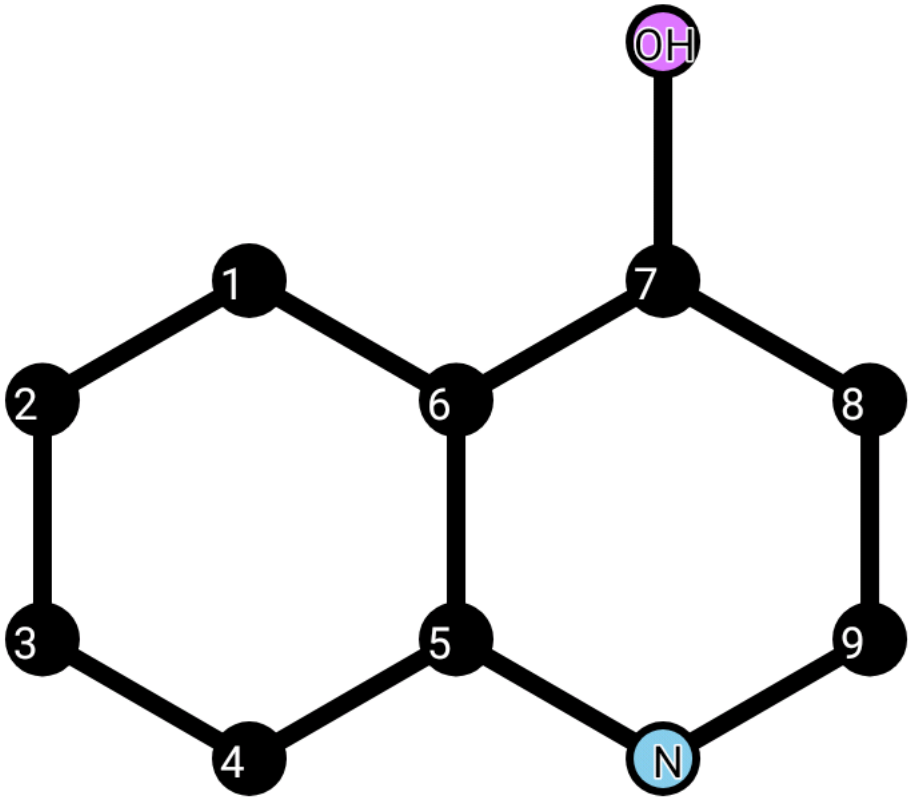
Print calculated values

Report generated by:root, 16.05.2020 - 18:44:53

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	1.06	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	0.9
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	1.06	0.0
0.0	0.0	0.0	0.0	1.06	0.0	0.0	0.0	1.06	-x+0.83	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.9	0.0	0.0	0.0	-x+2.0

It is about this molecule:

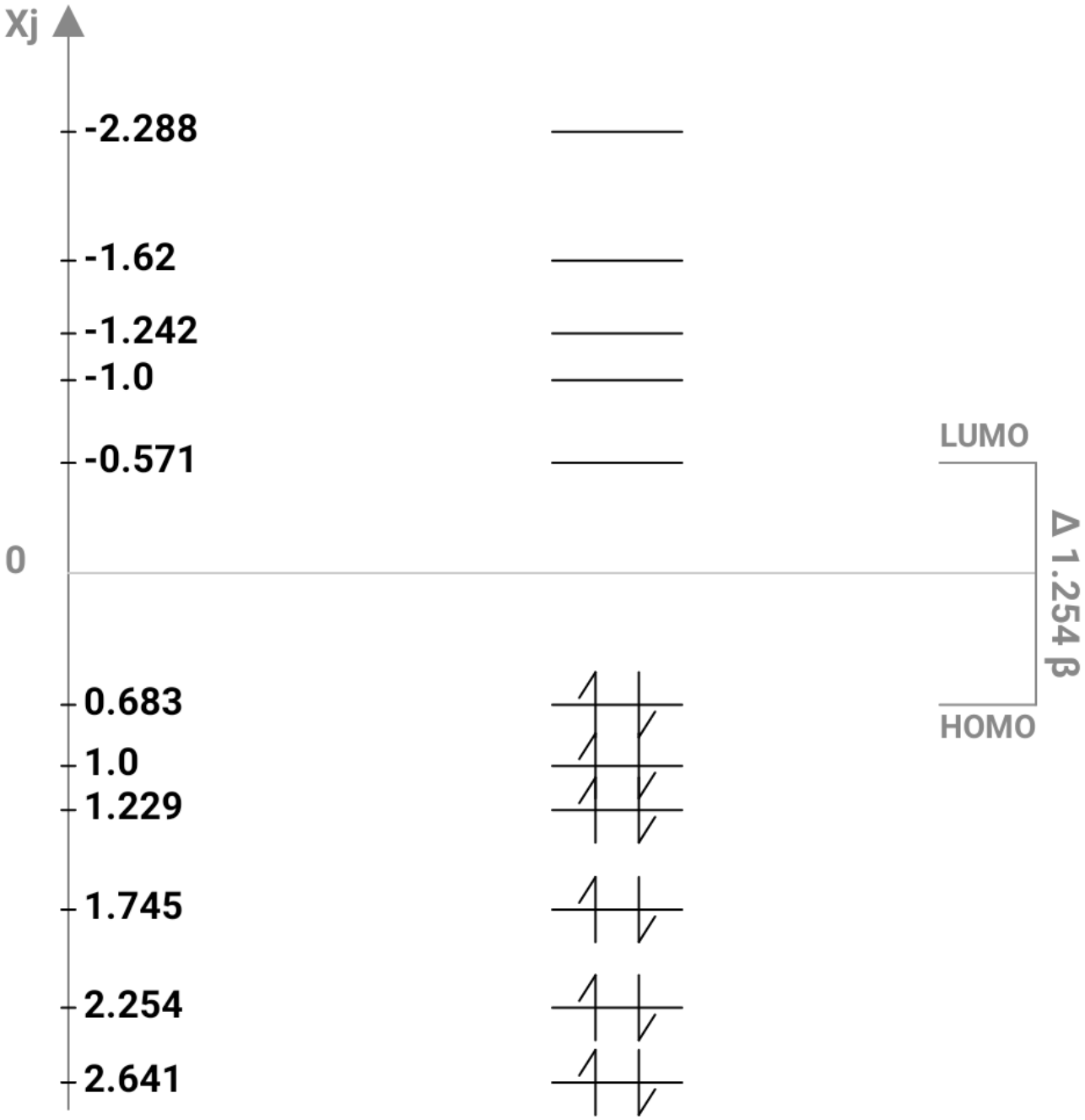


HMO-Energies

x1 = 2.641; x2 = 2.254; x3 = 1.745; x4 = 1.229; x5 = 1.0; x6 = 0.683; x7 = -0.571; x8 = -1.0;
x9 = -1.242; x10 = -1.62; x11 = -2.288;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 11α + 19.104β -

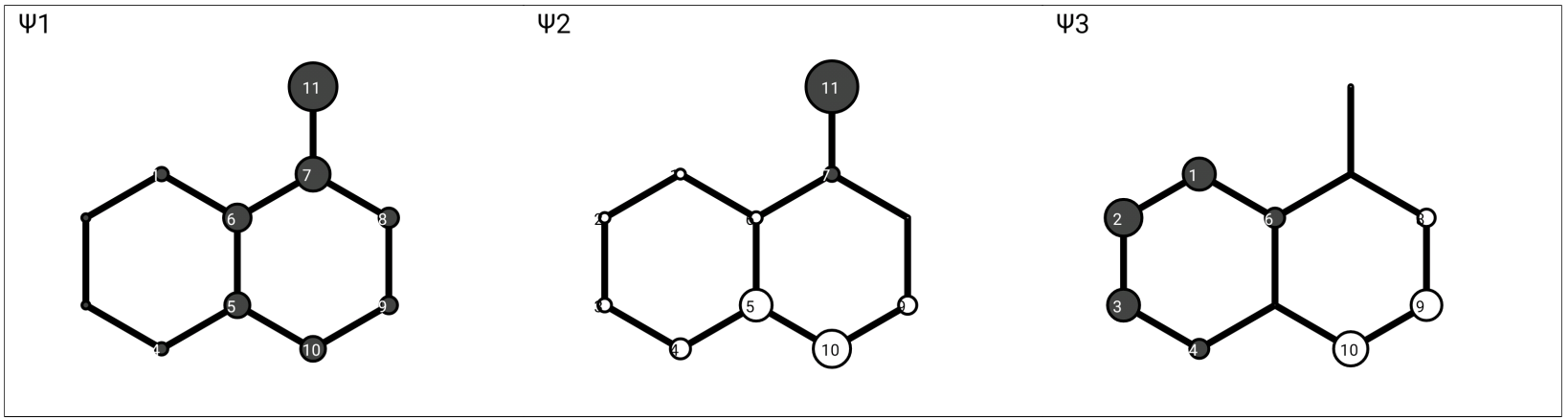
this corresponds to one πelectron: 1.592β

2. Hueckel-coefficient

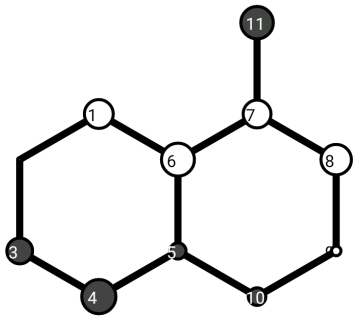
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11
	x1= 2.641	x2= 2.254	x3= 1.745	x4= 1.229	x5= 1.0	x6= 0.683	x7= -0.571	x8= -1.0	x9= -1.242	x10= -1.62	x11= -2.288
1	-0.166	0.123	-0.397	0.341	0.0	0.415	-0.411	0.0	0.449	0.204	-0.315
2	-0.099	0.129	-0.454	0.03	0.408	0.329	0.197	0.408	-0.271	-0.394	0.24
3	-0.095	0.167	-0.395	-0.304	0.408	-0.191	0.298	-0.408	-0.112	0.434	-0.234
4	-0.153	0.248	-0.235	-0.403	0.0	-0.459	-0.367	0.0	0.41	-0.309	0.295
5	-0.309	0.392	-0.015	-0.191	-0.408	-0.123	-0.088	0.408	-0.398	0.066	-0.442
6	-0.339	0.149	-0.239	0.389	-0.408	-0.045	0.037	-0.408	-0.287	0.063	0.481
7	-0.42	-0.18	-0.005	0.328	0.0	-0.323	0.477	0.0	0.305	-0.373	-0.344
8	-0.24	0.02	0.215	0.359	0.408	-0.374	-0.16	0.408	-0.016	0.458	0.241
9	-0.213	0.225	0.379	0.113	0.408	0.068	-0.386	-0.408	-0.285	-0.368	-0.208
10	-0.306	0.46	0.422	-0.208	0.0	0.397	0.359	0.0	0.349	0.131	0.221
11	-0.589	-0.639	0.018	-0.383	0.0	0.221	-0.167	0.0	-0.085	0.093	0.072

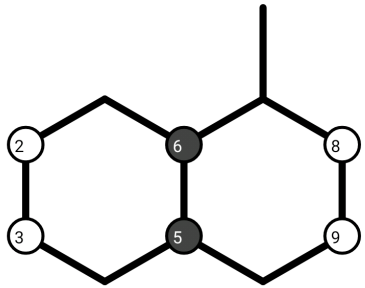
2.2. Molecule orbital presentation:



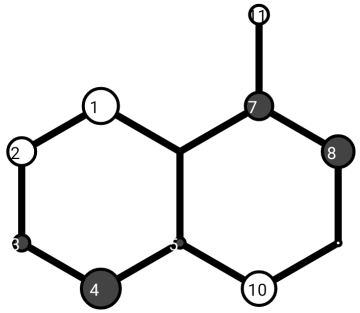
Ψ4



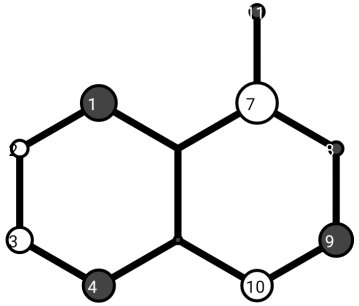
Ψ5



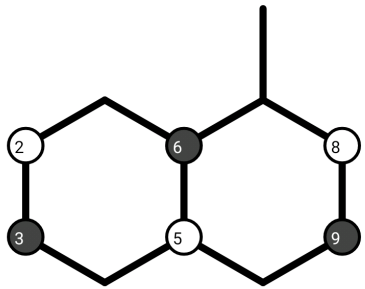
Ψ6



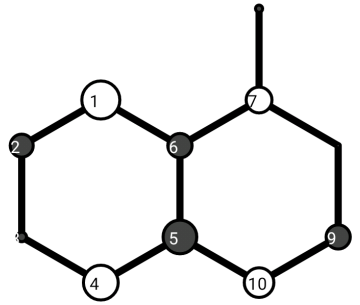
Ψ7



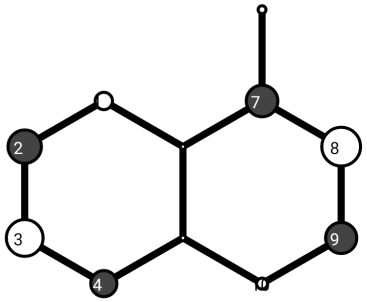
Ψ8



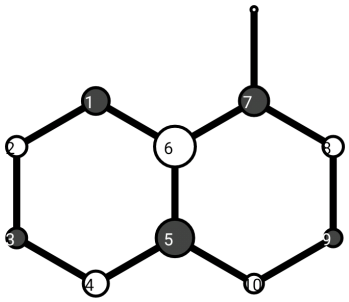
Ψ9



Ψ10



Ψ11

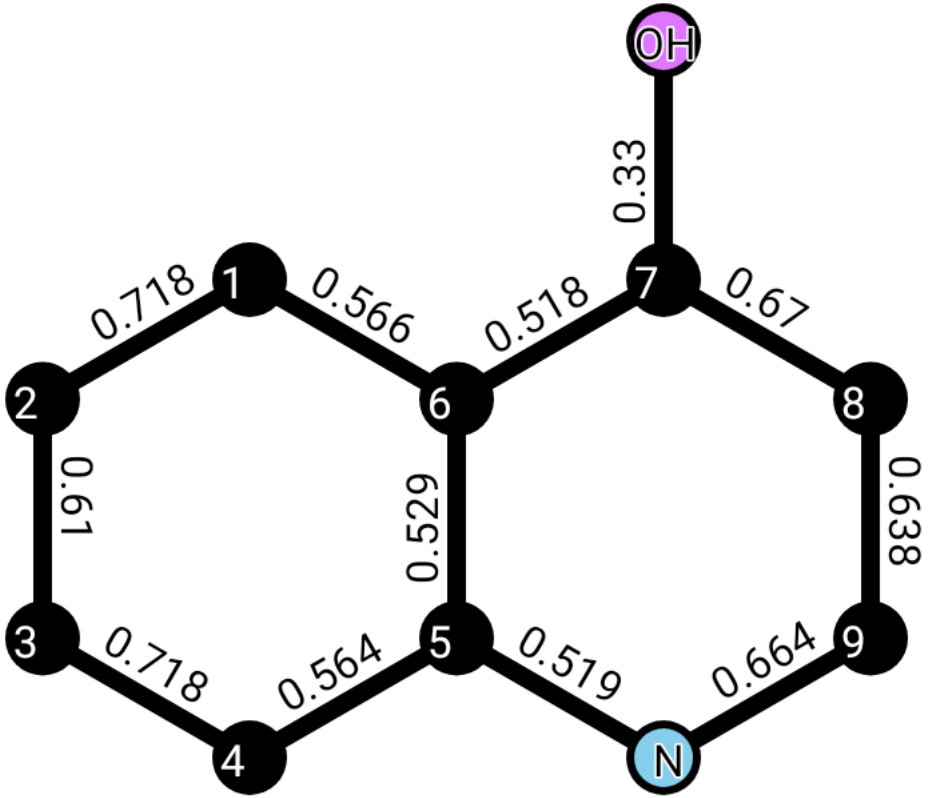


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.977										
2	0.718	1.016									
3	0.02	0.61	0.977								
4	-0.358	-0.018	0.718	1.027							
5	-0.021	-0.249	0.032	0.564	0.936						
6	0.566	-0.018	-0.25	0.018	0.529	1.028					
7	0.054	-0.152	-0.053	0.073	0.072	0.518	0.842				
8	-0.152	-0.034	0.14	0.036	-0.222	0.046	0.67	1.08			
9	-0.042	0.141	0.055	-0.155	-0.096	-0.221	0.125	0.638	0.848		
10	0.067	0.045	-0.146	-0.073	0.519	-0.056	-0.306	-0.1	0.664	1.367	
11	-0.054	0.059	0.034	-0.039	-0.045	-0.117	0.33	-0.176	-0.079	0.123	1.902

3.2. Presentation of bond order:

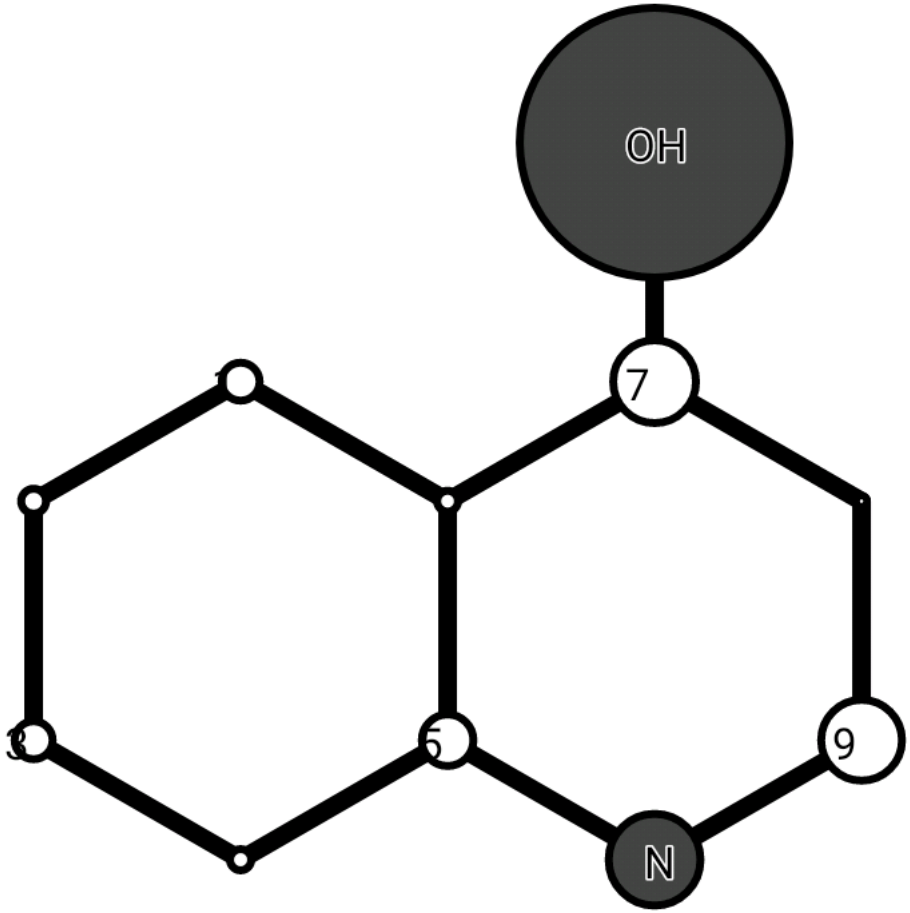

OH
0.33
0.718
1
0.566
0.518
7
0.67
2
6
8
0.61
0.529
0.638
3
0.718
0.564
5
0.519
0.664
9
4
N

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.114										
2		0.075									
3			0.114								
4				0.064							
5					0.155						
6						0.063					
7							0.249				
8								0.011			
9									0.243		
10										-0.276	
11											-0.811

4.2. Presentation of molecule:

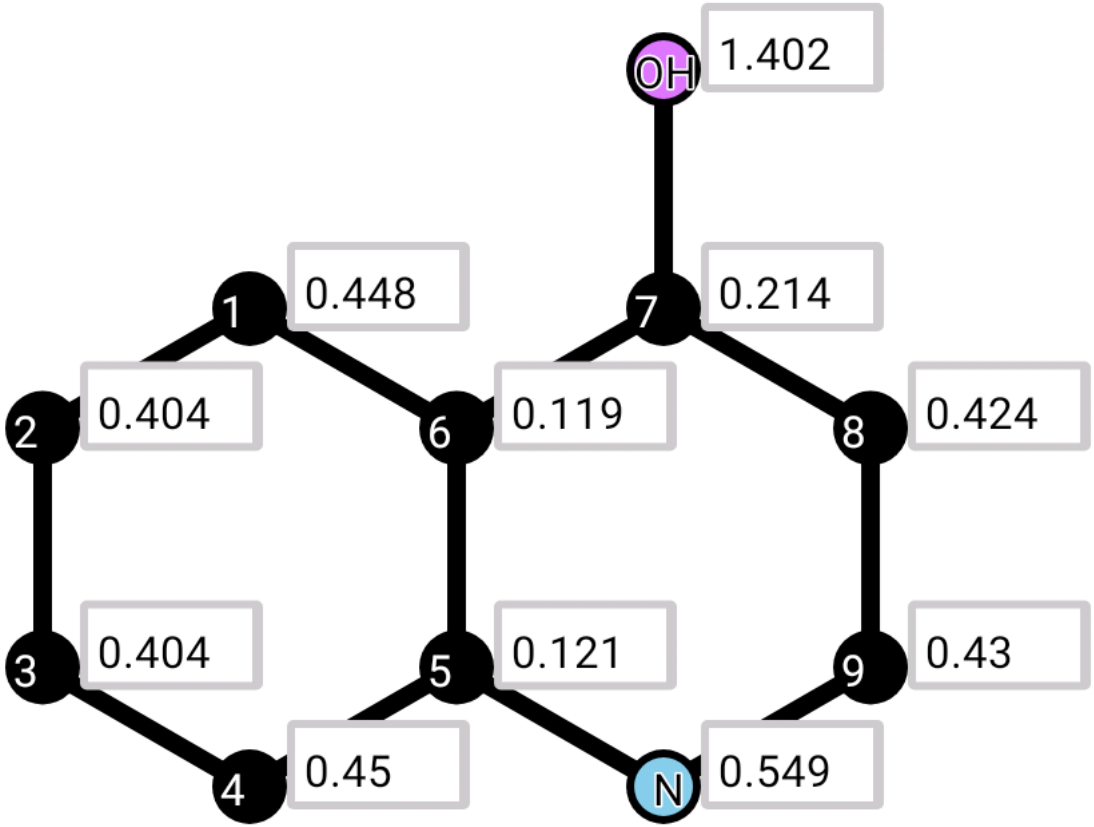

OH
7
9
N

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11
0.448	0.404	0.404	0.45	0.121	0.119	0.214	0.424	0.43	0.549	1.402

5.2. Presentation of molecule:

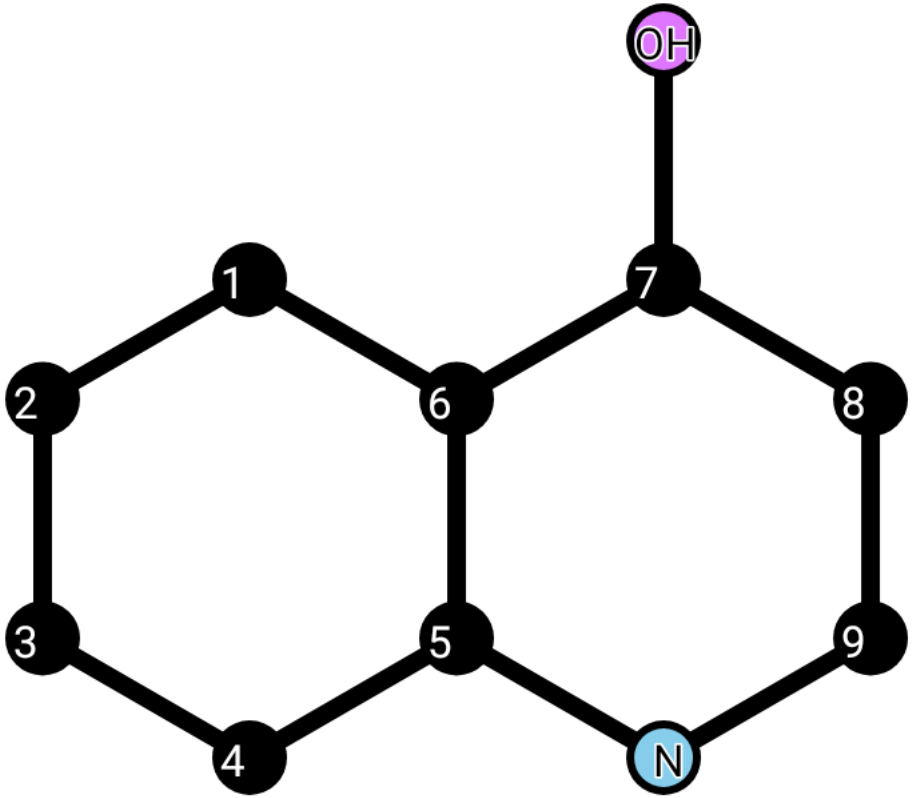

OH
1.402
1
0.448
7
0.214
2
0.404
6
0.119
8
0.424
3
0.404
5
0.121
9
0.43
4
0.45
N
0.549

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.437										
2	-0.206	0.404									
3	0.016	-0.114	0.404								
4	-0.134	0.016	-0.206	0.438							
5	0.003	-0.053	0.006	-0.094	0.329						
6	-0.095	0.007	-0.053	0.003	-0.082	0.335					
7	0.018	-0.025	0.001	-0.017	-0.003	-0.073	0.374				
8	-0.025	-0.002	-0.026	0.004	-0.039	0.004	-0.172	0.407			
9	0.002	-0.025	-0.005	-0.023	-0.002	-0.04	-0.006	-0.133	0.385		
10	-0.016	0.003	-0.022	0.017	-0.063	0.001	-0.095	0.006	-0.148	0.338	
11	0.001	-0.005	-0.001	-0.004	-0.001	-0.007	-0.001	-0.023	-0.004	-0.018	0.064

6.2. Presentation of molecule:

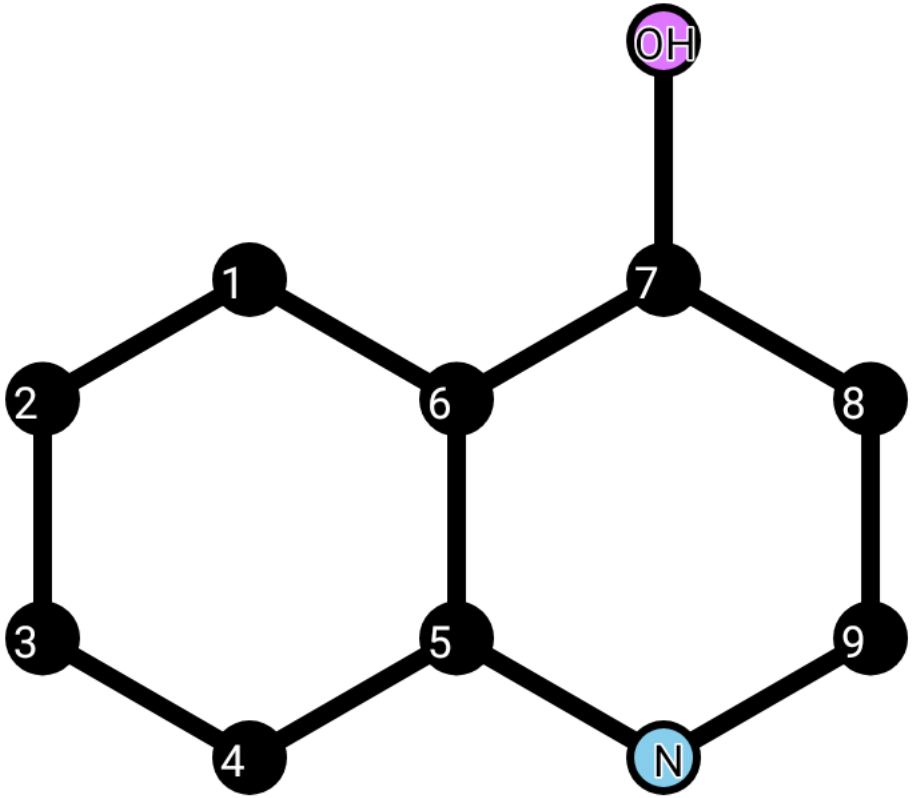

OH
1
7
2
6
8
3
5
9
4
N

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1 2	0.013	-0.007	-0.008	-0.009	-0.006	0.006	0.01	-0.007	0.008	-0.005	0.003
1 6	0.003	0.009	0.006	0.007	0.007	-0.011	-0.017	0.008	-0.011	0.005	-0.006
2 3	-0.012	-0.004	0.009	0.011	0.009	-0.005	-0.011	0.007	-0.011	0.009	-0.003
3 4	0.01	0.006	0.008	-0.017	-0.012	0.004	0.007	-0.007	0.011	-0.012	0.002
4 5	-0.012	-0.003	-0.015	0.004	0.024	-0.005	-0.009	0.01	-0.017	0.025	-0.002
5 6	0.008	-0.004	0.008	-0.007	0.017	-0.005	-0.019	0.008	-0.018	0.015	-0.004
5 10	0.004	0.01	0.004	0.014	-0.016	0.013	0.023	-0.021	0.041	-0.077	0.005
6 7	-0.015	-0.004	-0.015	-0.001	-0.02	0.0	0.046	-0.02	0.028	-0.016	0.018
7 8	0.013	-0.007	0.011	-0.007	0.014	-0.013	0.07	-0.026	-0.048	-0.034	0.026
7 11	-0.005	0.011	0.001	0.008	0.002	0.024	-0.051	0.065	0.006	0.043	-0.103
8 9	-0.011	0.007	-0.011	0.01	-0.019	0.009	-0.058	-0.02	0.06	0.047	-0.014
9 10	0.008	-0.009	0.01	-0.015	0.026	-0.01	0.041	0.03	0.014	-0.106	0.011

7.2. Presentation of molecule:

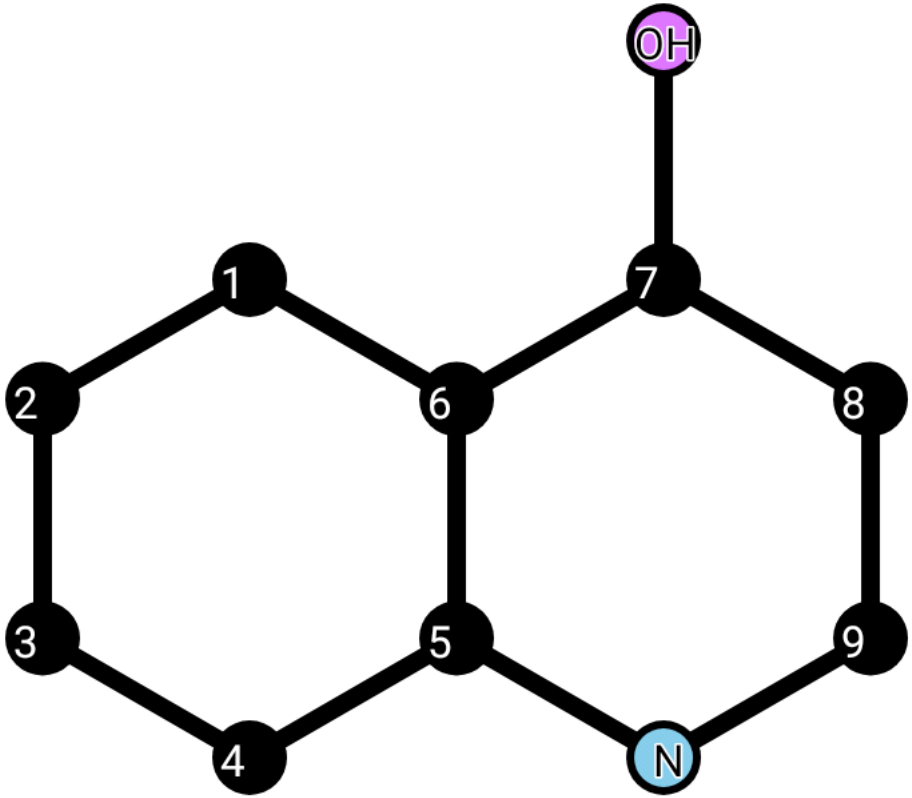

OH
1
7
2
6
8
3
5
9
4
N

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	0.215											
1 6	-0.185	0.285										
2 3	-0.21	0.114	0.291									
3 4	0.126	-0.077	-0.21	0.216								
4 5	-0.077	0.099	0.115	-0.186	0.285							
5 6	0.071	-0.115	-0.045	0.071	-0.114	0.253						
5 10	0.023	-0.023	-0.042	0.056	-0.137	-0.103	0.293					
6 7	0.057	-0.138	-0.043	0.024	-0.025	-0.105	0.088	0.294				
7 8	-0.022	0.044	0.022	-0.012	0.015	0.051	-0.046	-0.141	0.248			
7 11	-0.013	0.025	0.011	-0.008	0.009	0.02	-0.023	-0.079	-0.112	0.364		
8 9	0.023	-0.033	-0.023	0.022	-0.031	-0.029	0.076	0.083	-0.221	0.061	0.293	
9 10	-0.011	0.015	0.02	-0.018	0.038	0.047	-0.12	-0.047	0.132	-0.044	-0.217	0.26

8.2. Presentation of molecule:


OH
1
7
2
6
8
3
5
9
4
N