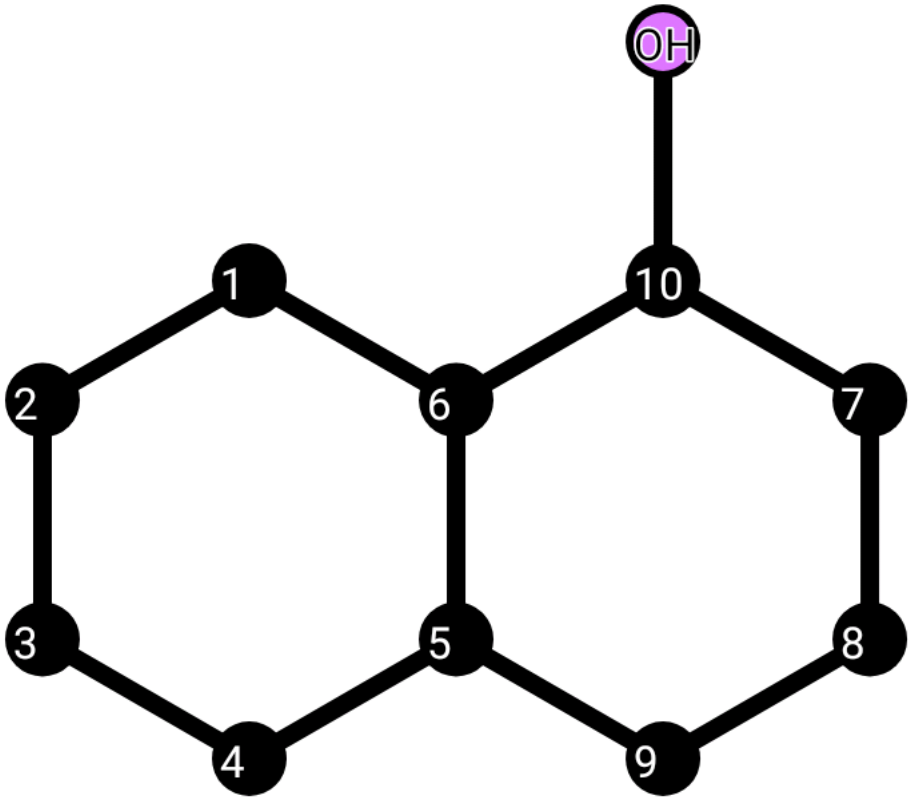
Print calculated values

Report generated by:root, 16.05.2020 - 18:47:44

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	1.0	0.0	0.0
1.0	0.0	0.0	0.0	1.0	-x	0.0	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	1.0	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	1.0	0.0	0.0	1.0	-x	0.0	0.0
0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	-x	0.9
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.9	-x+2.0

It is about this molecule:

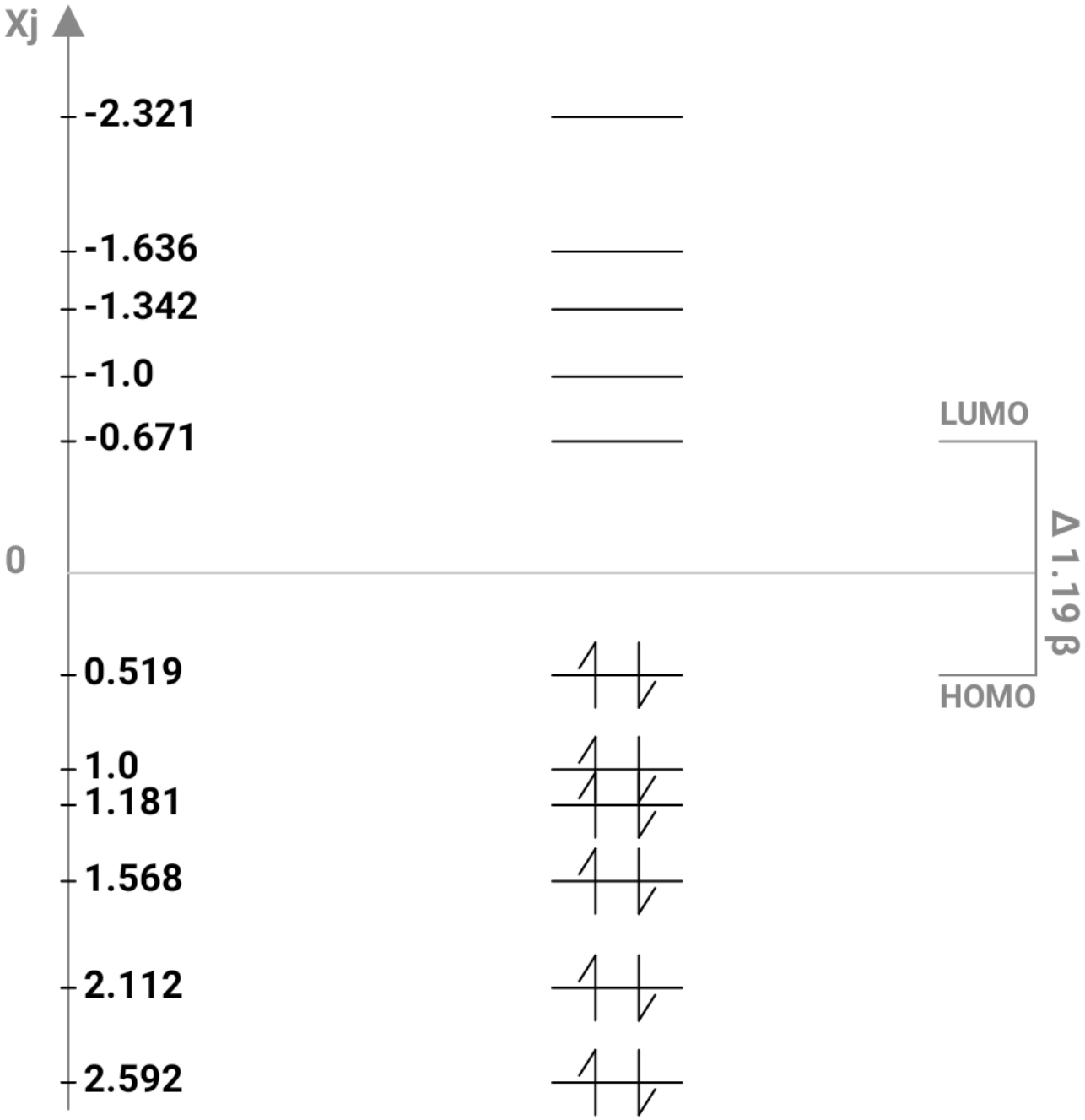


HMO-Energies

x1 = 2.592; x2 = 2.112; x3 = 1.568; x4 = 1.181; x5 = 1.0; x6 = 0.519; x7 = -0.671; x8 = -1.0;
x9 = -1.342; x10 = -1.636; x11 = -2.321;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 11α + 17.944β -

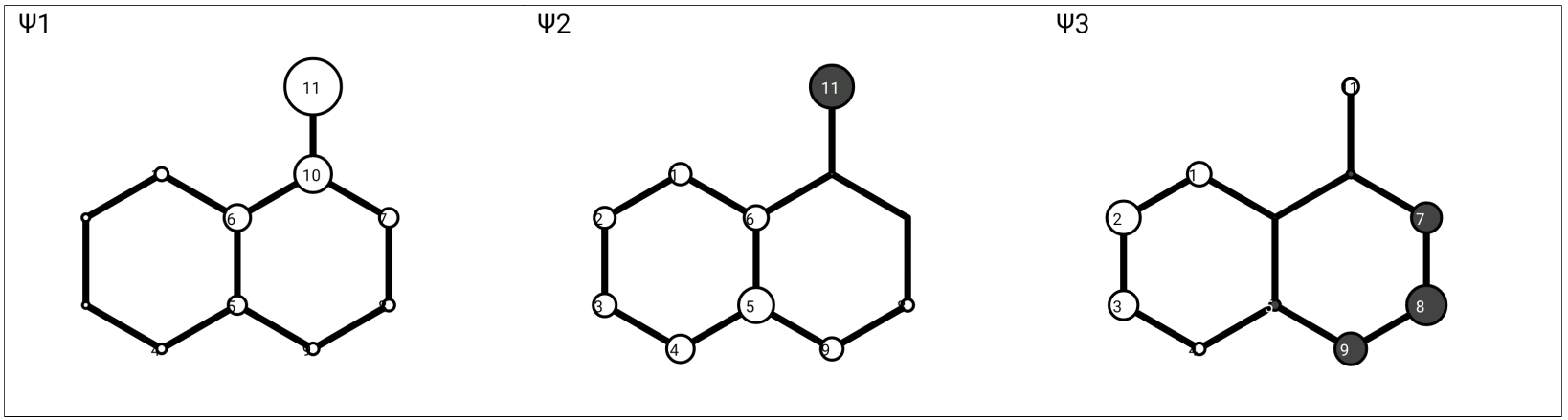
this corresponds to one πelectron: 1.495β

2. Hueckel-coefficient

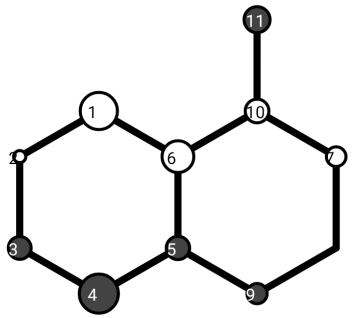
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11
	x1= 2.592	x2= 2.112	x3= 1.568	x4= 1.181	x5= 1.0	x6= 0.519	x7= -0.671	x8= -1.0	x9= -1.342	x10= -1.636	x11= -2.321
1	0.162	0.265	0.293	0.439	0.0	0.347	-0.455	0.0	0.382	0.251	0.296
2	0.095	0.26	0.415	0.144	0.408	0.265	0.254	-0.408	-0.194	-0.42	-0.222
3	0.083	0.284	0.358	-0.27	0.408	-0.21	0.285	0.408	-0.122	0.435	0.22
4	0.12	0.34	0.146	-0.462	0.0	-0.374	-0.445	0.0	0.358	-0.293	-0.289
5	0.228	0.434	-0.129	-0.276	-0.408	0.016	0.014	-0.408	-0.358	0.044	0.451
6	0.327	0.3	0.044	0.375	-0.408	-0.085	0.052	0.408	-0.32	0.009	-0.464
7	0.232	0.04	-0.37	0.232	0.408	-0.349	-0.202	-0.408	-0.126	0.428	-0.242
8	0.145	0.15	-0.486	-0.006	0.408	0.226	-0.271	0.408	-0.236	-0.392	0.231
9	0.144	0.276	-0.392	-0.239	0.0	0.467	0.384	0.0	0.442	0.213	-0.294
10	0.456	-0.066	-0.095	0.28	0.0	-0.407	0.407	0.0	0.405	-0.309	0.331
11	0.694	-0.532	0.197	-0.307	0.0	0.247	-0.137	0.0	-0.109	0.077	-0.069

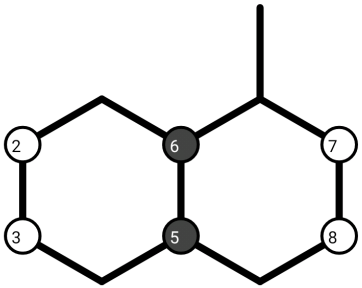
2.2. Molecule orbital presentation:



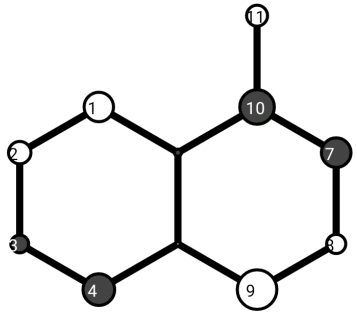
Ψ4



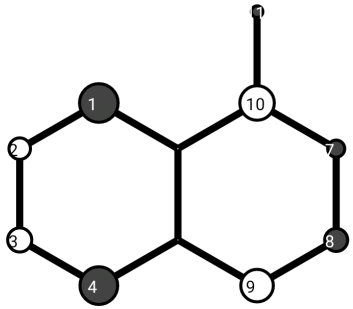
Ψ5



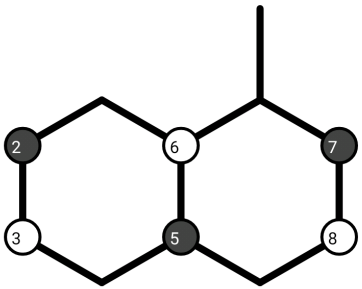
Ψ6



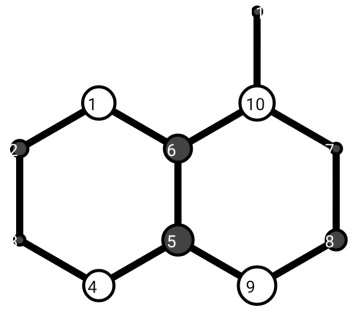
Ψ7



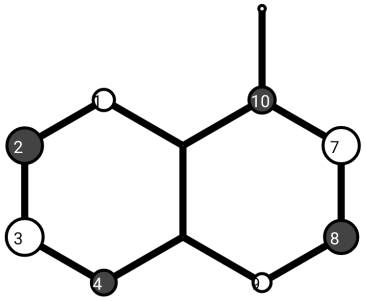
Ψ8



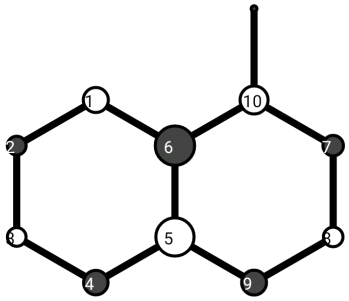
Ψ9



Ψ10



Ψ11

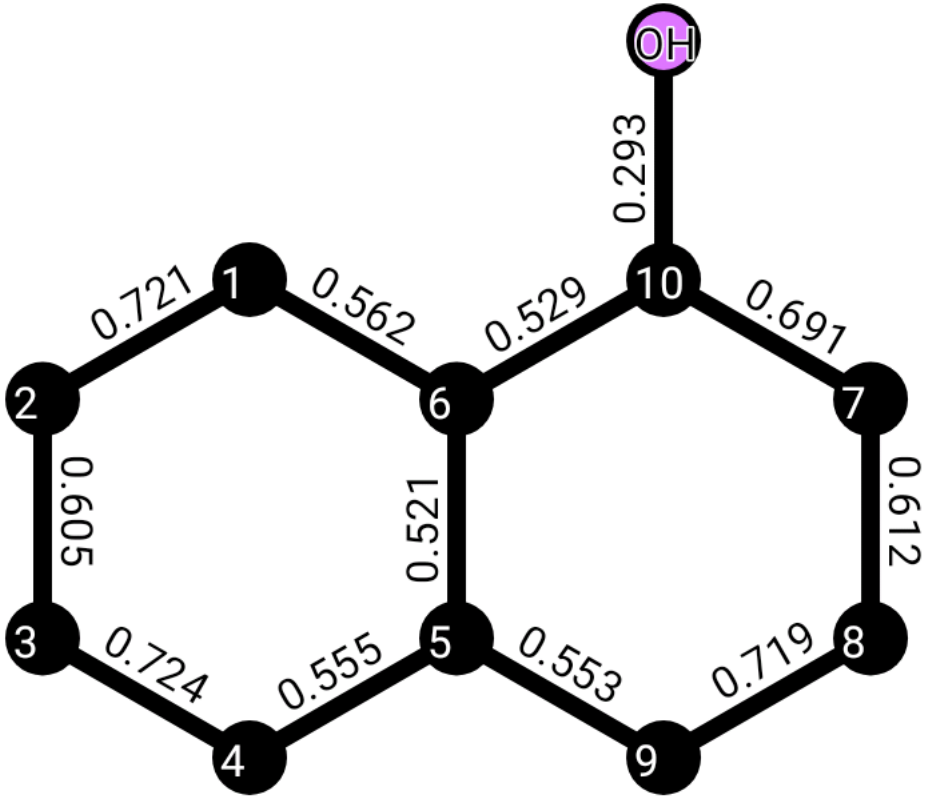


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.992										
2	0.721	1.012									
3	0.004	0.605	0.998								
4	-0.361	-0.01	0.724	1.009							
5	-0.002	-0.242	0.001	0.555	0.999						
6	0.562	-0.016	-0.244	0.012	0.521	1.026					
7	-0.16	-0.028	0.151	0.021	-0.237	0.042	1.07				
8	-0.006	0.153	0.003	-0.169	-0.002	-0.235	0.612	0.995			
9	0.078	0.025	-0.166	-0.02	0.553	-0.033	-0.058	0.719	1.051		
10	0.021	-0.162	-0.01	0.083	0.007	0.529	0.691	0.017	-0.345	0.931	
11	-0.039	0.061	0.015	-0.039	-0.019	-0.121	-0.182	-0.034	0.129	0.293	1.917

3.2. Presentation of bond order:

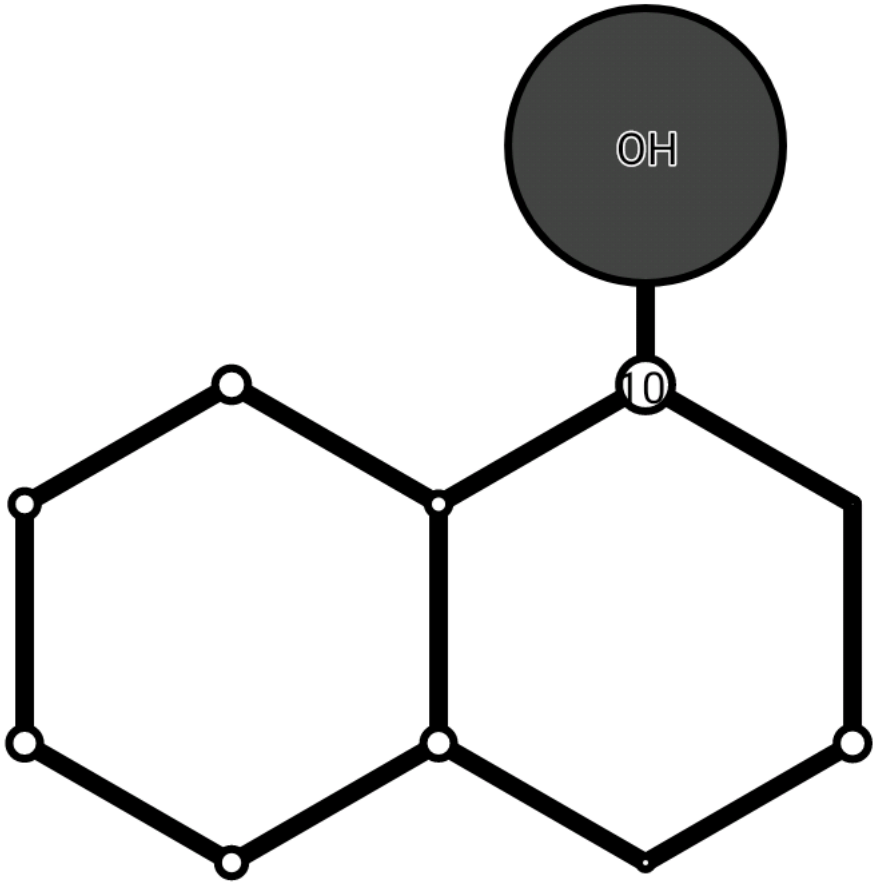

OH
0.293
1
10
0.721
0.562
0.529
0.691
2
6
7
0.605
0.521
0.612
3
5
8
0.724
0.555
0.553
0.719
4
9

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.099										
2		0.079									
3			0.093								
4				0.082							
5					0.092						
6						0.065					
7							0.021				
8								0.096			
9									0.04		
10										0.16	
11											-0.827

4.2. Presentation of molecule:

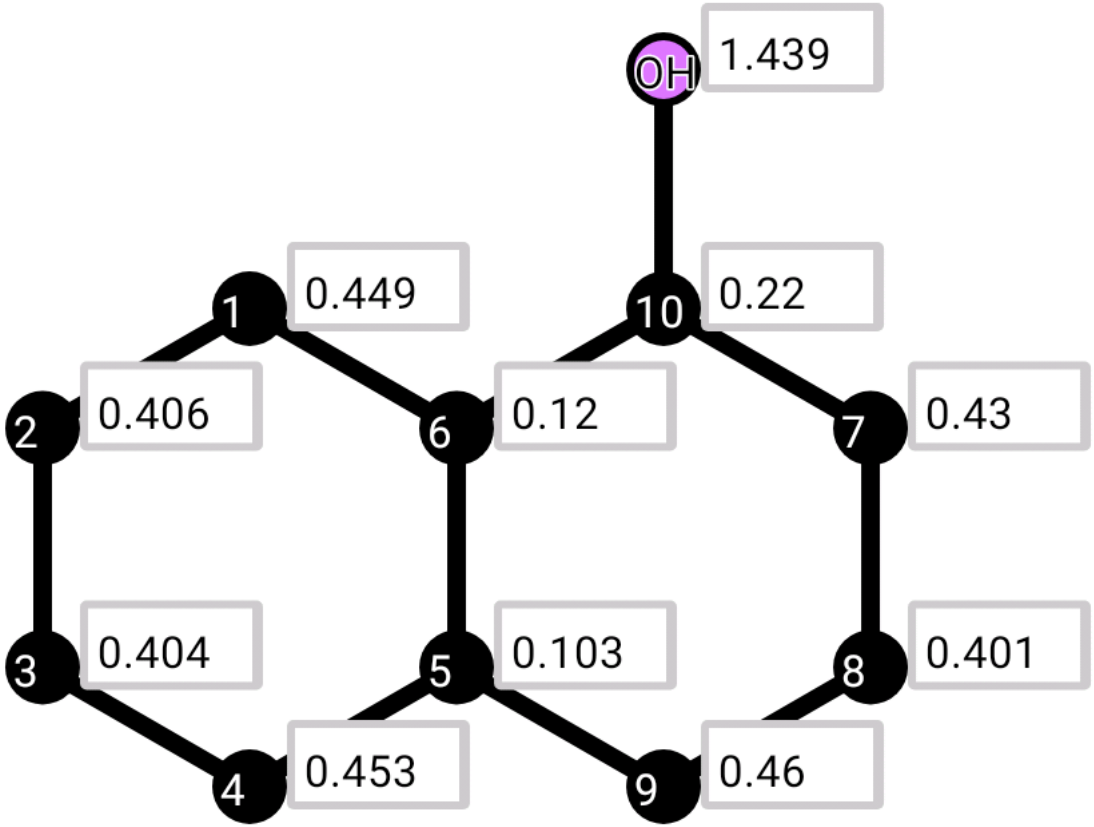

OH
10

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11
0.449	0.406	0.404	0.453	0.103	0.12	0.43	0.401	0.46	0.22	1.439

5.2. Presentation of molecule:

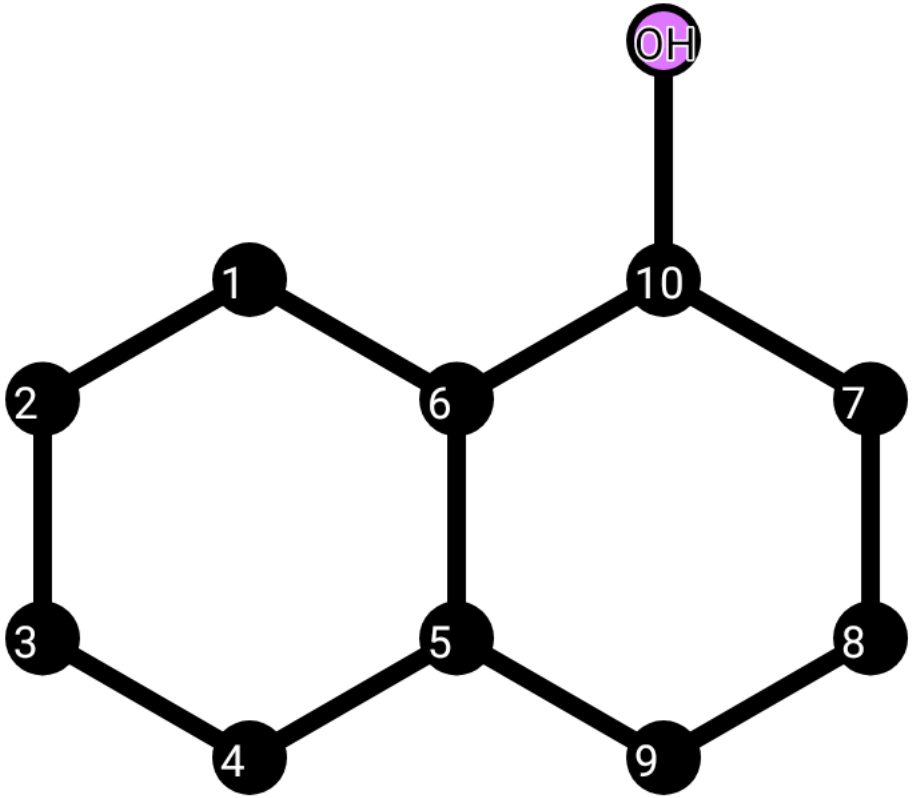

OH
1.439
1
0.449
10
0.22
2
0.406
6
0.12
7
0.43
3
0.404
5
0.103
8
0.401
4
0.453
9
0.46

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.439										
2	-0.211	0.406									
3	0.017	-0.111	0.404								
4	-0.138	0.018	-0.213	0.443							
5	0.004	-0.049	0.007	-0.089	0.329						
6	-0.092	0.008	-0.05	0.003	-0.078	0.336					
7	-0.029	-0.001	-0.031	0.006	-0.048	0.003	0.415				
8	0.006	-0.032	0.0	-0.032	0.008	-0.047	-0.114	0.403			
9	-0.021	0.006	-0.031	0.027	-0.088	0.003	0.016	-0.209	0.447		
10	0.023	-0.03	0.006	-0.022	0.003	-0.079	-0.192	0.015	-0.129	0.398	
11	0.002	-0.005	0.001	-0.004	0.0	-0.008	-0.025	0.001	-0.021	0.007	0.052

6.2. Presentation of molecule:

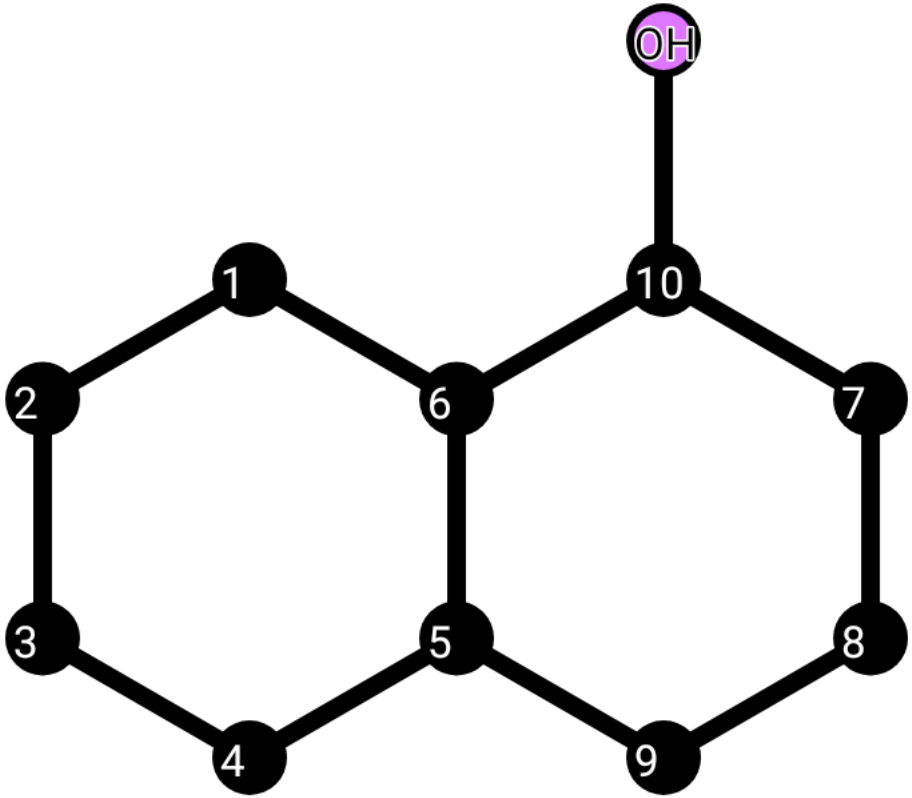

OH
1
10
2
6
7
3
5
8
4
9

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1 2	0.006	-0.005	-0.001	-0.005	-0.001	0.006	-0.006	0.001	-0.004	0.005	0.002
1 6	-0.003	0.008	0.0	0.007	0.001	-0.011	0.009	-0.002	0.005	-0.01	-0.005
2 3	-0.003	-0.005	0.0	0.006	0.0	-0.005	0.007	-0.001	0.005	-0.003	-0.001
3 4	0.002	0.004	0.002	-0.005	0.0	0.003	-0.005	0.001	-0.004	0.002	0.001
4 5	0.0	-0.003	-0.001	-0.003	0.0	-0.003	0.006	0.0	0.006	-0.001	0.0
5 6	0.001	-0.004	0.0	-0.004	-0.001	-0.008	0.01	0.0	0.01	-0.003	-0.002
5 9	-0.001	0.007	0.001	0.007	0.001	0.01	-0.015	0.0	-0.014	0.003	0.001
6 10	-0.003	-0.002	-0.001	-0.003	-0.001	0.003	-0.023	0.004	-0.013	0.026	0.015
7 8	-0.003	0.007	-0.001	0.006	0.0	0.011	-0.028	-0.004	0.03	-0.012	-0.006
7 10	0.006	-0.006	0.002	-0.004	0.001	-0.013	-0.016	-0.003	-0.023	0.037	0.02
8 9	0.002	-0.006	0.001	-0.005	0.0	-0.008	0.022	0.006	-0.024	0.008	0.004
10 11	-0.008	0.012	-0.002	0.01	-0.001	0.026	0.071	-0.005	0.053	-0.066	-0.09

7.2. Presentation of molecule:

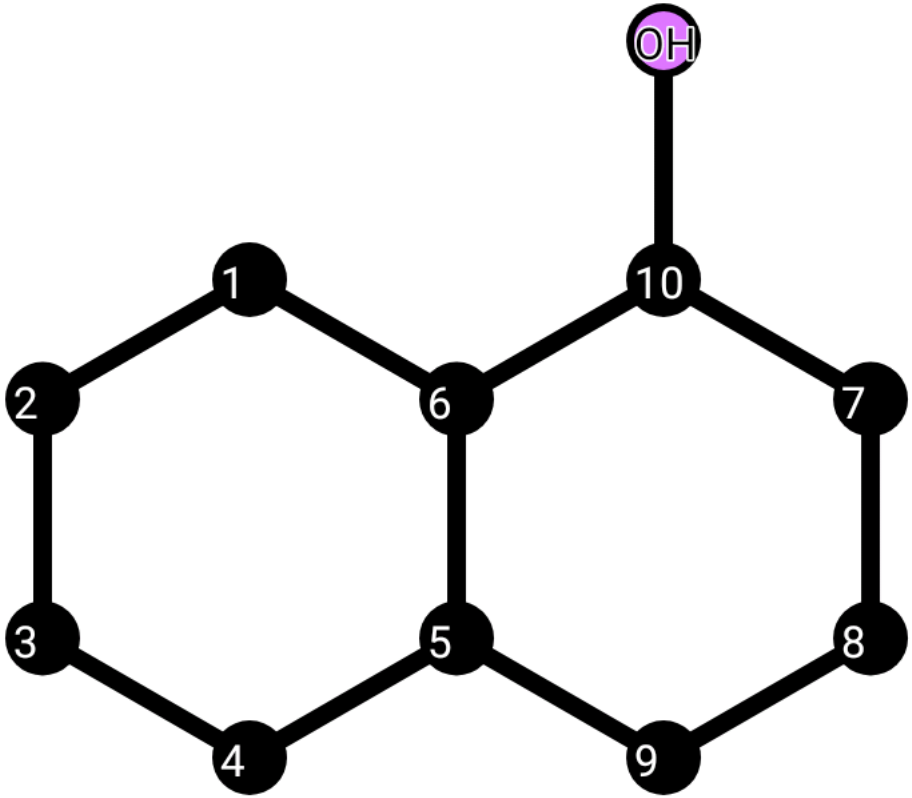

OH
1
10
2
6
7
3
5
8
4
9

8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	2 3	3 4	4 5	5 6	5 9	6 10	7 8	7 10	8 9	10 11
1 2	0.211											
1 6	-0.185	0.289										
2 3	-0.208	0.112	0.295									
3 4	0.124	-0.075	-0.21	0.21								
4 5	-0.073	0.096	0.111	-0.181	0.288							
5 6	0.068	-0.112	-0.042	0.067	-0.109	0.256						
5 9	0.023	-0.024	-0.045	0.059	-0.145	-0.112	0.292					
6 10	0.059	-0.14	-0.044	0.025	-0.025	-0.104	0.093	0.287				
7 8	0.029	-0.04	-0.031	0.031	-0.045	-0.041	0.11	0.101	0.299			
7 10	-0.027	0.051	0.029	-0.018	0.024	0.061	-0.069	-0.156	-0.205	0.221		
8 9	-0.018	0.022	0.031	-0.031	0.059	0.065	-0.181	-0.068	-0.216	0.124	0.217	
10 11	-0.008	0.018	0.004	-0.002	0.001	0.007	-0.005	-0.062	0.022	-0.083	-0.015	0.338

8.2. Presentation of molecule:


OH
1
10
2
6
7
3
5
8
4
9