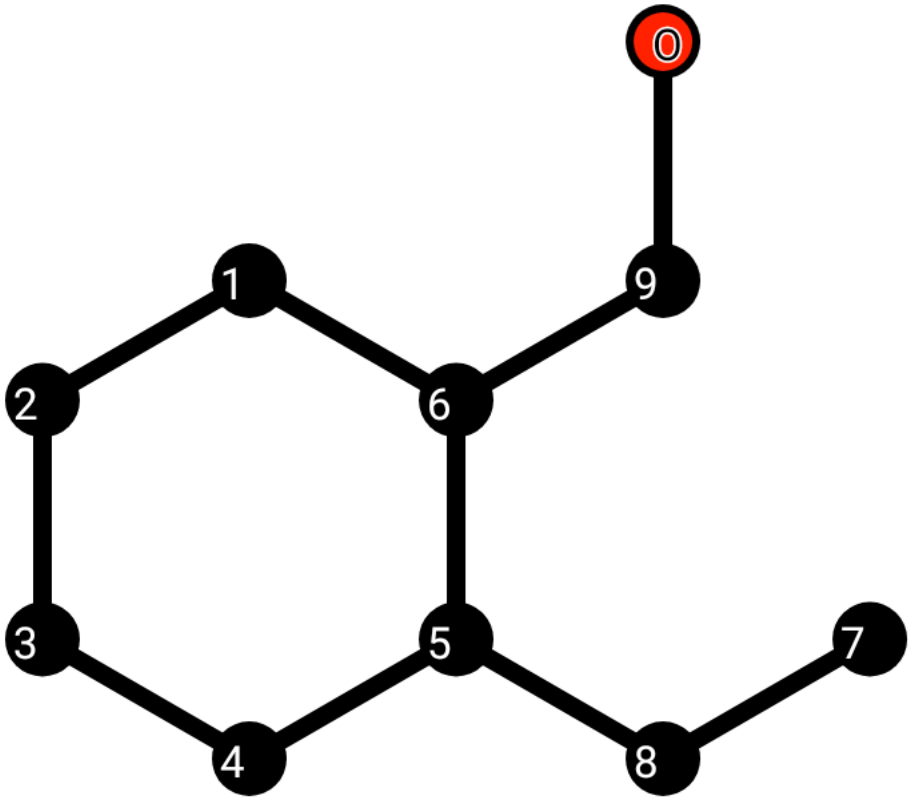
Print calculated values

Report generated by:root, 16.05.2020 - 18:48:24

The following determinant is calculated:

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

It is about this molecule:

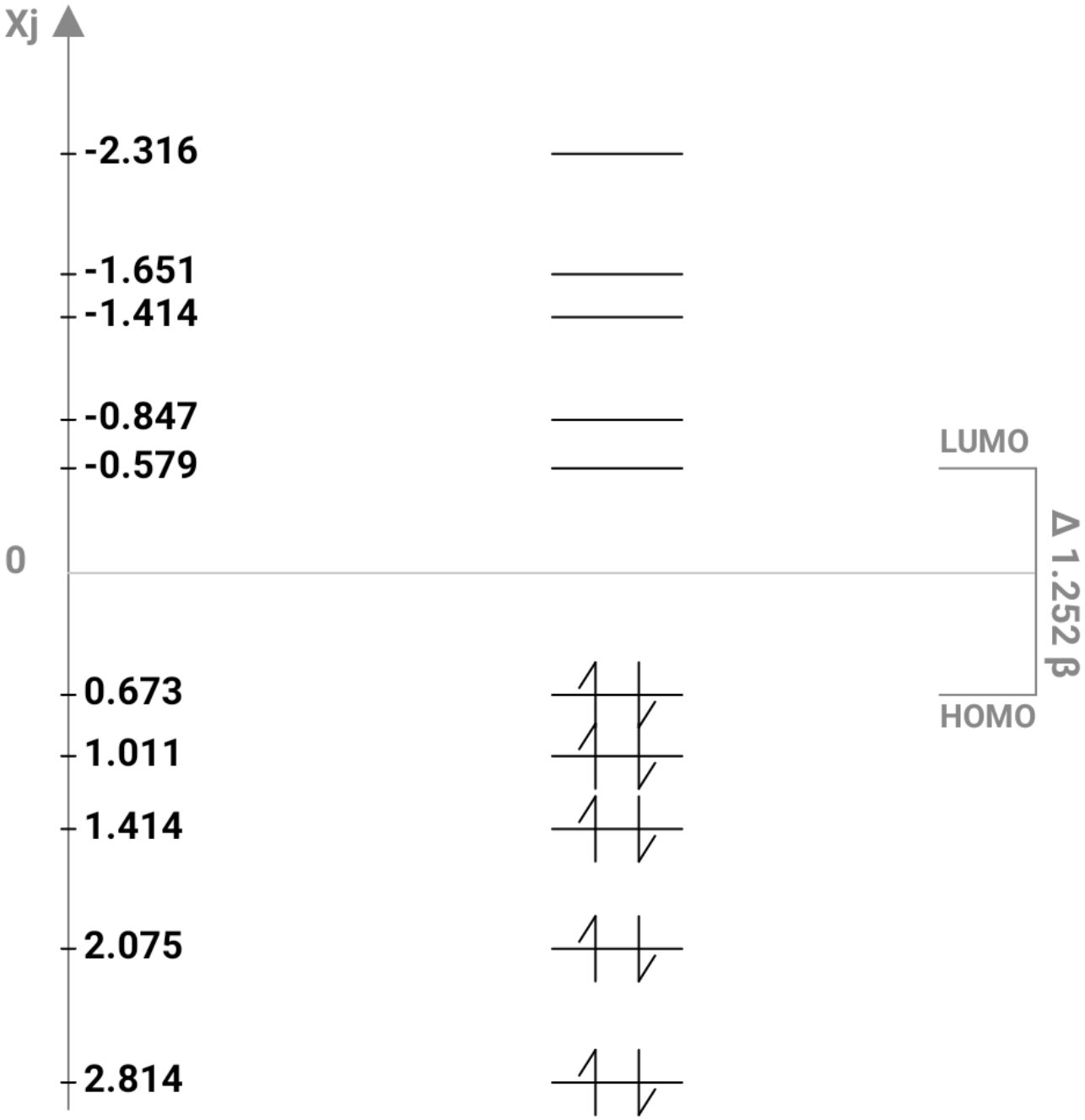


HMO-Energies

x1 = 2.814; x2 = 2.075; x3 = 1.414; x4 = 1.011; x5 = 0.673; x6 = -0.579; x7 = -0.847; x8 = -1.414; x9 = -1.651; x10 = -2.316;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 10α + 15.974β -

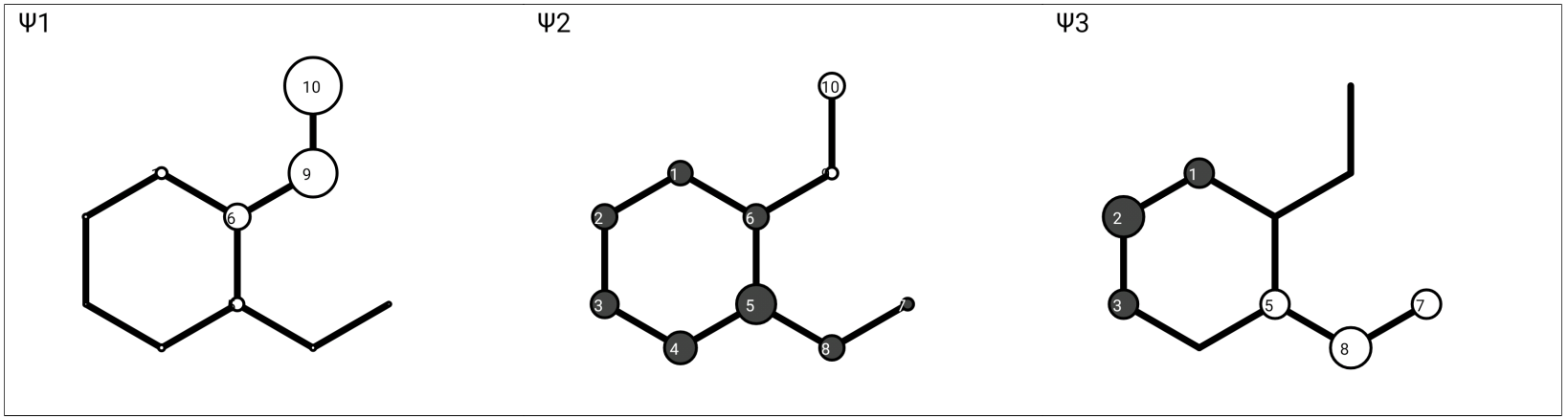
this corresponds to one πelectron: 1.597β

2. Hueckel-coefficient

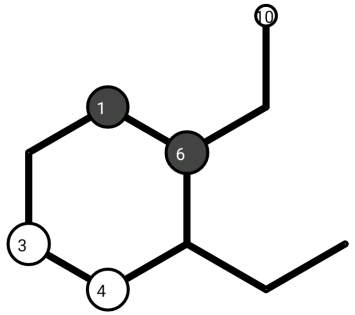
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10
	x1= 2.814	x2= 2.075	x3= 1.414	x4= 1.011	x5= 0.673	x6= -0.579	x7= -0.847	x8= -1.414	x9= -1.651	x10= -2.316
1	0.136	-0.292	-0.354	-0.477	-0.165	0.088	0.533	-0.354	0.021	0.316
2	0.066	-0.302	-0.5	0.01	-0.394	0.317	-0.2	0.5	-0.232	-0.233
3	0.05	-0.336	-0.354	0.487	-0.1	-0.271	-0.363	-0.354	0.362	0.225
4	0.076	-0.394	0.0	0.482	0.327	-0.16	0.508	0.0	-0.366	-0.287
5	0.163	-0.482	0.354	0.0	0.32	0.364	-0.067	0.354	0.242	0.44
6	0.316	-0.303	0.0	-0.492	0.283	-0.368	-0.251	0.0	0.198	-0.498
7	0.024	-0.146	0.354	0.01	-0.586	-0.547	0.236	0.354	0.14	0.101
8	0.066	-0.302	0.5	0.01	-0.394	0.317	-0.2	-0.5	-0.232	-0.233
9	0.591	0.145	0.0	-0.021	0.035	-0.239	-0.253	0.0	-0.59	0.398
10	0.698	0.313	0.0	0.244	-0.134	0.262	0.241	0.0	0.402	-0.22

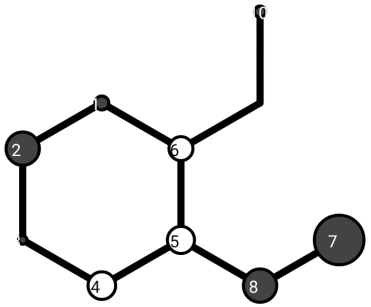
2.2. Molecule orbital presentation:



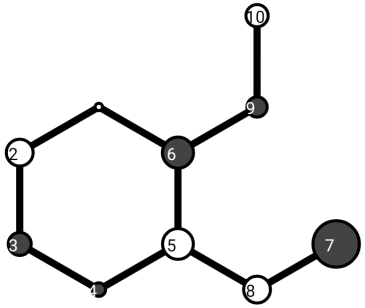
Ψ4



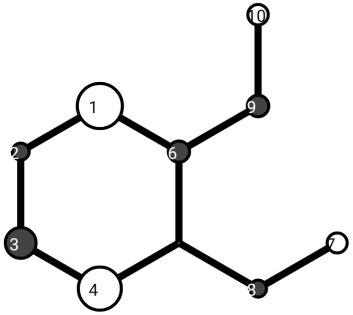
Ψ5



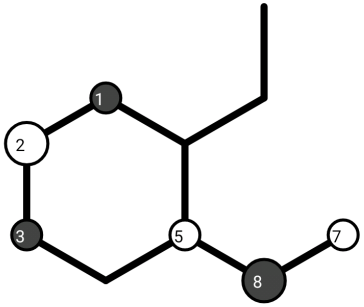
Ψ6



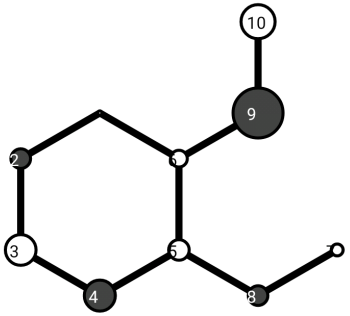
Ψ7



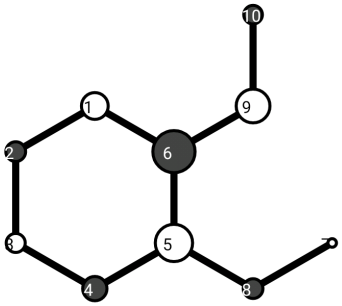
Ψ8



Ψ9



Ψ10

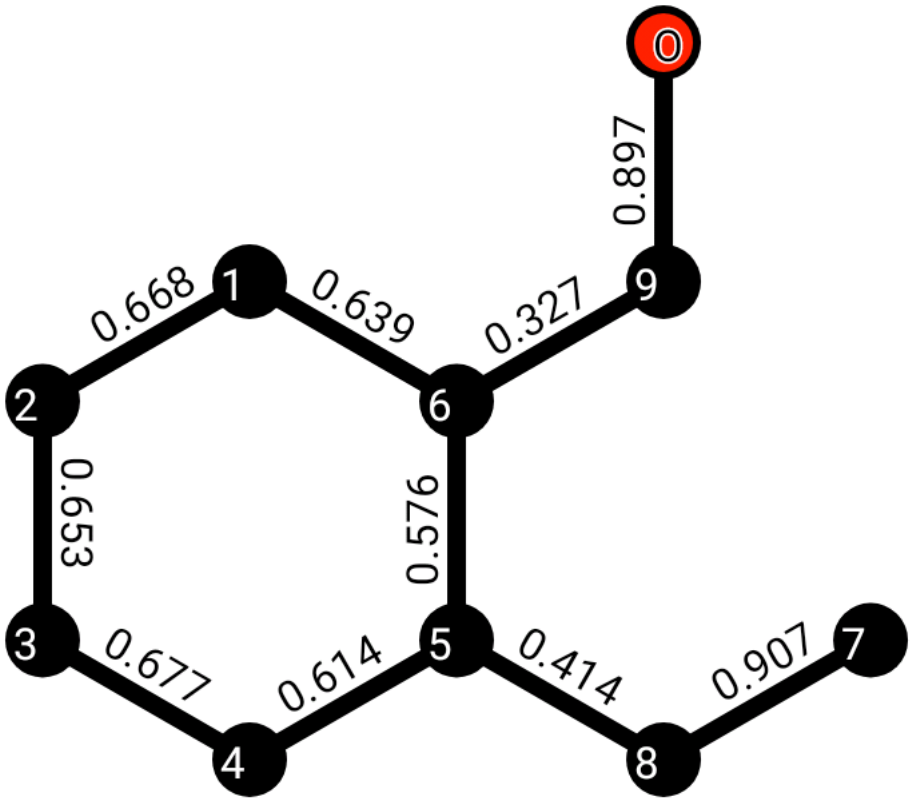


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.966									
2	0.668	1.003								
3	0.028	0.653	0.976							
4	-0.317	0.001	0.677	1.0						
5	-0.03	-0.293	0.026	0.614	0.972					
6	0.639	-0.008	-0.301	-0.003	0.576	1.029				
7	0.025	0.2	-0.022	-0.254	0.023	-0.239	0.98			
8	-0.039	0.003	-0.054	0.001	0.414	-0.008	0.907	1.003		
9	0.085	-0.038	-0.066	-0.022	0.075	0.327	-0.056	-0.038	0.745	
10	-0.181	0.014	0.125	0.007	-0.16	-0.064	0.104	0.014	0.897	1.326

3.2. Presentation of bond order:

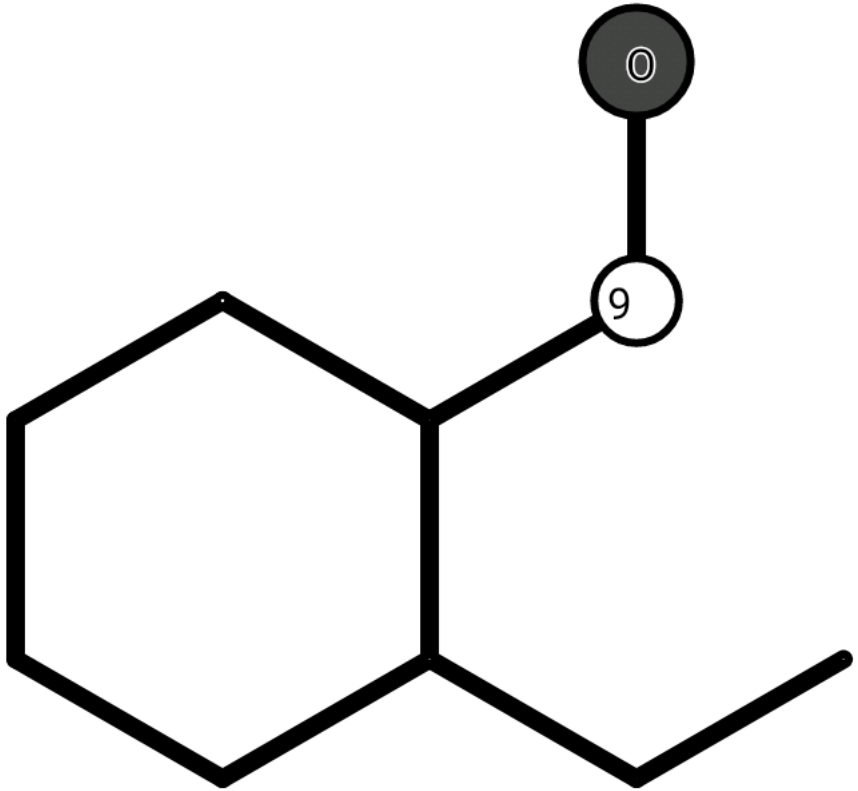

0
1
2
3
4
5
6
7
8
9
0.897
0.668
0.639
0.327
0.653
0.576
0.677
0.614
0.414
0.907

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.034									
2		-0.003								
3			0.024							
4				0.0						
5					0.028					
6						-0.029				
7							0.02			
8								-0.003		
9									0.255	
10										-0.326

4.2. Presentation of molecule:

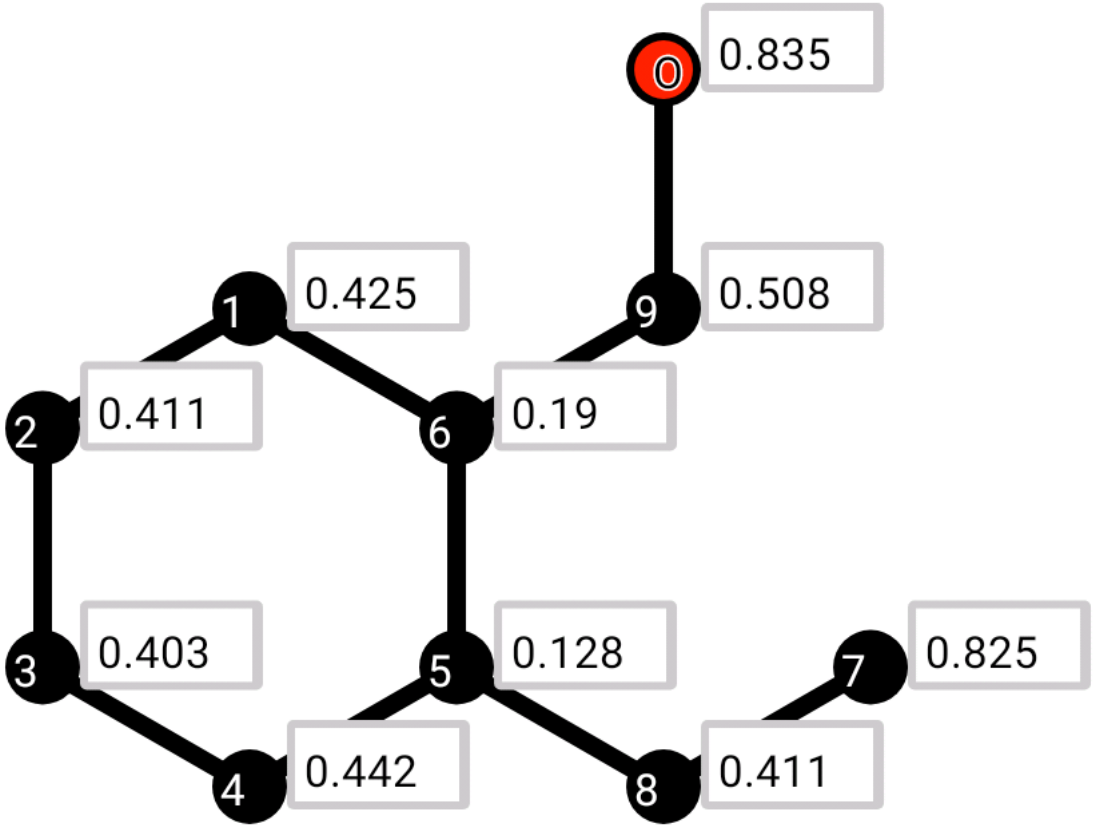

0
9

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10
0.425	0.411	0.403	0.442	0.128	0.19	0.825	0.411	0.508	0.835

5.2. Presentation of molecule:

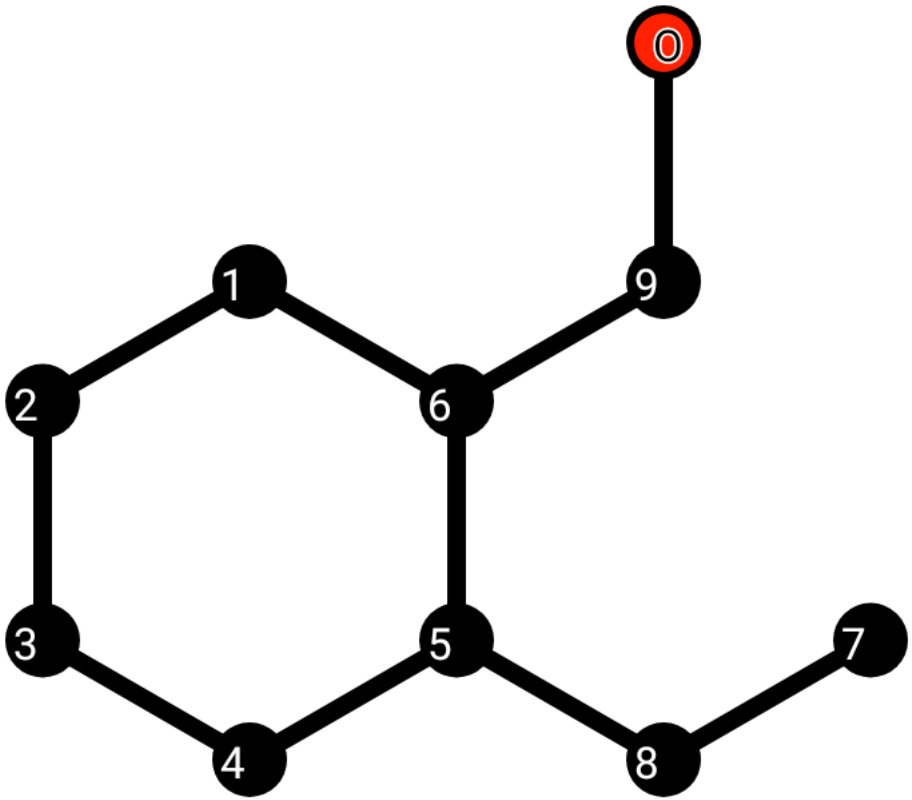

0
0.835
1
0.425
9
0.508
2
0.411
6
0.19
3
0.403
5
0.128
7
0.825
4
0.442
8
0.411

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.413									
2	-0.158	0.412								
3	0.012	-0.148	0.402							
4	-0.095	0.016	-0.164	0.429						
5	0.003	-0.084	0.008	-0.131	0.347					
6	-0.145	0.014	-0.087	0.003	-0.115	0.379				
7	0.0	-0.063	0.002	-0.075	0.033	-0.069	0.606			
8	-0.001	0.008	-0.002	0.016	-0.036	0.014	-0.414	0.412		
9	-0.003	0.0	-0.004	0.0	-0.003	-0.013	-0.004	0.0	0.217	
10	-0.026	0.002	-0.019	0.0	-0.022	0.021	-0.016	0.002	-0.189	0.247

6.2. Presentation of molecule:

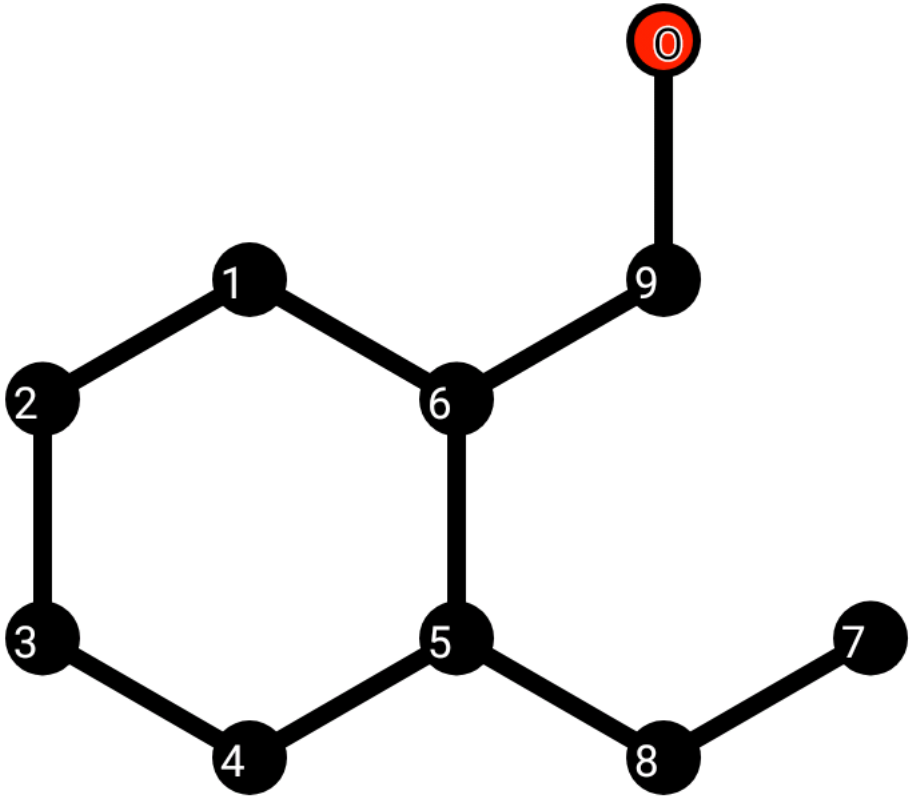

0
1
2
3
4
5
6
7
8
9

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1 2	0.017	0.002	-0.011	0.0	-0.011	0.006	-0.009	0.001	0.003	0.003
1 6	0.005	0.002	0.009	-0.001	0.013	-0.017	0.01	-0.001	-0.01	-0.01
2 3	-0.013	-0.003	0.009	0.0	0.009	-0.004	0.008	-0.001	-0.002	-0.002
3 4	0.011	0.001	0.011	-0.001	-0.011	-0.001	-0.009	0.001	-0.001	-0.001
4 5	-0.012	-0.001	-0.011	0.001	0.012	0.001	0.009	-0.001	0.001	0.001
5 6	0.014	-0.003	0.008	0.001	0.005	-0.014	0.006	0.0	-0.008	-0.009
5 8	-0.001	0.002	0.001	0.0	0.004	0.005	-0.018	0.002	0.003	0.003
6 9	-0.03	0.002	-0.023	0.0	-0.025	0.024	-0.019	0.002	0.033	0.035
7 8	0.001	-0.001	-0.001	0.0	-0.003	-0.003	0.015	-0.003	-0.002	-0.002
9 10	0.012	-0.001	0.01	0.0	0.011	-0.004	0.009	-0.001	0.049	-0.085

7.2. Presentation of molecule:

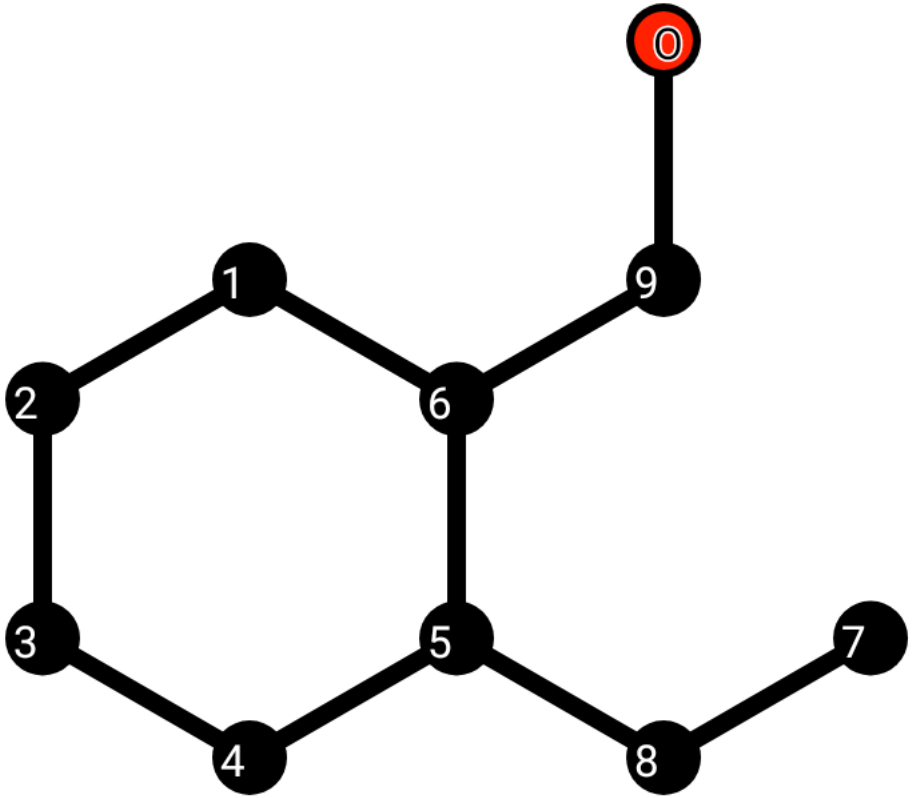

0
1
2
3
4
5
6
7
8
9

8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	2 3	3 4	4 5	5 6	5 8	6 9	7 8	9 10
1 2	0.256									
1 6	-0.206	0.252								
2 3	-0.209	0.124	0.26							
3 4	0.127	-0.086	-0.214	0.252						
4 5	-0.081	0.104	0.122	-0.195	0.254					
5 6	0.111	-0.16	-0.074	0.107	-0.149	0.248				
5 8	-0.01	0.014	-0.017	0.025	-0.104	-0.095	0.343			
6 9	0.019	-0.076	-0.012	-0.004	0.007	-0.065	0.016	0.301		
7 8	0.006	-0.007	0.011	-0.014	0.047	0.043	-0.161	-0.009	0.079	
9 10	-0.008	0.028	0.006	0.002	-0.003	0.023	-0.007	-0.112	0.005	0.086

8.2. Presentation of molecule:


0
1
9
2
6
3
5
7
4
8