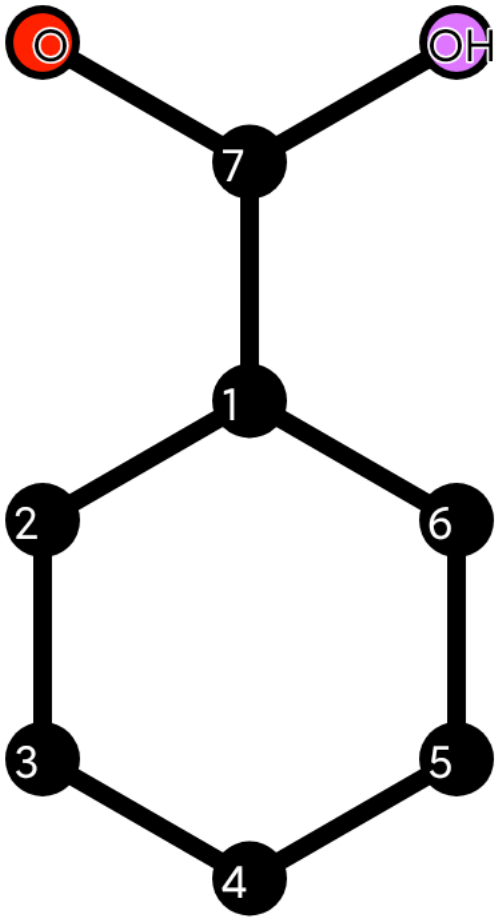


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9
1 2	-0.013	0.005	0.001	0.009	-0.002	0.014	-0.007	-0.006	-0.001
1 6	-0.013	0.014	-0.002	0.009	0.001	0.005	-0.007	-0.006	-0.001
1 7	0.021	-0.028	0.001	-0.022	0.001	-0.028	0.028	0.023	0.005
2 3	0.003	0.015	0.001	-0.011	0.0	-0.012	0.002	0.002	0.0
3 4	-0.002	-0.012	-0.002	0.009	0.0	0.01	-0.001	-0.001	0.0
4 5	-0.002	0.01	0.0	0.009	-0.002	-0.012	-0.001	-0.001	0.0
5 6	0.003	-0.012	0.0	-0.011	0.001	0.015	0.002	0.002	0.0
7 8	-0.004	0.011	0.0	0.009	0.0	0.011	0.049	-0.097	0.022
7 9	0.0	0.002	0.0	0.002	0.0	0.002	0.002	0.069	-0.079

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	1 7	2 3	3 4	4 5	5 6	7 8	7 9
1 2	0.243								
1 6	-0.178	0.243							
1 7	-0.063	-0.063	0.281						
2 3	-0.196	0.12	0.012	0.244					
3 4	0.127	-0.087	-0.008	-0.209	0.246				
4 5	-0.087	0.127	-0.008	0.128	-0.203	0.246			
5 6	0.12	-0.196	0.012	-0.092	0.128	-0.209	0.244		
7 8	0.02	0.02	-0.089	-0.005	0.003	0.003	-0.005	0.109	
7 9	0.007	0.007	-0.032	-0.002	0.001	0.001	-0.002	-0.097	0.314

8.2. Presentation of molecule: