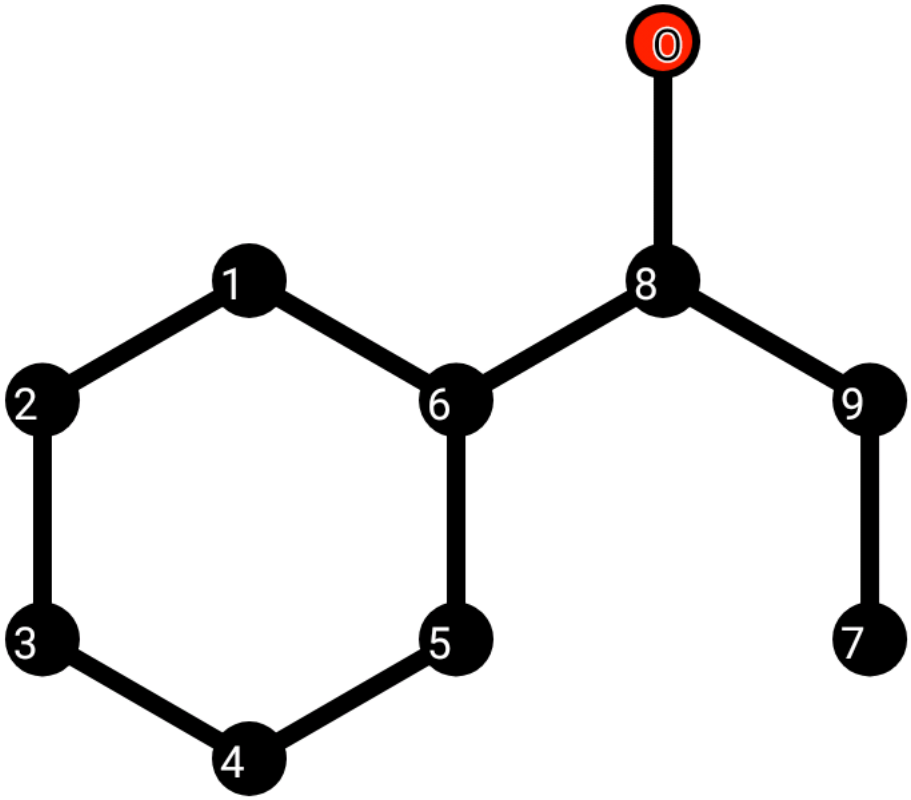
Print calculated values

Report generated by:root, 16.05.2020 - 18:49:12

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

It is about this molecule:

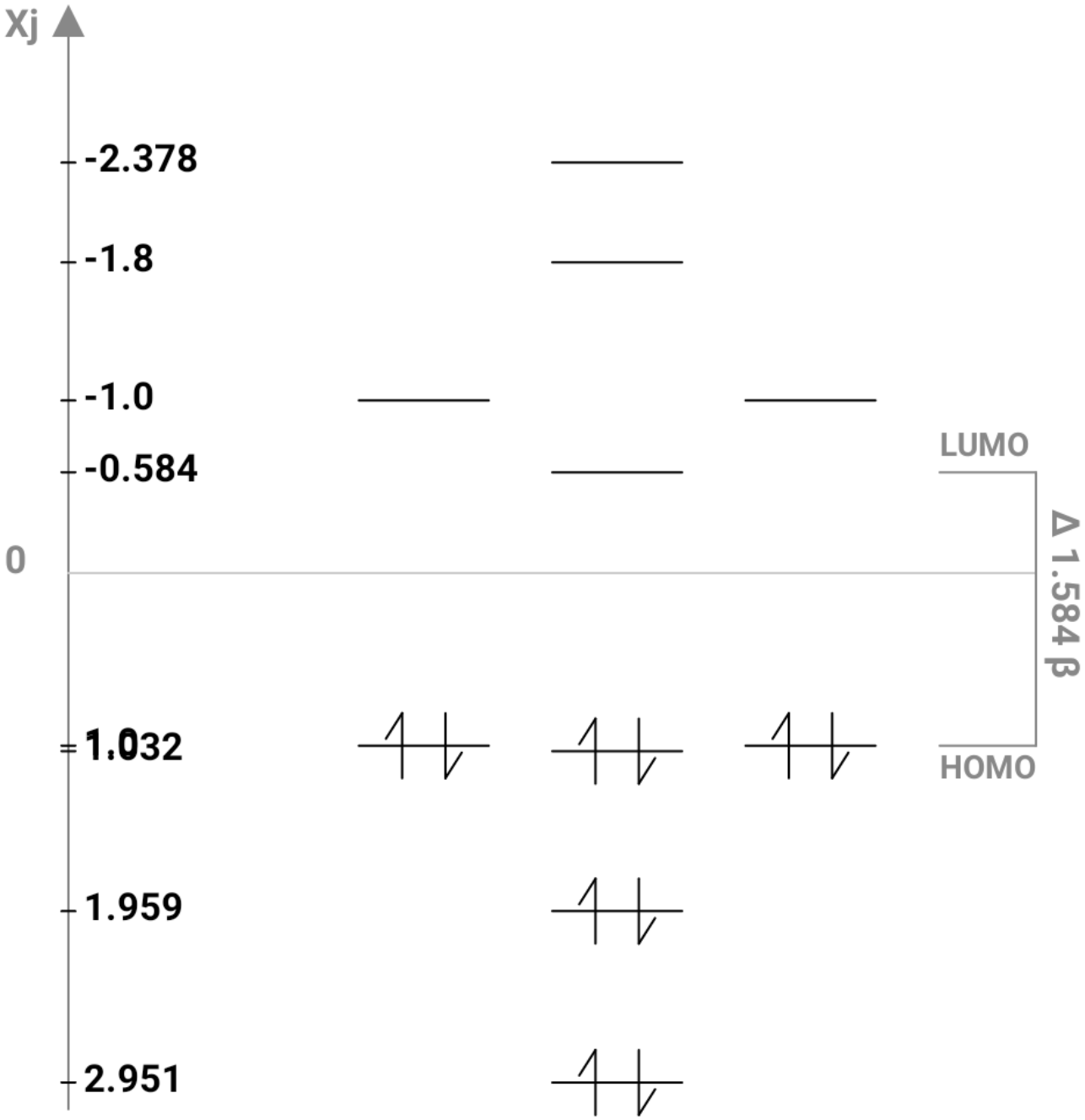


HMO-Energies

x1 = 2.951; x2 = 1.959; x3 = 1.032; x4 = 1.0; x5 = 1.0; x6 = -0.584; x7 = -1.0; x8 = -1.0;
x9 = -1.8; x10 = -2.378;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 10α + 15.884β -

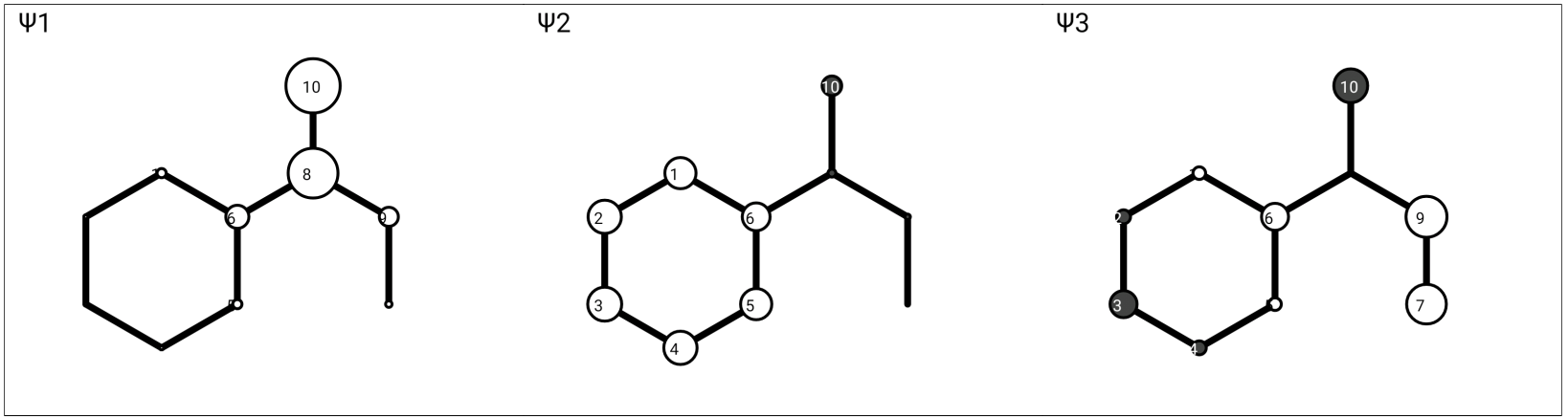
this corresponds to one πelectron: 1.588β

2. Hueckel-coefficient

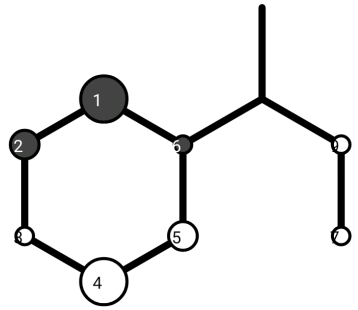
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10
	x1= 2.951	x2= 1.959	x3= 1.032	x4= 1.0	x5= 1.0	x6= -0.584	x7= -1.0	x8= -1.0	x9= -1.8	x10= -2.378
1	0.114	0.385	0.156	-0.547	-0.034	0.252	-0.034	-0.547	-0.275	0.275
2	0.05	0.41	-0.172	-0.339	-0.43	0.089	0.43	0.339	0.399	-0.179
3	0.034	0.419	-0.334	0.208	-0.396	-0.304	-0.396	0.208	-0.444	0.15
4	0.05	0.41	-0.172	0.547	0.034	0.089	-0.034	-0.547	0.399	-0.179
5	0.114	0.385	0.156	0.339	0.43	0.252	0.43	0.339	-0.275	0.275
6	0.285	0.343	0.333	-0.208	0.396	-0.236	-0.396	0.208	0.096	-0.475
7	0.08	-0.034	0.489	0.208	-0.396	0.556	-0.396	0.208	0.169	0.124
8	0.614	-0.098	0.032	0.0	0.0	-0.366	0.0	0.0	0.378	0.579
9	0.235	-0.067	0.505	0.208	-0.396	-0.324	0.396	-0.208	-0.304	-0.296
10	0.669	-0.242	-0.417	0.0	0.0	0.401	0.0	0.0	-0.245	-0.314

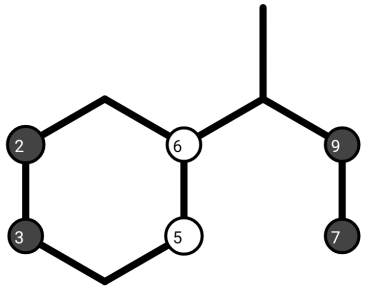
2.2. Molecule orbital presentation:



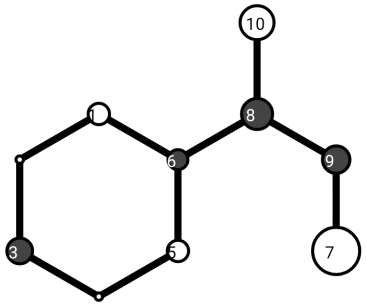
Ψ4



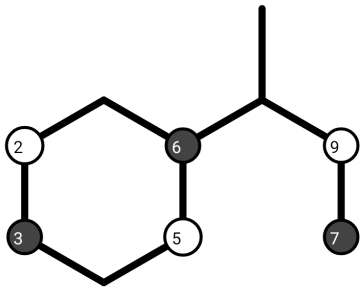
Ψ5



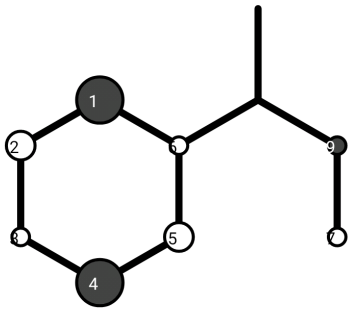
Ψ6



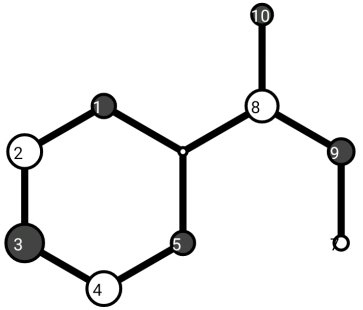
Ψ7



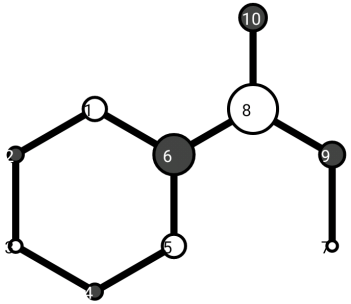
Ψ8



Ψ9



Ψ10

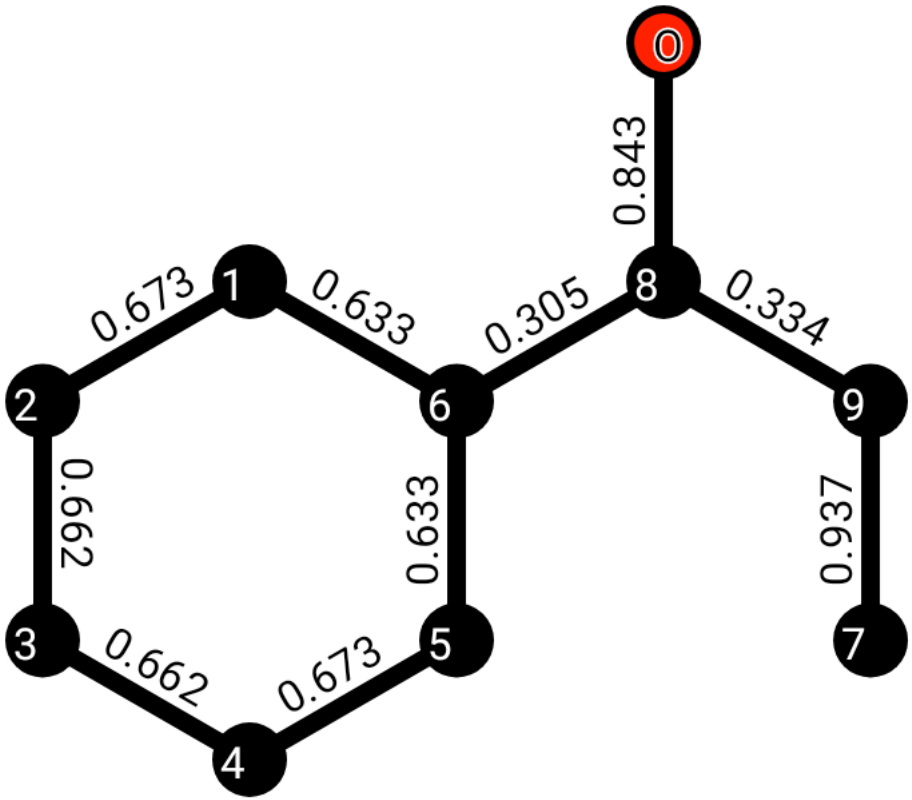


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.97									
2	0.673	1.001								
3	0.026	0.662	0.976							
4	-0.327	0.001	0.662	1.001						
5	-0.03	-0.327	0.026	0.673	0.97					
6	0.633	-0.005	-0.315	-0.005	0.633	1.02				
7	-0.056	0.011	0.05	0.011	-0.056	-0.052	0.894			
8	0.074	-0.03	-0.062	-0.03	0.074	0.305	0.136	0.775		
9	-0.041	-0.006	0.022	-0.006	-0.041	0.024	0.937	0.334	1.03	
10	-0.164	0.012	0.121	0.012	-0.164	-0.062	-0.285	0.843	-0.074	1.361

3.2. Presentation of bond order:

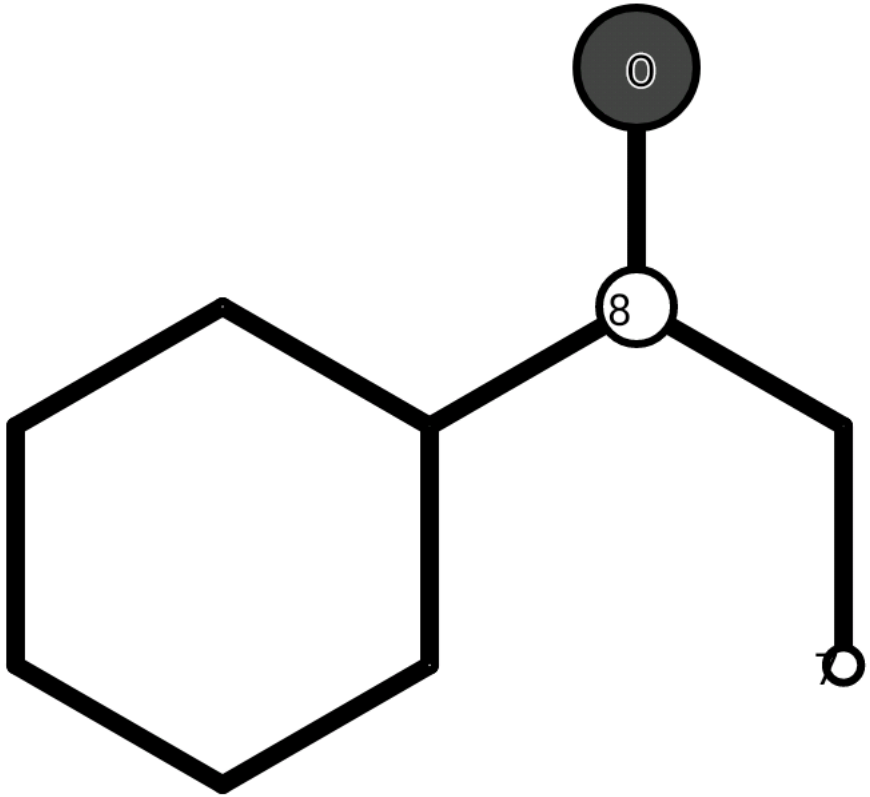

0
1
2
3
4
5
6
7
8
9
0.843
0.673
0.633
0.305
0.334
0.662
0.633
0.662
0.673
0.937

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.03									
2		-0.001								
3			0.024							
4				-0.001						
5					0.03					
6						-0.02				
7							0.106			
8								0.225		
9									-0.03	
10										-0.361

4.2. Presentation of molecule:

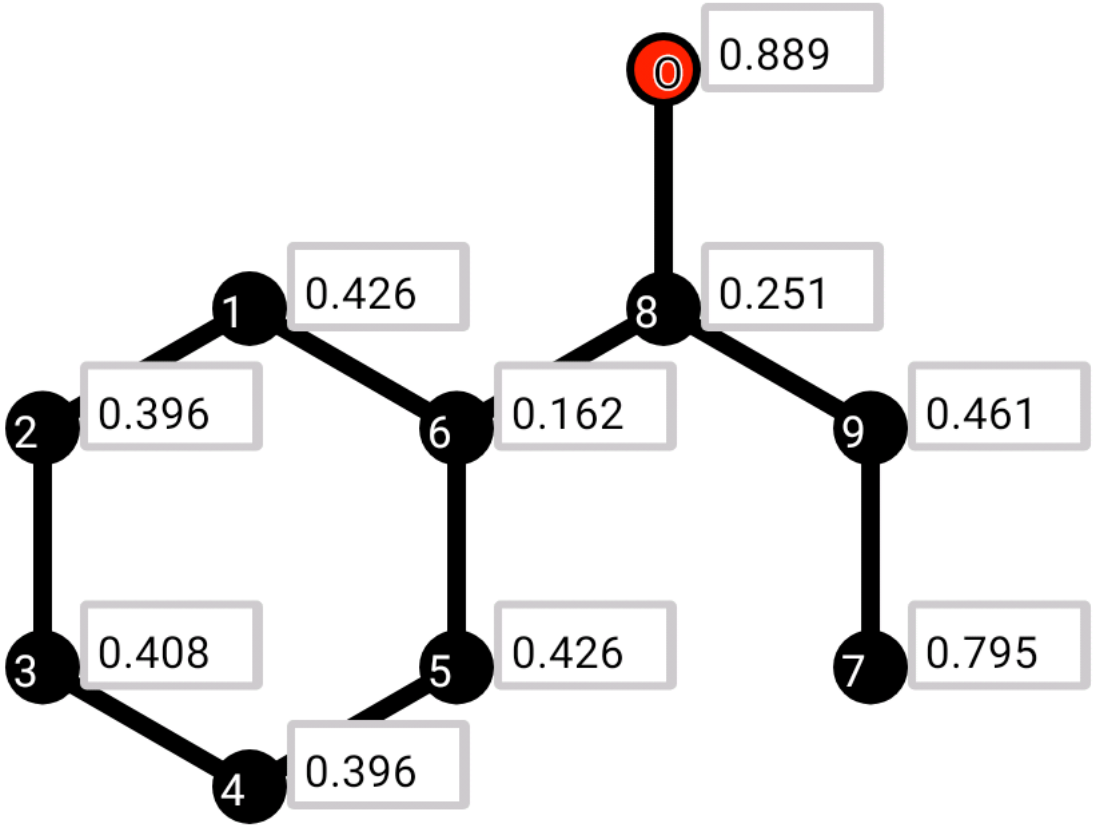

O
8
O

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10
0.426	0.396	0.408	0.396	0.426	0.162	0.795	0.251	0.461	0.889

5.2. Presentation of molecule:

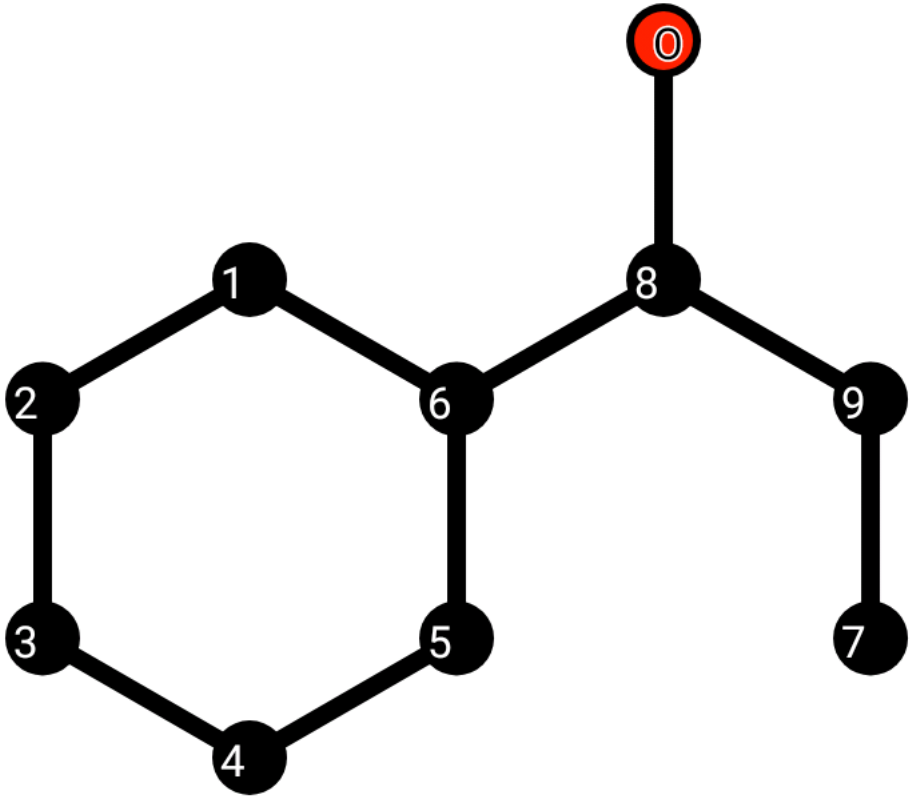

0
0.889
1
0.426
8
0.251
2
0.396
6
0.162
9
0.461
3
0.408
5
0.426
7
0.795
4
0.396

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.414									
2	-0.161	0.397								
3	0.011	-0.154	0.405							
4	-0.099	0.01	-0.154	0.397						
5	0.004	-0.099	0.011	-0.161	0.414					
6	-0.141	0.008	-0.094	0.008	-0.141	0.357				
7	-0.004	0.0	-0.004	0.0	-0.004	-0.001	0.544			
8	-0.002	0.0	-0.004	0.0	-0.002	-0.012	-0.012	0.205		
9	0.0	0.0	0.0	0.0	0.0	0.002	-0.441	-0.015	0.435	
10	-0.022	0.001	-0.018	0.001	-0.022	0.013	-0.079	-0.159	0.02	0.265

6.2. Presentation of molecule:


0
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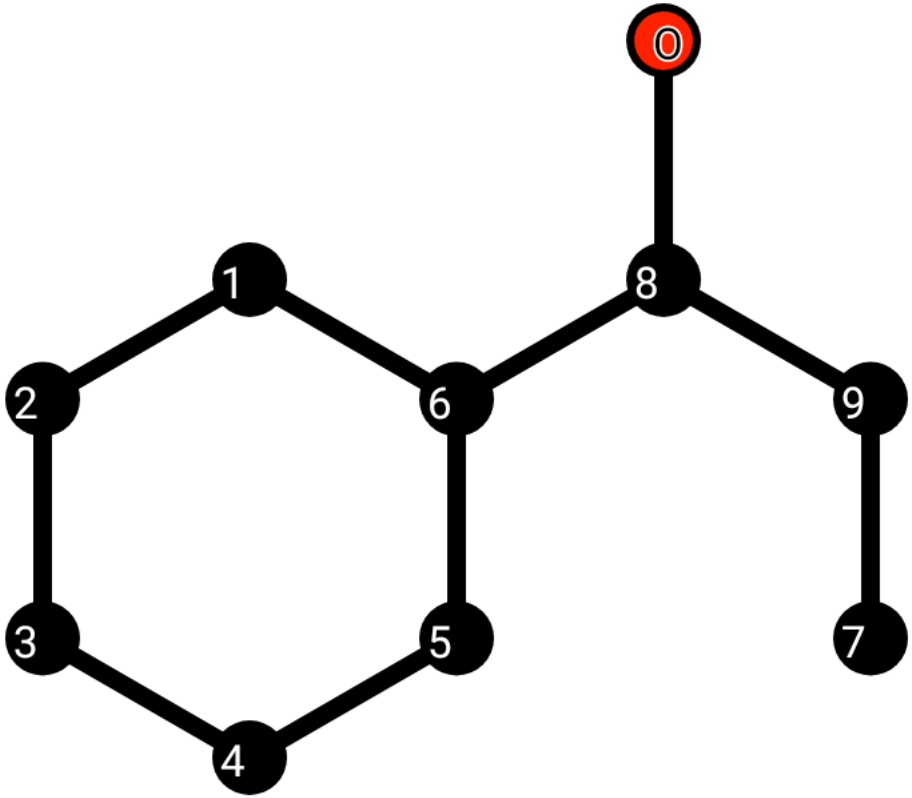
7
4

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1 2	0.014	0.001	-0.011	0.0	-0.012	0.003	0.001	0.002	0.0	0.002
1 6	0.006	0.001	0.009	-0.001	0.013	-0.011	-0.003	-0.007	0.001	-0.009
2 3	-0.012	-0.002	0.009	0.0	0.01	-0.002	-0.001	-0.001	0.0	-0.002
3 4	0.01	0.0	0.009	-0.002	-0.012	-0.002	-0.001	-0.001	0.0	-0.002
4 5	-0.012	0.0	-0.011	0.001	0.014	0.003	0.001	0.002	0.0	0.002
5 6	0.013	-0.001	0.009	0.001	0.006	-0.011	-0.003	-0.007	0.001	-0.009
6 8	-0.027	0.001	-0.022	0.001	-0.027	0.017	0.007	0.024	-0.004	0.031
7 9	-0.002	0.0	-0.001	0.0	-0.002	0.002	0.067	-0.015	-0.029	-0.02
8 9	0.003	0.0	0.002	0.0	0.003	-0.004	-0.096	0.03	0.025	0.038
8 10	0.01	0.0	0.009	0.0	0.01	-0.001	0.038	0.035	-0.003	-0.098

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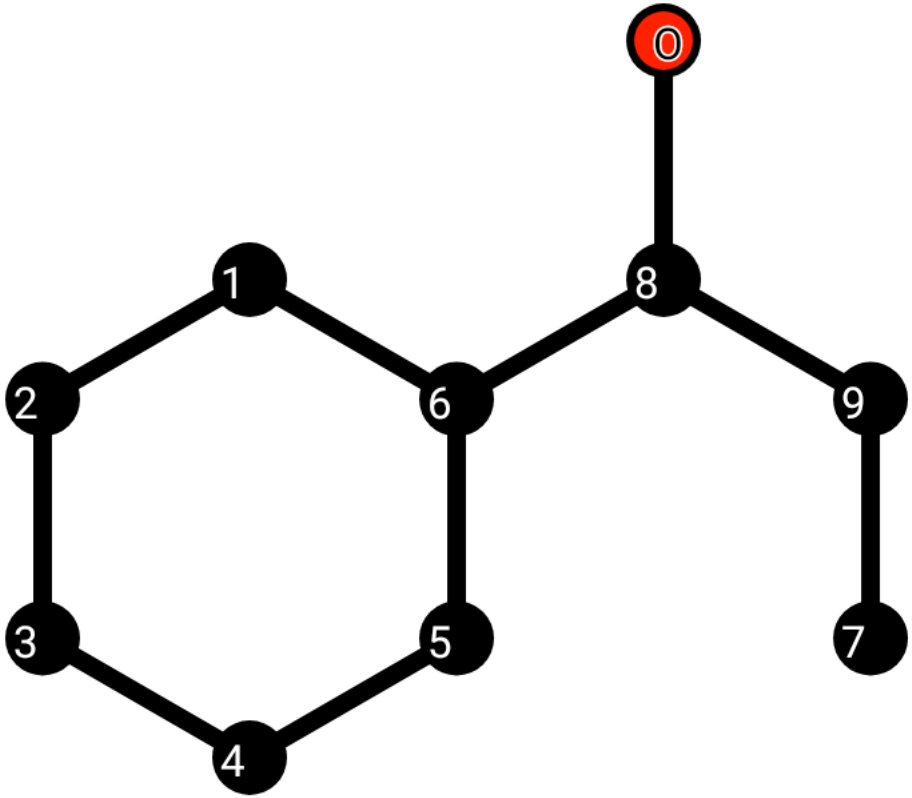
8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	2 3	3 4	4 5	5 6	6 8	7 9	8 9	8 10
1 2	0.244									
1 6	-0.196	0.244								
2 3	-0.21	0.126	0.247							
3 4	0.128	-0.086	-0.203	0.247						
4 5	-0.092	0.119	0.128	-0.21	0.244					
5 6	0.119	-0.176	-0.086	0.126	-0.196	0.244				
6 8	0.013	-0.065	-0.009	-0.009	0.013	-0.065	0.281			
7 9	0.0	-0.001	0.0	0.0	0.0	-0.001	0.005	0.054		
8 9	-0.001	0.004	0.0	0.0	-0.001	0.004	-0.026	-0.121	0.305	
8 10	-0.005	0.021	0.004	0.004	-0.005	0.021	-0.091	0.045	-0.108	0.119

8.2. Presentation of molecule: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