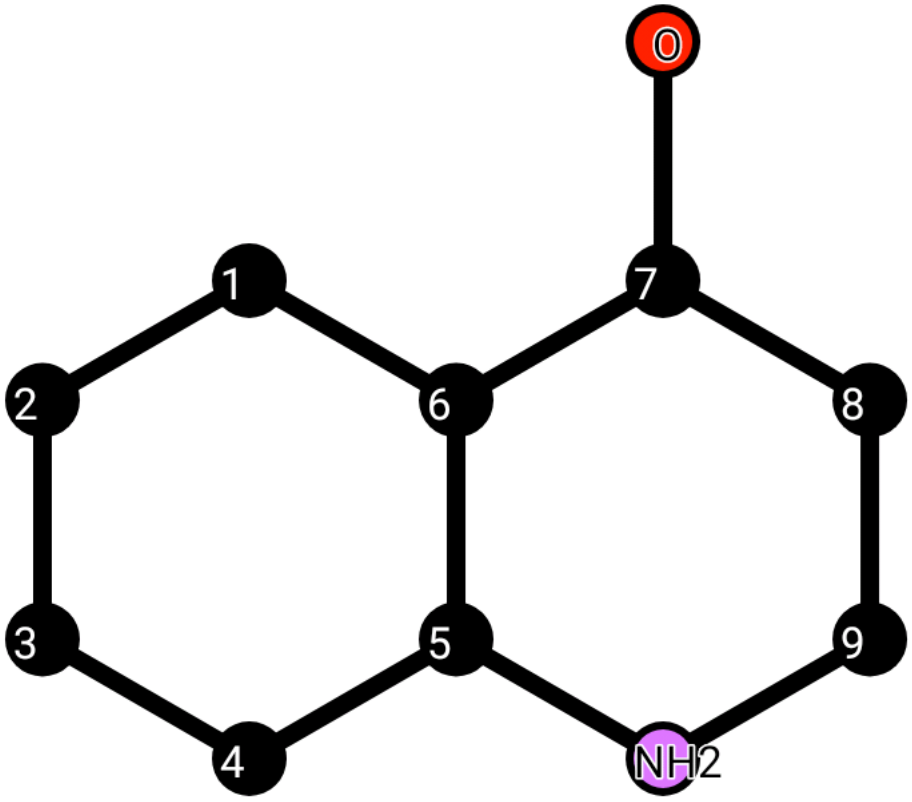
Print calculated values

Report generated by:root, 16.05.2020 - 18:43:39

The following determinant is calculated:

-x	1.0	0.0	0.0	0.0	1.0	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
0.0	1.0	-x	1.0	0.0	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	0.0	1.0	-x	1.0	0.0	0.0	0.0	1.3	0.0
1.0	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	0.0	1.0	-x	1.0	0.0	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	0.0	0.0	0.0	0.0	1.0	-x	1.3	0.0
0.0	0.0	0.0	0.0	1.3	0.0	0.0	0.0	1.3	-x+1.47	0.0
0.0	0.0	0.0	0.0	0.0	0.0	1.93	0.0	0.0	0.0	-x+1.18

It is about this molecule:

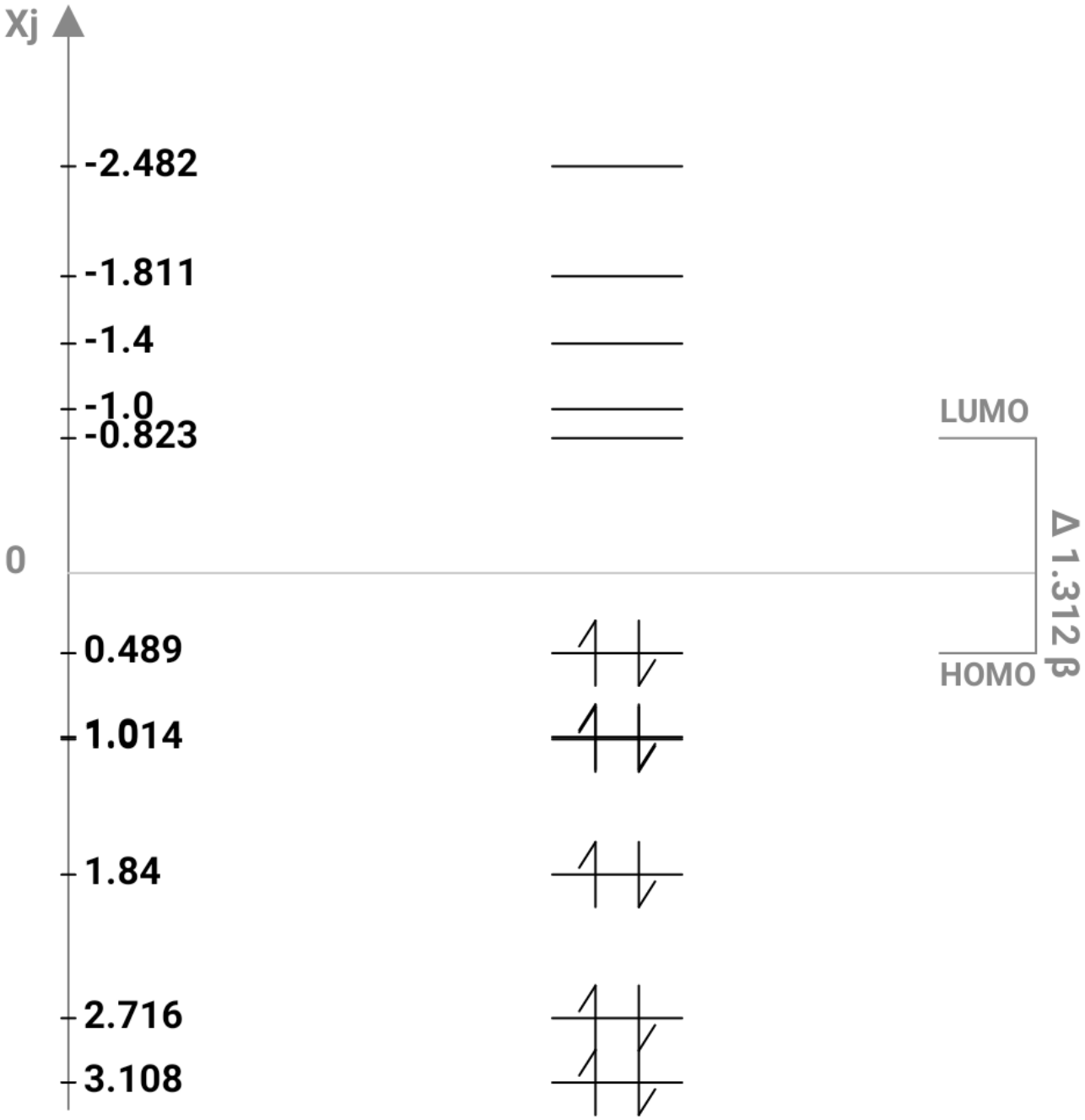


HMO-Energies

x1 = 3.108; x2 = 2.716; x3 = 1.84; x4 = 1.014; x5 = 1.0; x6 = 0.489; x7 = -0.823; x8 = -1.0;
x9 = -1.4; x10 = -1.811; x11 = -2.482;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 11α + 20.334β -

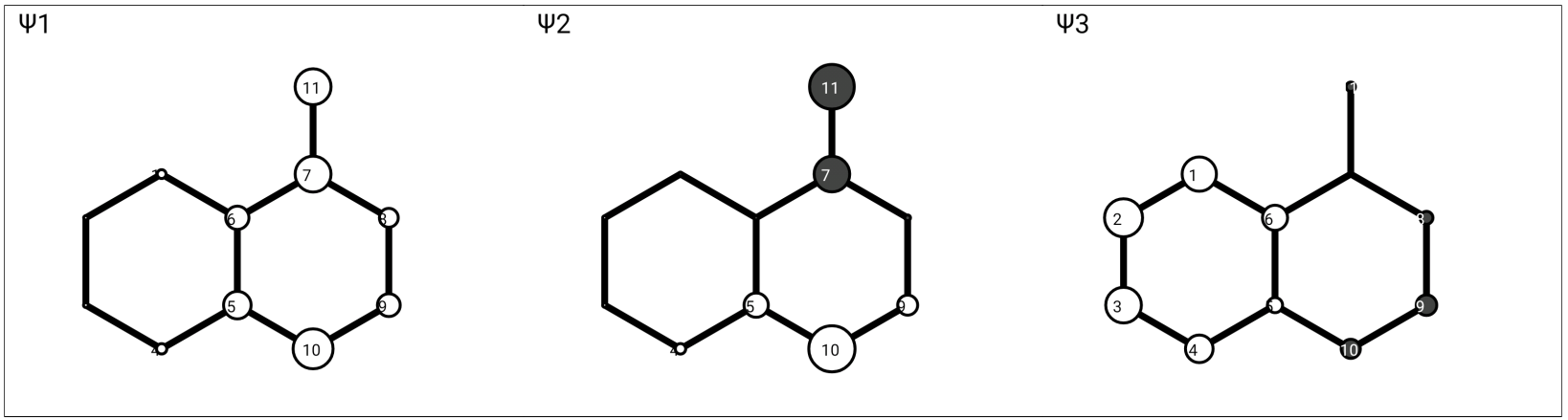
this corresponds to one πelectron: 1.695β

2. Hueckel-coefficient

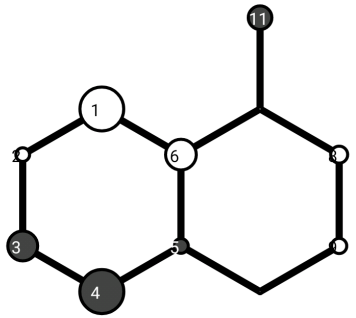
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11
	x1= 3.108	x2= 2.716	x3= 1.84	x4= 1.014	x5= 1.0	x6= 0.489	x7= -0.823	x8= -1.0	x9= -1.4	x10= -1.811	x11= -2.482
1	0.11	-0.016	0.423	0.517	0.0	0.172	0.511	0.0	0.371	0.228	0.247
2	0.054	0.014	0.469	0.162	0.408	0.328	-0.183	0.408	-0.35	-0.358	-0.159
3	0.059	0.053	0.44	-0.353	0.408	-0.011	-0.36	-0.408	0.119	0.42	0.148
4	0.128	0.13	0.34	-0.52	0.0	-0.334	0.48	0.0	0.183	-0.403	-0.208
5	0.34	0.3	0.186	-0.174	-0.408	-0.152	-0.035	0.408	-0.375	0.31	0.368
6	0.287	-0.057	0.31	0.362	-0.408	-0.245	-0.237	-0.408	-0.17	-0.055	-0.454
7	0.442	-0.439	-0.04	0.024	0.0	-0.139	-0.281	0.0	0.242	-0.438	0.511
8	0.233	-0.071	-0.159	0.2	0.408	-0.573	-0.054	0.408	0.18	0.303	-0.295
9	0.281	0.247	-0.254	0.179	0.408	-0.141	0.325	-0.408	-0.494	-0.111	0.22
10	0.493	0.57	-0.236	-0.014	0.0	0.388	-0.164	0.0	0.394	-0.079	-0.194
11	0.443	-0.551	-0.116	-0.279	0.0	0.388	0.271	0.0	-0.181	0.283	-0.27

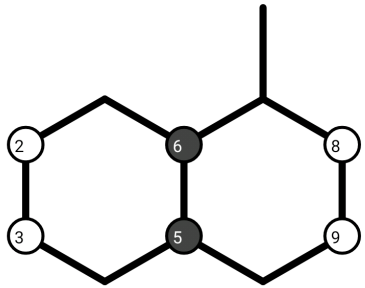
2.2. Molecule orbital presentation:



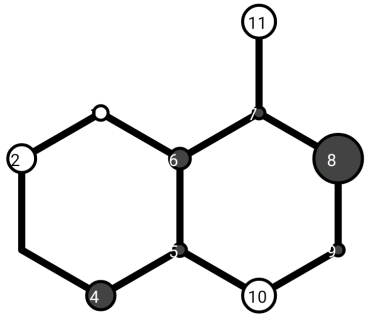
Ψ4



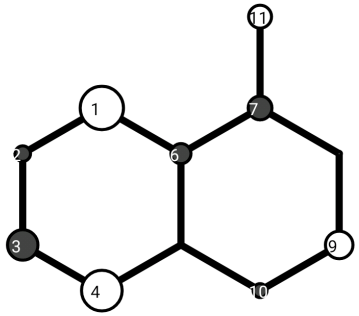
Ψ5



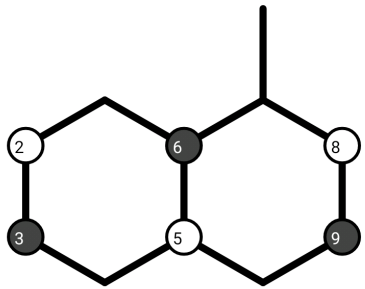
Ψ6



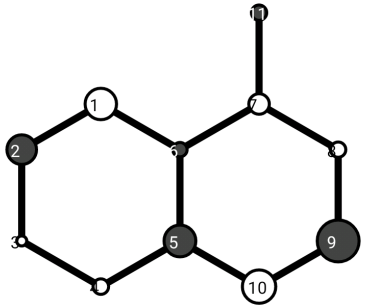
Ψ7



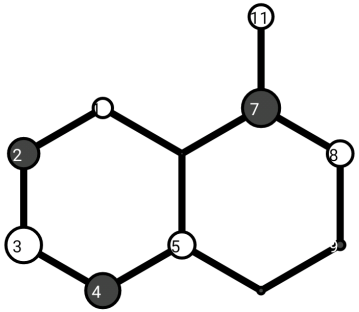
Ψ8



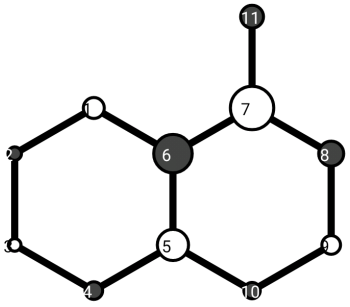
Ψ9



Ψ10



Ψ11

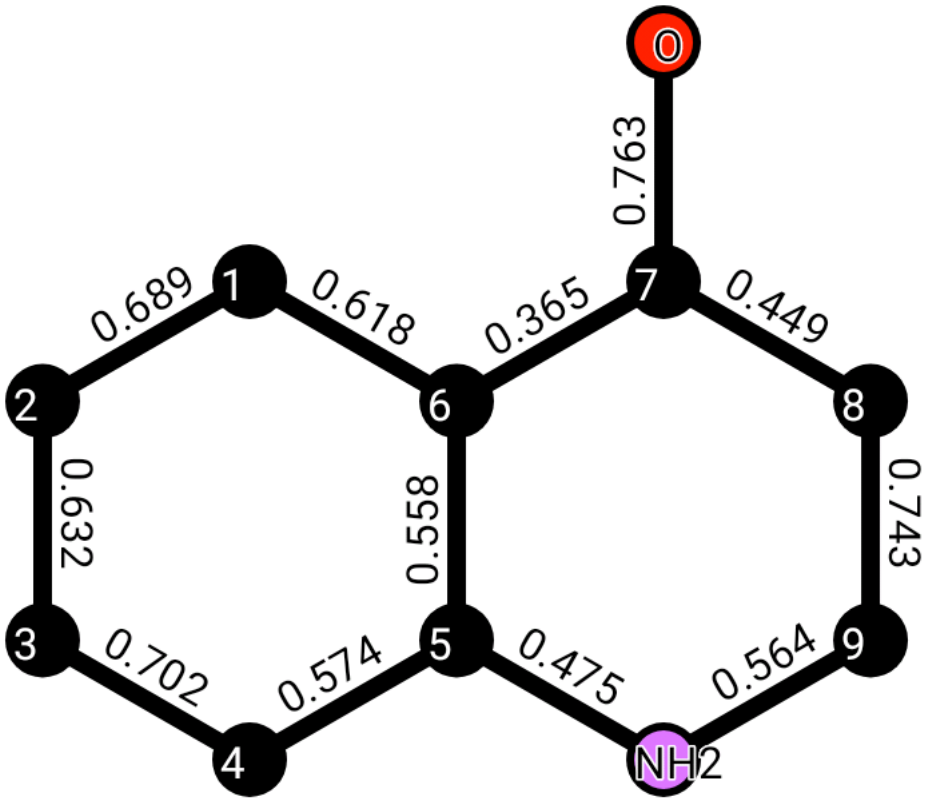


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.976										
2	0.689	1.048									
3	0.015	0.632	0.982								
4	-0.34	-0.051	0.702	1.061							
5	-0.009	-0.27	0.028	0.574	0.92						
6	0.618	-0.056	-0.283	0.057	0.558	1.078					
7	0.055	-0.085	-0.043	0.041	0.057	0.365	0.819				
8	-0.071	-0.104	0.084	0.107	-0.172	0.135	0.449	1.239			
9	-0.024	0.098	0.046	-0.129	-0.108	-0.159	0.1	0.743	0.845		
10	0.008	0.097	-0.088	-0.13	0.475	-0.129	-0.154	-0.226	0.564	1.548	
11	-0.138	0.089	0.08	-0.078	-0.094	-0.147	0.763	-0.236	-0.174	0.172	1.483

3.2. Presentation of bond order:

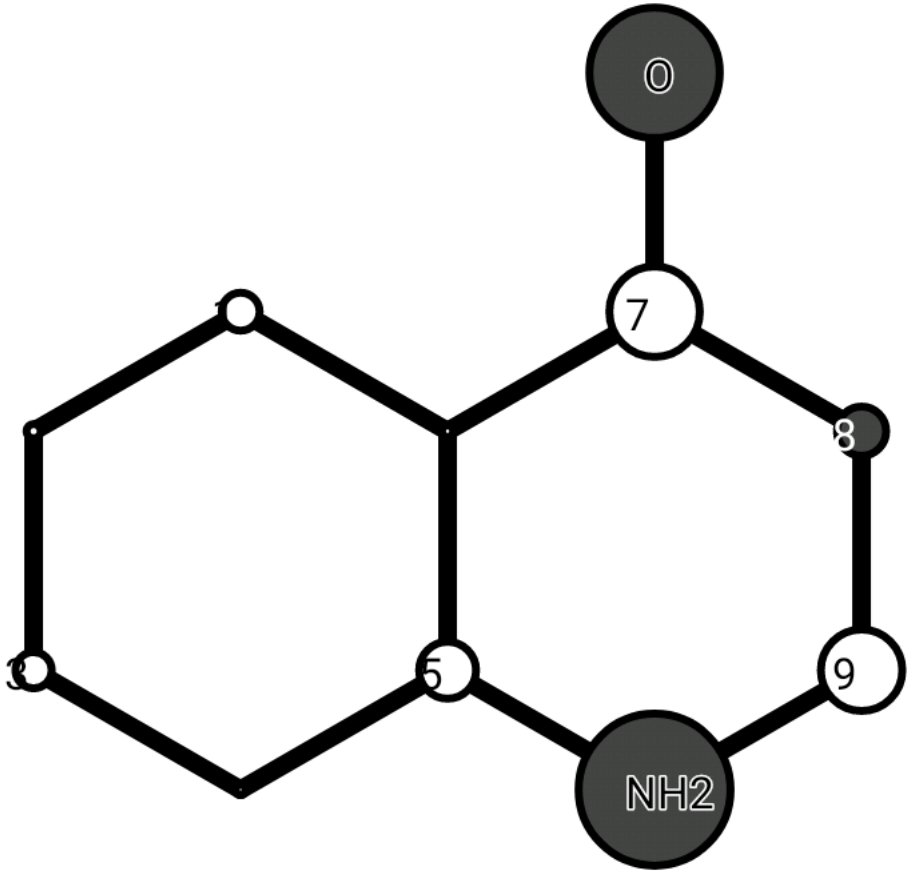

0
0.763
1
0.689
0.618
0.365
7
0.449
2
6
8
0.632
0.558
0.743
3
0.702
0.574
5
0.475
0.564
9
4
NH2

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.114										
2		0.043									
3			0.109								
4				0.03							
5					0.171						
6						0.013					
7							0.272				
8								-0.148			
9									0.245		
10										-0.457	
11											-0.392

4.2. Presentation of molecule:

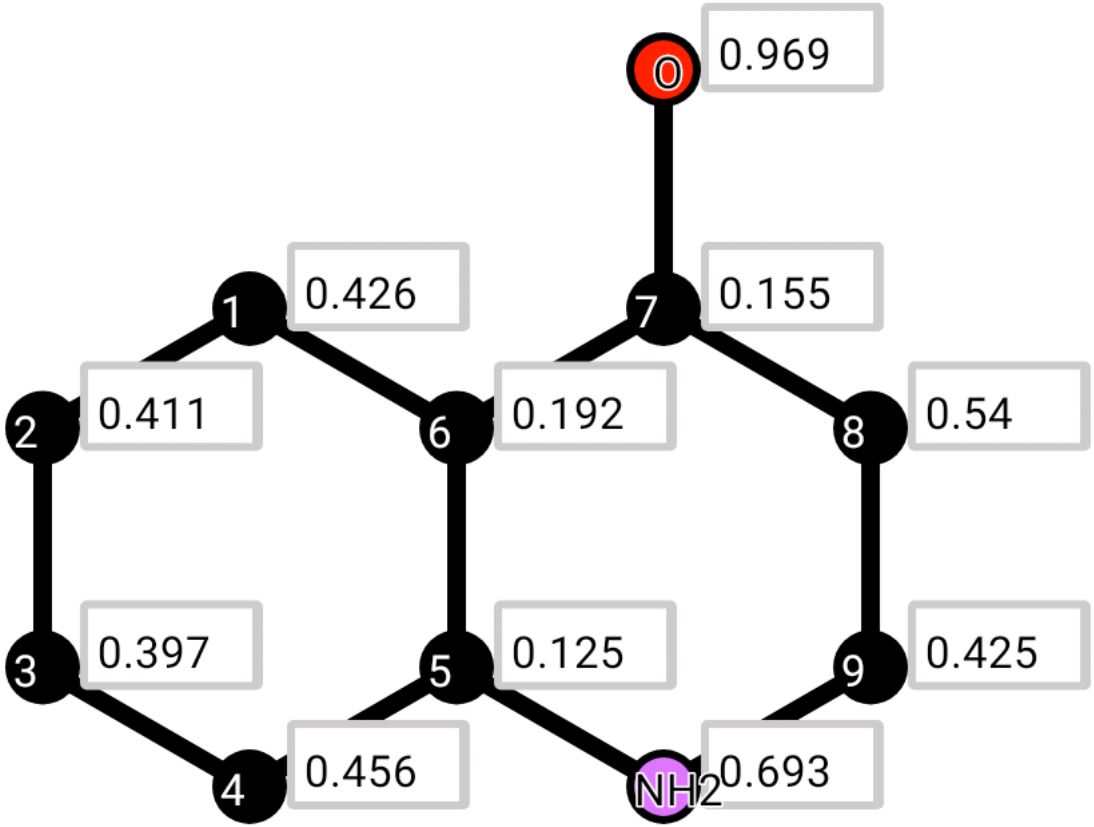

0
7
8
5
9
NH2

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11
0.426	0.411	0.397	0.456	0.125	0.192	0.155	0.54	0.425	0.693	0.969

5.2. Presentation of molecule:

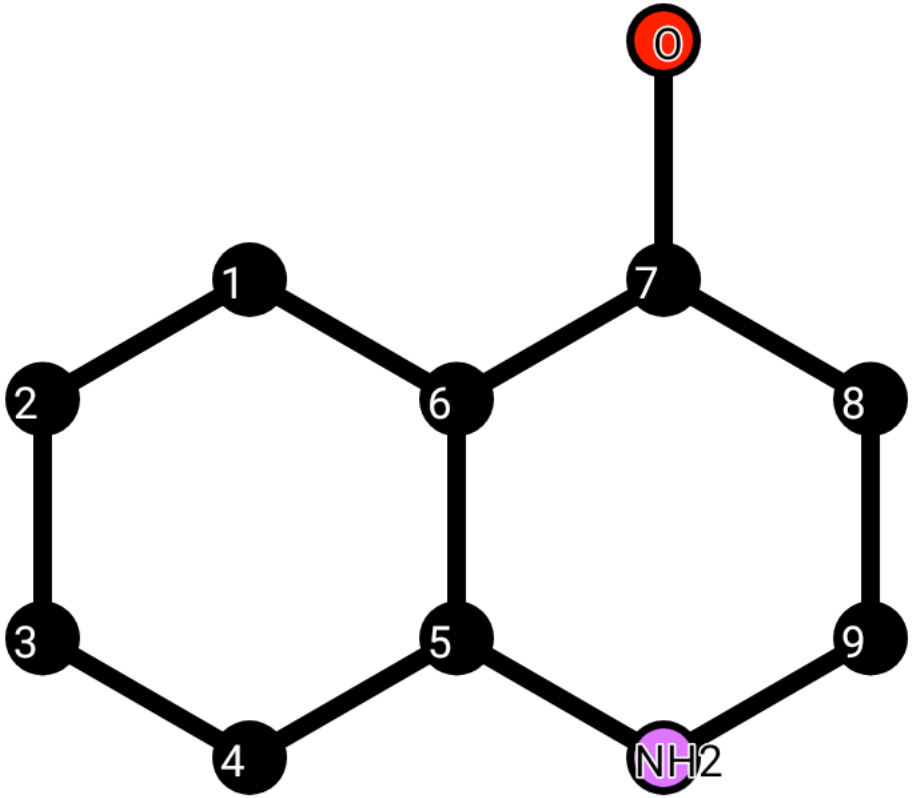

0
0.969
1
0.426
7
0.155
2
0.411
6
0.192
8
0.54
3
0.397
5
0.125
9
0.425
4
0.456
NH2
0.693

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.415										
2	-0.178	0.407									
3	0.012	-0.131	0.398								
4	-0.115	0.013	-0.187	0.435							
5	0.005	-0.066	0.006	-0.104	0.316						
6	-0.126	0.007	-0.073	-0.002	-0.101	0.366					
7	0.002	-0.007	-0.002	-0.005	-0.002	-0.023	0.214				
8	-0.003	-0.018	-0.008	-0.013	-0.017	-0.023	-0.048	0.423			
9	0.0	-0.009	-0.002	-0.01	0.003	-0.016	-0.008	-0.232	0.361		
10	-0.002	-0.008	-0.005	-0.001	-0.033	-0.01	-0.019	-0.036	-0.059	0.204	
11	-0.011	-0.01	-0.007	-0.012	-0.006	0.001	-0.104	-0.025	-0.027	-0.031	0.232

6.2. Presentation of molecule:

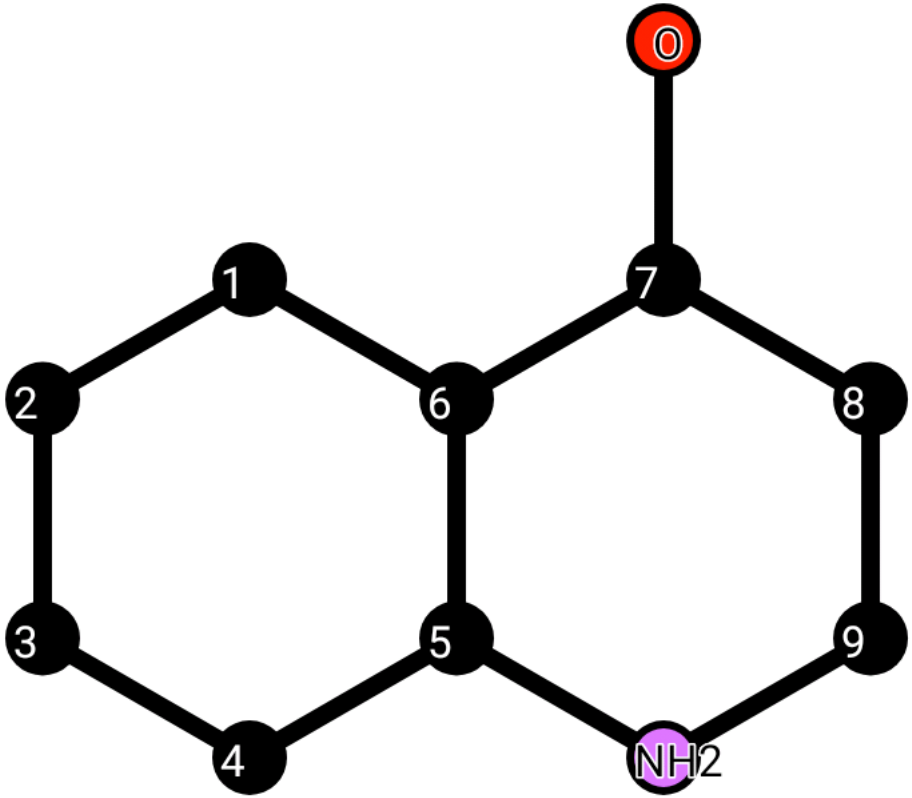

0
1
7
2
6
8
3
5
9
4
NH2

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1 2	0.015	-0.019	-0.006	-0.021	-0.003	0.024	0.006	-0.008	0.003	-0.003	0.014
1 6	-0.001	0.025	0.005	0.024	0.003	-0.035	-0.01	0.01	-0.003	0.003	-0.022
2 3	-0.009	-0.017	0.008	0.027	0.009	-0.019	-0.004	0.012	-0.005	0.01	-0.01
3 4	0.008	0.019	0.005	-0.033	-0.011	0.018	0.003	-0.012	0.006	-0.012	0.009
4 5	-0.005	-0.014	-0.011	-0.004	0.029	-0.02	-0.003	0.02	-0.013	0.028	-0.008
5 6	0.006	-0.016	0.007	-0.021	0.024	-0.016	-0.007	0.02	-0.012	0.025	-0.009
5 10	-0.001	0.028	0.001	0.033	-0.028	0.036	0.007	-0.037	0.031	-0.083	0.014
6 7	-0.017	-0.004	-0.013	-0.005	-0.017	0.008	0.03	-0.03	0.012	-0.017	0.053
7 8	0.007	-0.011	0.004	-0.011	0.007	-0.017	0.043	-0.025	-0.049	-0.032	0.084
7 11	0.003	0.008	0.004	0.008	0.004	0.011	0.008	0.038	0.017	0.026	-0.127
8 9	-0.004	0.015	-0.004	0.018	-0.015	0.018	-0.023	-0.107	0.077	0.065	-0.04
9 10	0.003	-0.013	0.004	-0.02	0.023	-0.017	0.014	0.104	-0.021	-0.108	0.031

7.2. Presentation of molecule:

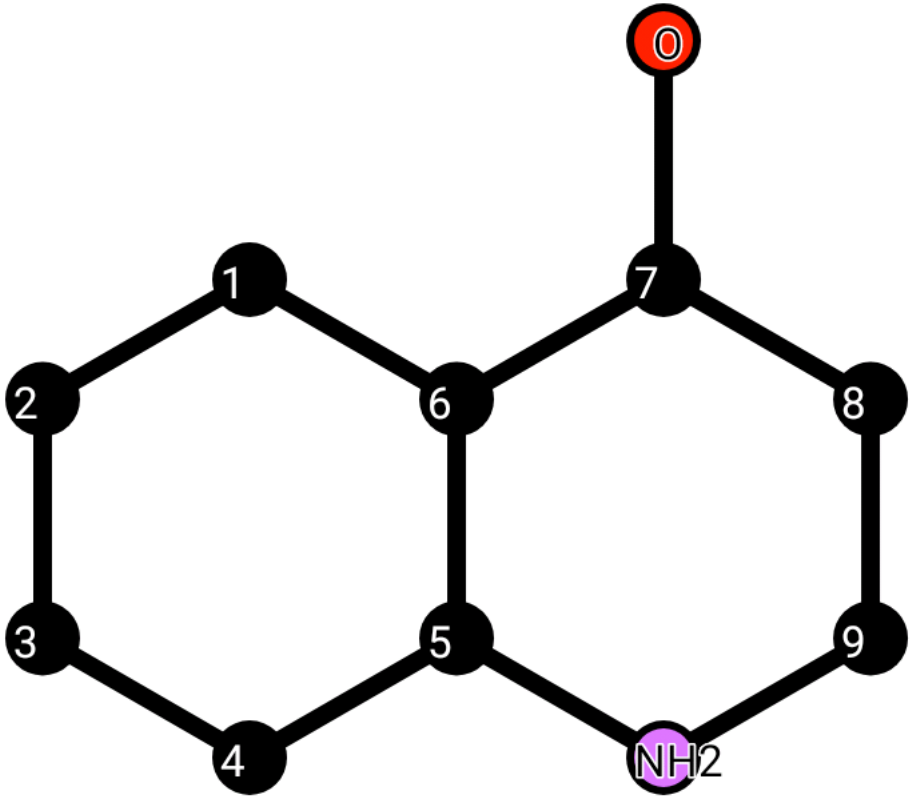

0
1
7
2
6
8
3
5
9
4
NH2

8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	2 3	3 4	4 5	5 6	5 10	6 7	7 8	7 11	8 9	9 10
1 2	0.238											
1 6	-0.205	0.27										
2 3	-0.208	0.123	0.275									
3 4	0.128	-0.087	-0.216	0.232								
4 5	-0.079	0.106	0.12	-0.186	0.27							
5 6	0.094	-0.147	-0.059	0.085	-0.125	0.247						
5 10	0.006	-0.004	-0.028	0.038	-0.115	-0.098	0.274					
6 7	0.039	-0.094	-0.029	0.019	-0.02	-0.064	0.05	0.276				
7 8	0.005	-0.002	-0.001	0.003	-0.001	0.014	-0.004	-0.02	0.309			
7 11	-0.02	0.036	0.014	-0.011	0.011	0.02	-0.022	-0.116	-0.163	0.187		
8 9	0.001	-0.003	-0.003	0.004	-0.011	-0.005	0.026	0.013	-0.166	0.068	0.236	
9 10	0.003	-0.004	0.002	-0.003	0.016	0.019	-0.061	0.0	0.097	-0.045	-0.217	0.289

8.2. Presentation of molecule:


0
1
7
2
6
8
3
5
9
4
NH2