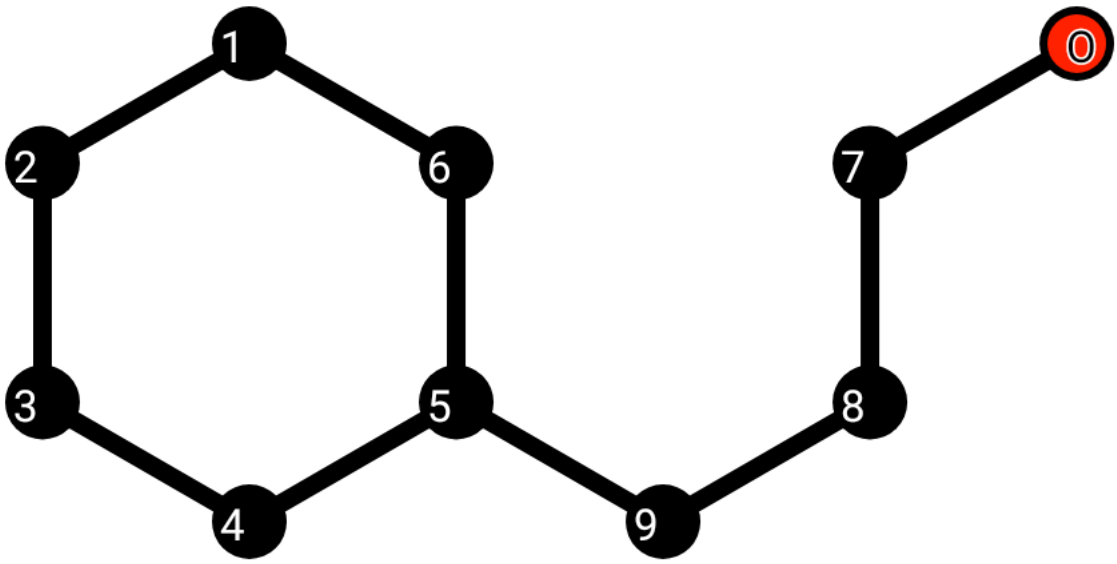
Print calculated values

Report generated by:root, 16.05.2020 - 18:46:51

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

It is about this molecule:

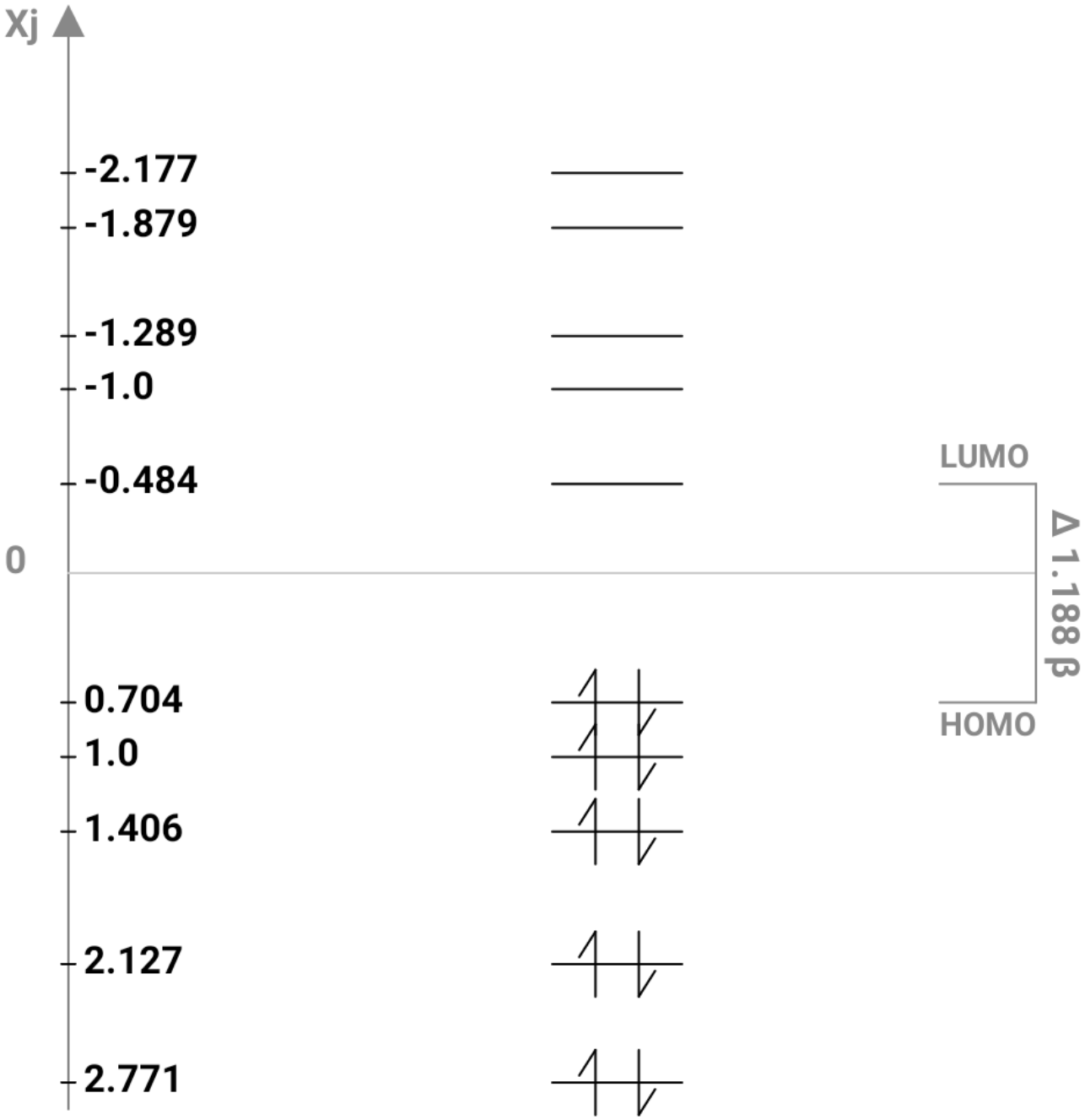


HMO-Energies

x1 = 2.771; x2 = 2.127; x3 = 1.406; x4 = 1.0; x5 = 0.704; x6 = -0.484; x7 = -1.0; x8 = -1.289; x9 = -1.879; x10 = -2.177;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 10α + 16.016β -

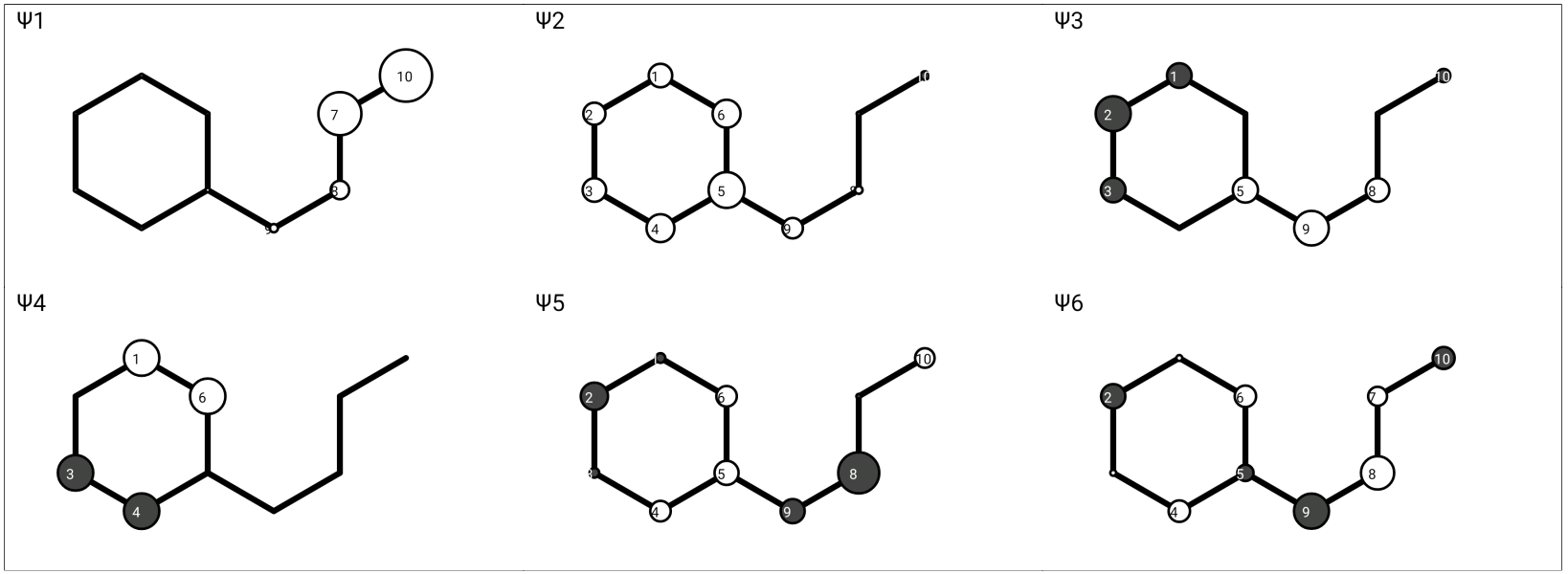
this corresponds to one πelectron: 1.602β

2. Hueckel-coefficient

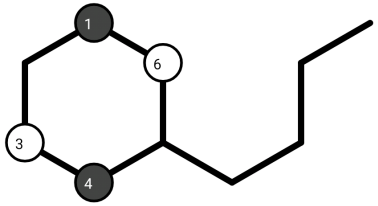
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10
	x1= 2.771	x2= 2.127	x3= 1.406	x4= 1.0	x5= 0.704	x6= -0.484	x7= -1.0	x8= -1.289	x9= -1.879	x10= -2.177
1	0.013	0.332	-0.348	0.5	-0.136	0.083	-0.5	-0.329	0.239	-0.278
2	0.009	0.313	-0.495	0.0	-0.385	-0.343	0.0	0.511	-0.254	0.256
3	0.013	0.332	-0.348	-0.5	-0.136	0.083	0.5	-0.329	0.239	-0.278
4	0.027	0.394	0.006	-0.5	0.29	0.303	-0.5	-0.087	-0.195	0.35
5	0.061	0.507	0.356	0.0	0.34	-0.23	0.0	0.441	0.127	-0.484
6	0.027	0.394	0.006	0.5	0.29	0.303	0.5	-0.087	-0.195	0.35
7	0.608	-0.06	-0.022	0.0	-0.068	0.267	0.0	0.307	0.62	0.267
8	0.261	0.108	0.332	0.0	-0.579	0.469	0.0	0.068	-0.41	-0.285
9	0.116	0.289	0.489	0.0	-0.34	-0.495	0.0	-0.395	0.151	0.353
10	0.737	-0.122	-0.188	0.0	0.275	-0.31	0.0	-0.24	-0.391	-0.153

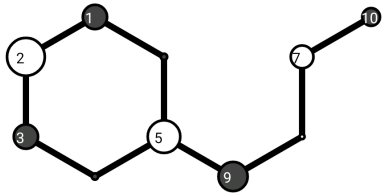
2.2. Molecule orbital presentation:



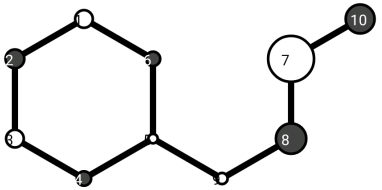
Ψ7



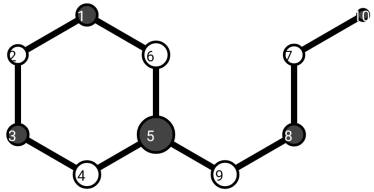
Ψ8



Ψ9



Ψ10

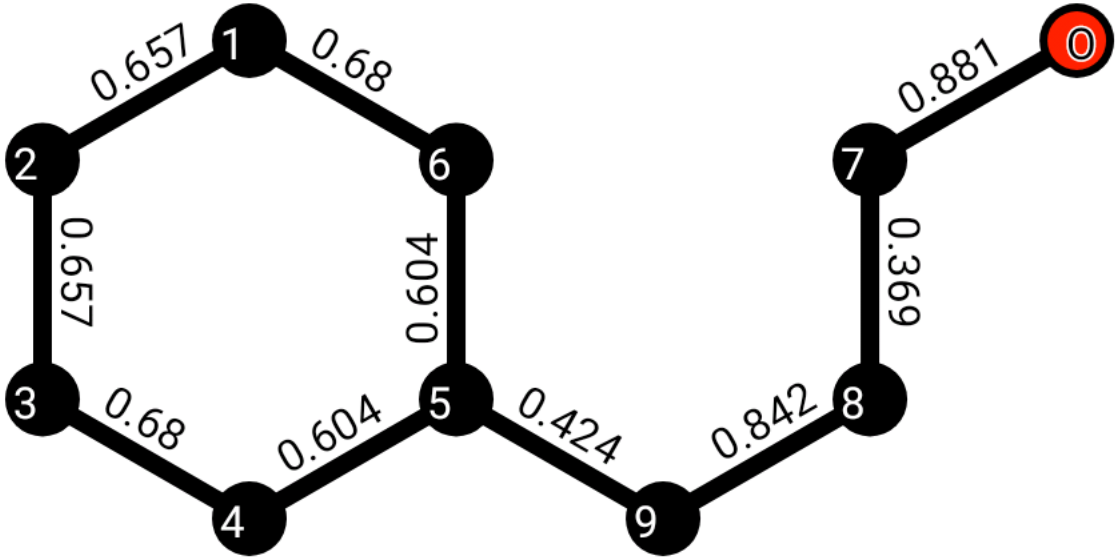


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	1.0									
2	0.657	0.982								
3	0.0	0.657	1.0							
4	-0.32	0.018	0.68	0.981						
5	-0.001	-0.296	-0.001	0.604	1.005					
6	0.68	0.018	-0.32	-0.019	0.604	0.981				
7	0.01	0.048	0.01	-0.054	-0.048	-0.054	0.756			
8	0.004	0.19	0.004	-0.233	-0.016	-0.233	0.369	1.052		
9	-0.053	-0.04	-0.053	0.043	0.424	0.043	0.132	0.842	0.904	
10	-0.005	-0.088	-0.005	0.101	0.02	0.101	0.881	-0.085	-0.27	1.339

3.2. Presentation of bond order:

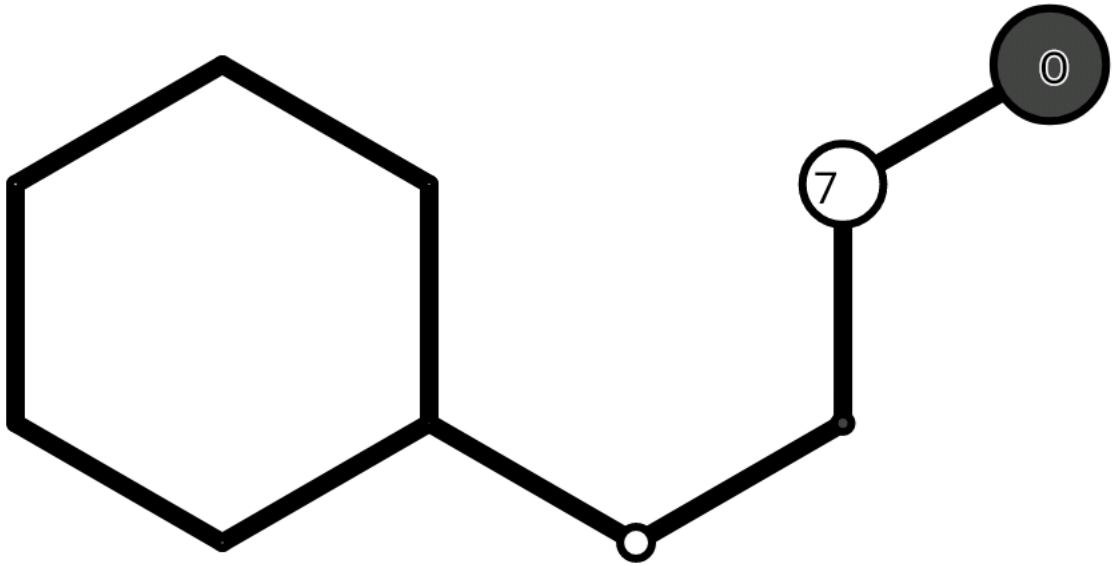

0.657
1
0.68
0.881
0
2
6
7
0.657
0.604
0.369
3
0.68
0.604
5
0.424
0.842
8
4
9

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.0									
2		0.018								
3			0.0							
4				0.019						
5					-0.005					
6						0.019				
7							0.244			
8								-0.052		
9									0.096	
10										-0.339

4.2. Presentation of molecule: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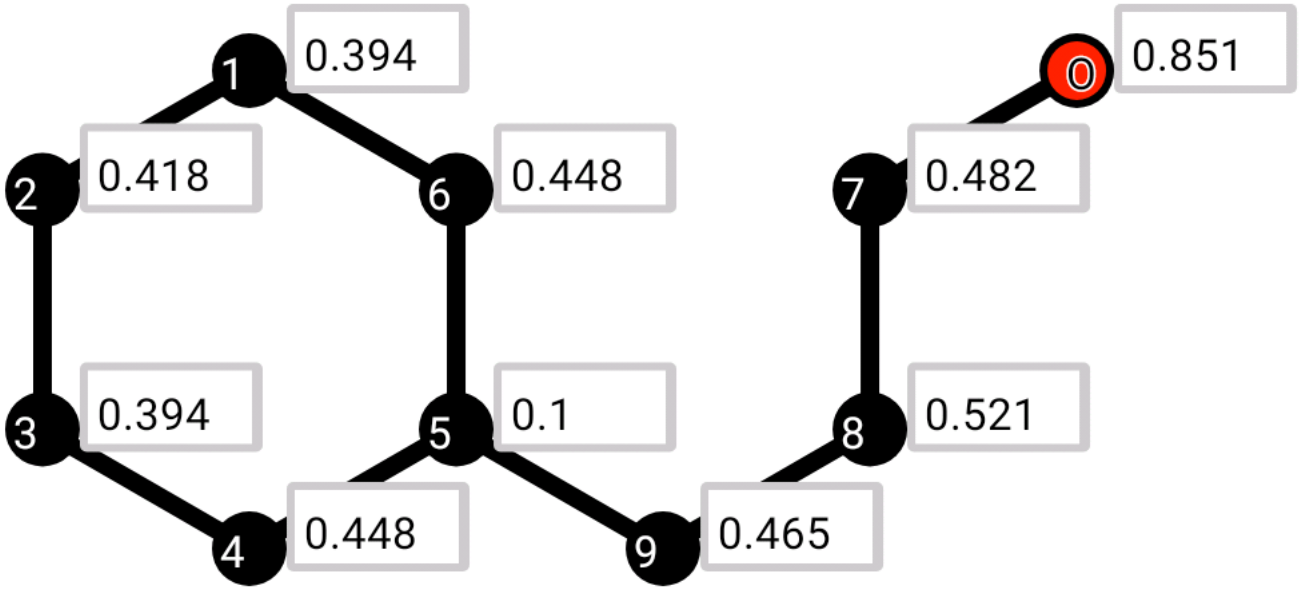
5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10
0.394	0.418	0.394	0.448	0.1	0.448	0.482	0.521	0.465	0.851

5.2. Presentation of molecule:

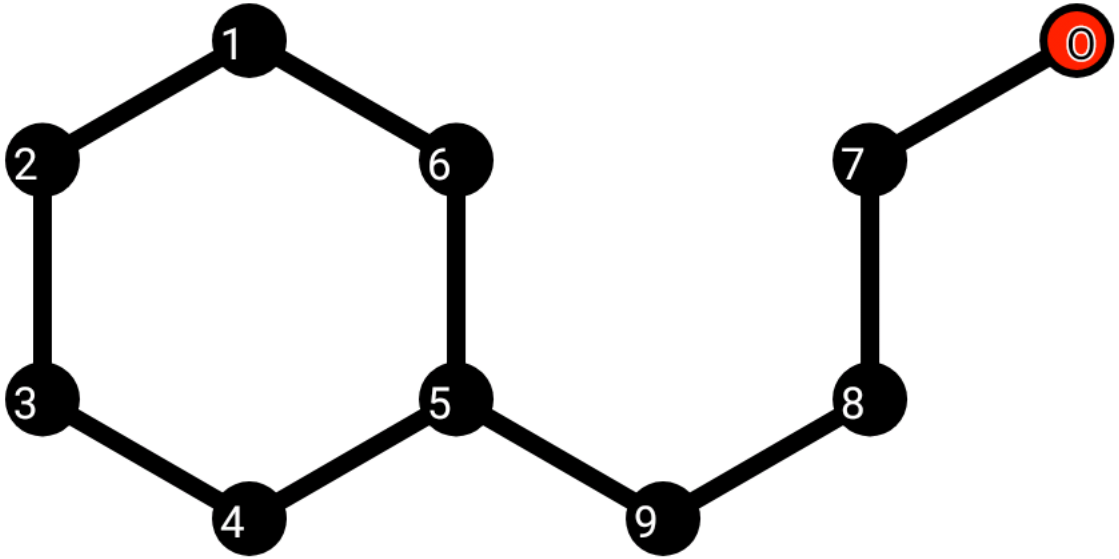


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.395									
2	-0.151	0.418								
3	0.01	-0.151	0.395							
4	-0.095	0.017	-0.166	0.434						
5	0.007	-0.084	0.007	-0.125	0.333					
6	-0.166	0.017	-0.095	0.002	-0.125	0.434				
7	0.0	-0.004	0.0	-0.004	0.0	-0.004	0.218			
8	0.002	-0.058	0.002	-0.066	0.023	-0.066	-0.017	0.502		
9	-0.002	0.009	-0.002	0.018	-0.038	0.018	-0.013	-0.358	0.441	
10	0.0	-0.014	0.0	-0.015	0.004	-0.015	-0.177	0.036	-0.074	0.254

6.2. Presentation of molecule: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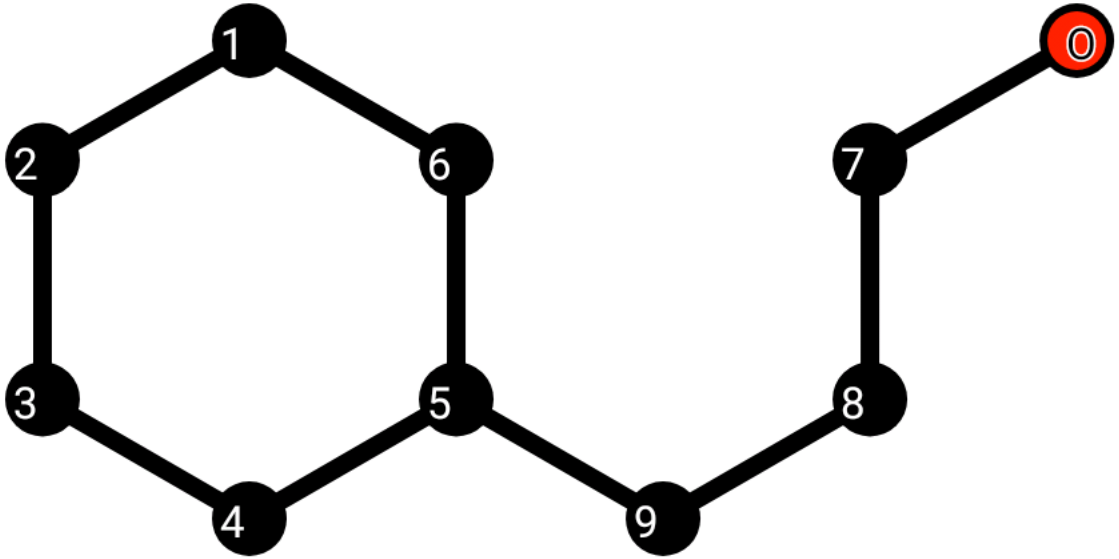
7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1 2	-0.001	0.008	0.0	0.008	-0.001	-0.009	-0.001	-0.002	-0.002	-0.001
1 6	0.0	-0.008	0.0	-0.008	0.001	0.01	0.001	0.002	0.002	0.001
2 3	0.0	0.008	-0.001	-0.009	-0.001	0.008	-0.001	-0.002	-0.002	-0.001
3 4	0.0	-0.008	0.0	0.01	0.001	-0.008	0.001	0.002	0.002	0.001
4 5	-0.001	0.007	0.0	0.006	-0.003	0.009	-0.002	-0.007	-0.006	-0.003
5 6	0.0	0.007	-0.001	0.009	-0.003	0.006	-0.002	-0.007	-0.006	-0.003
5 9	0.0	-0.016	0.0	-0.017	0.004	-0.017	0.006	0.017	0.015	0.008
7 8	0.0	-0.016	0.0	-0.018	0.004	-0.018	0.042	0.04	-0.084	0.048
7 10	0.0	0.008	0.0	0.008	-0.001	0.008	0.041	-0.009	0.037	-0.092
8 9	0.0	0.013	0.0	0.013	-0.001	0.013	-0.019	-0.048	0.053	-0.023

7.2. Presentation of molecule: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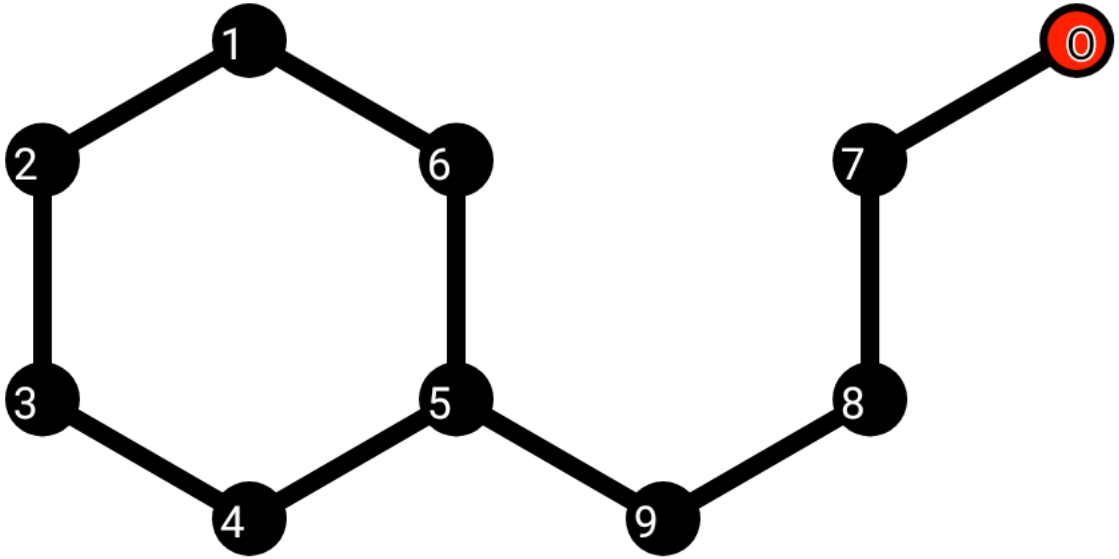
8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	2 3	3 4	4 5	5 6	5 9	7 8	7 10	8 9
1 2	0.255									
1 6	-0.216	0.247								
2 3	-0.201	0.126	0.255							
3 4	0.126	-0.09	-0.216	0.247						
4 5	-0.079	0.108	0.122	-0.188	0.253					
5 6	0.122	-0.188	-0.079	0.108	-0.151	0.253				
5 9	-0.016	0.024	-0.016	0.024	-0.109	-0.109	0.348			
7 8	-0.003	0.004	-0.003	0.004	-0.013	-0.013	0.037	0.335		
7 10	0.002	-0.002	0.002	-0.002	0.006	0.006	-0.017	-0.14	0.103	
8 9	0.01	-0.013	0.01	-0.013	0.047	0.047	-0.159	-0.134	0.054	0.126

8.2. Presentation of molecule: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