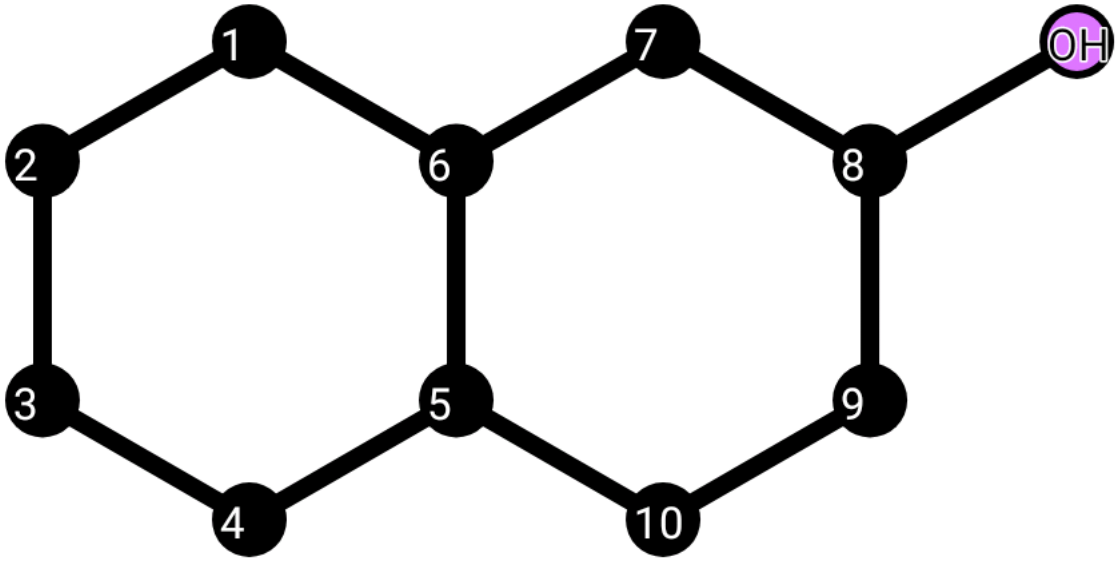
Print calculated values

Report generated by:root, 16.05.2020 - 18:45:56

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

It is about this molecule:

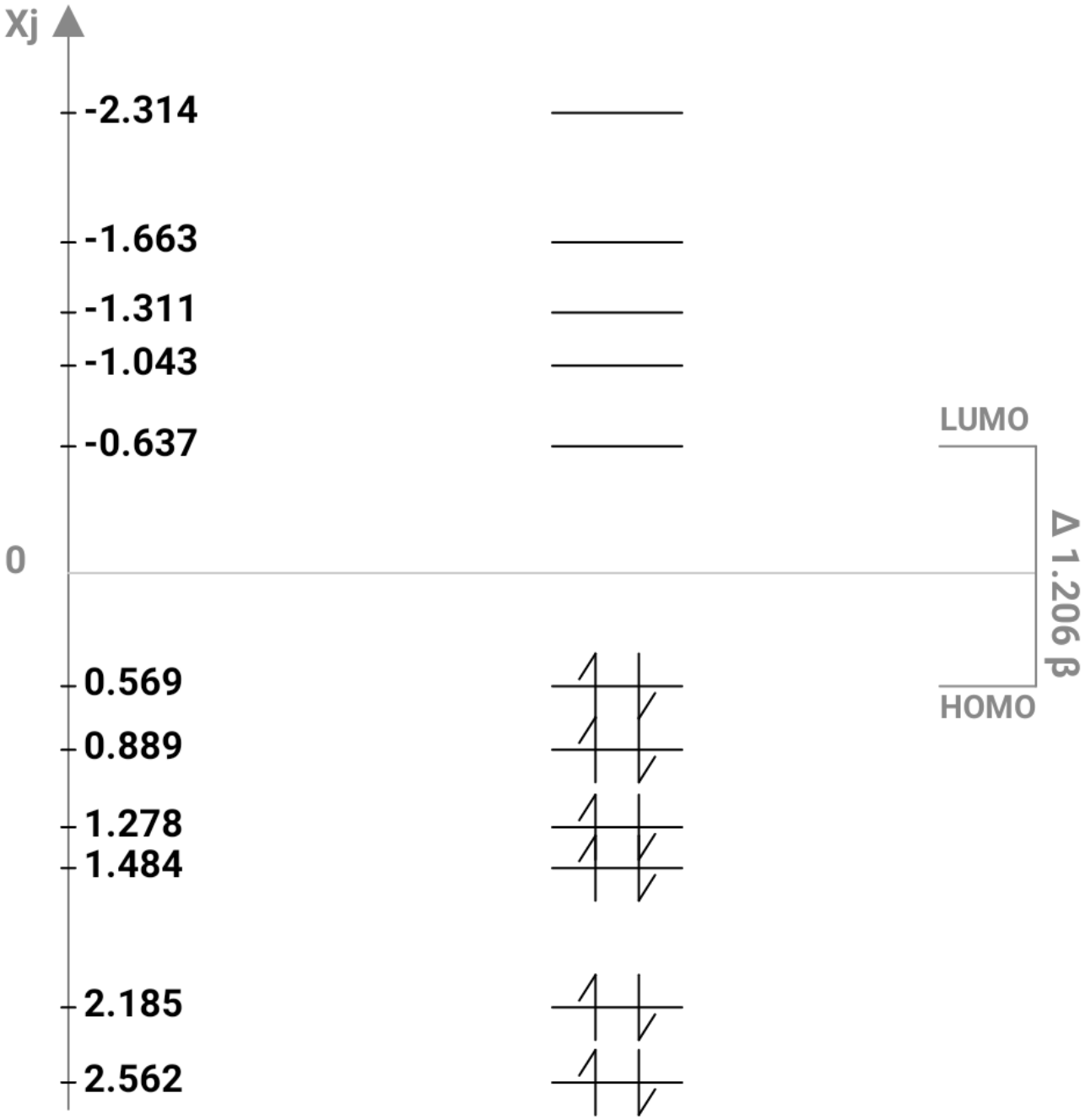


HMO-Energies

x1 = 2.562; x2 = 2.185; x3 = 1.484; x4 = 1.278; x5 = 0.889; x6 = 0.569; x7 = -0.637; x8 = -1.043; x9 = -1.311; x10 = -1.663; x11 = -2.314;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 11α + 17.934β -

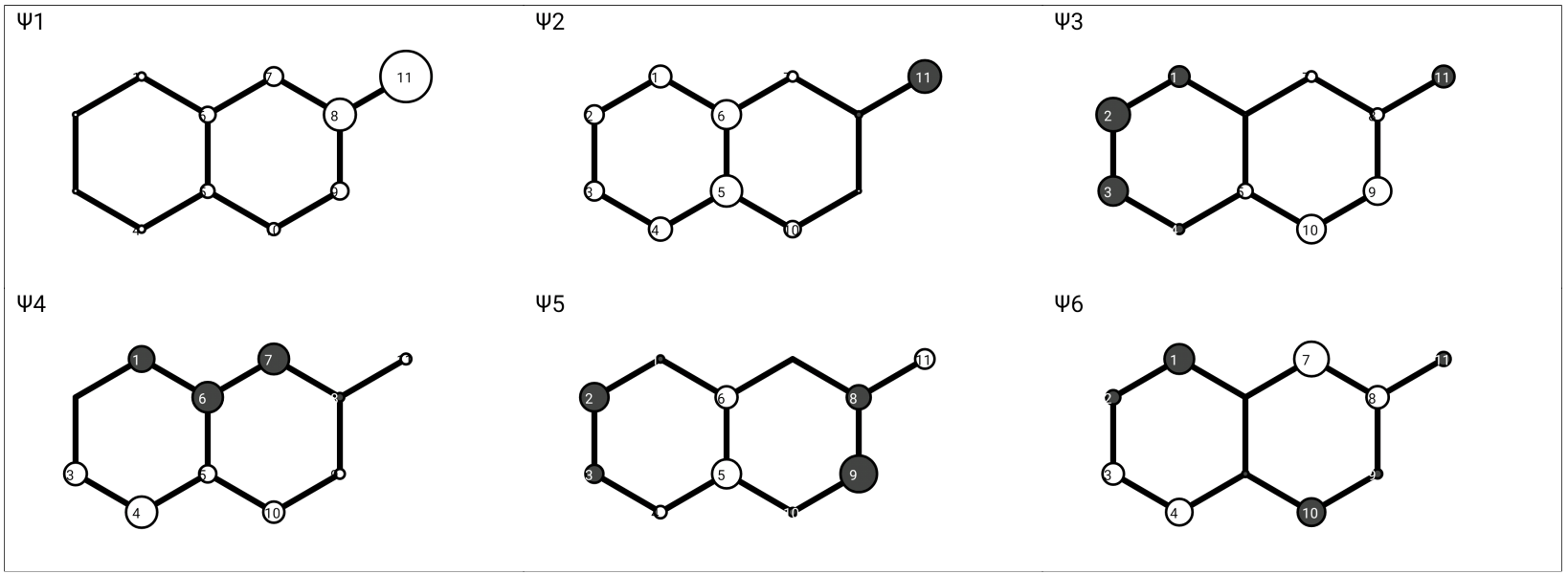
this corresponds to one πelectron: 1.494β

2. Hueckel-coefficient

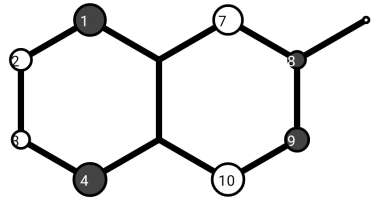
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11
	x1= 2.562	x2= 2.185	x3= 1.484	x4= 1.278	x5= 0.889	x6= 0.569	x7= -0.637	x8= -1.043	x9= -1.311	x10= -1.663	x11= -2.314
1	0.115	0.308	-0.289	-0.36	-0.101	-0.418	-0.419	0.035	0.406	-0.258	0.294
2	0.071	0.264	-0.473	-0.032	-0.4	-0.201	0.286	0.402	-0.216	0.401	-0.223
3	0.067	0.27	-0.412	0.319	-0.254	0.303	0.237	-0.454	-0.123	-0.409	0.223
4	0.102	0.325	-0.139	0.44	0.174	0.374	-0.437	0.072	0.377	0.279	-0.292
5	0.193	0.441	0.206	0.243	0.409	-0.091	0.041	0.379	-0.371	-0.055	0.453
6	0.222	0.408	0.044	-0.428	0.31	-0.037	-0.019	-0.438	-0.316	0.028	-0.457
7	0.263	0.144	0.148	-0.43	-0.032	0.487	0.39	0.043	0.379	0.267	0.309
8	0.451	-0.094	0.176	-0.121	-0.339	0.314	-0.229	0.393	-0.181	-0.471	-0.259
9	0.242	0.062	0.389	0.139	-0.516	-0.131	-0.314	-0.348	-0.186	0.413	0.242
10	0.17	0.23	0.401	0.299	-0.12	-0.389	0.429	-0.029	0.425	-0.215	-0.301
11	0.722	-0.458	-0.307	0.151	0.274	-0.198	0.078	-0.116	0.049	0.116	0.054

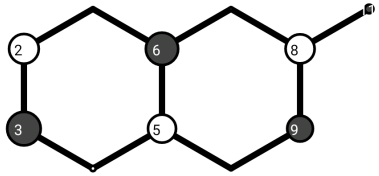
2.2. Molecule orbital presentation:



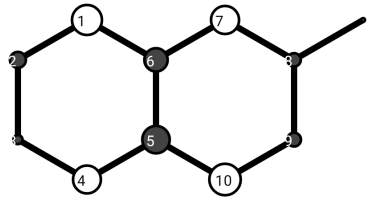
Ψ7



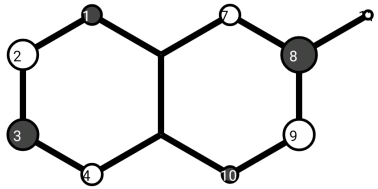
Ψ8



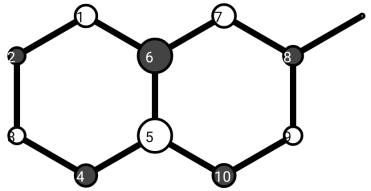
Ψ9



Ψ10



Ψ11

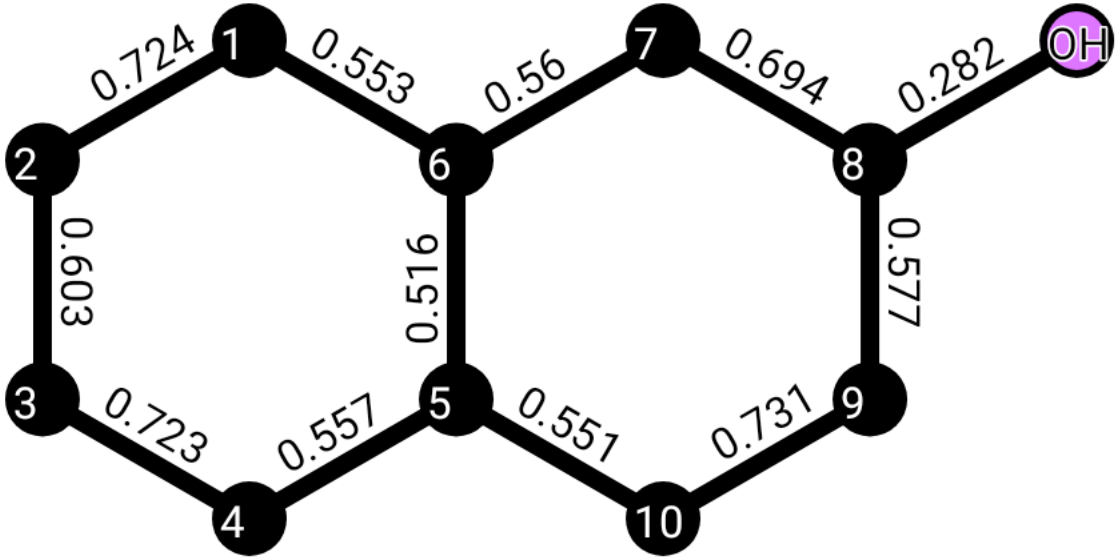


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	1.012										
2	0.724	1.0									
3	-0.012	0.603	1.012								
4	-0.361	0.0	0.723	0.998							
5	0.014	-0.241	-0.014	0.557	1.017						
6	0.553	0.0	-0.24	0.002	0.516	0.998					
7	-0.028	-0.17	0.028	0.08	-0.035	0.56	1.071				
8	-0.163	0.0	0.15	-0.008	-0.23	0.01	0.694	0.942			
9	-0.017	0.156	0.017	-0.173	-0.022	-0.236	0.047	0.577	1.032		
10	0.083	0.0	-0.168	0.003	0.551	-0.003	-0.354	0.015	0.731	0.995	
11	0.062	0.001	-0.06	0.015	0.082	-0.025	-0.184	0.282	-0.135	-0.034	1.923

3.2. Presentation of bond order:

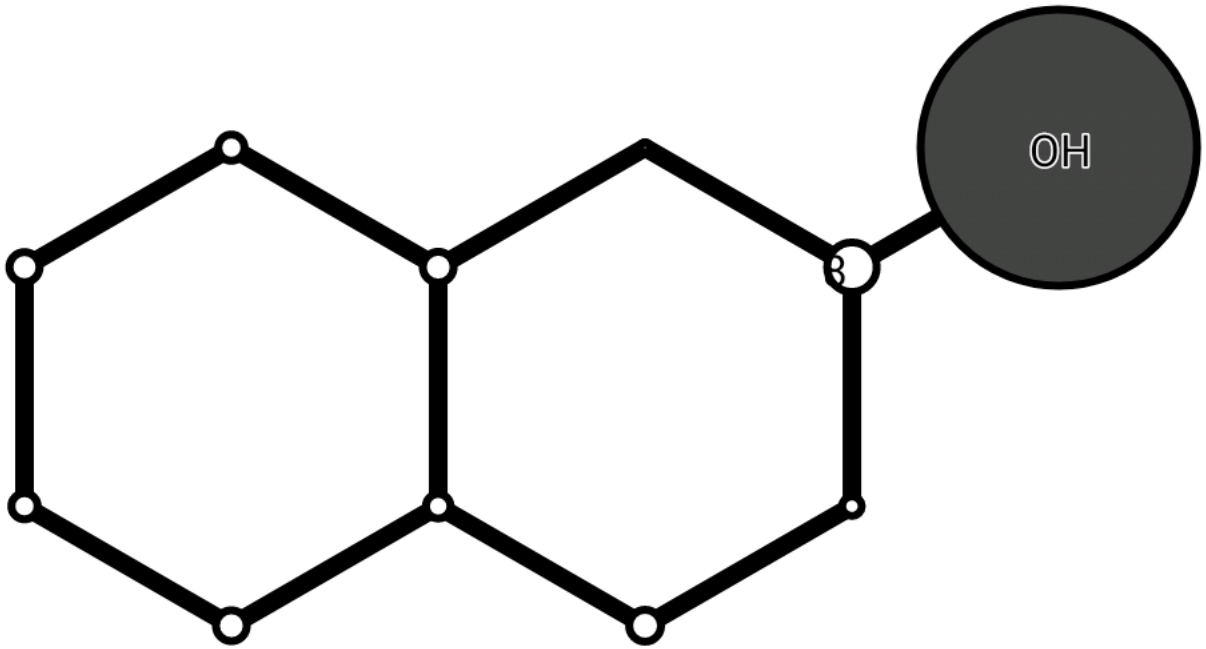

0.724
0.553
0.56
0.694
0.282
OH
1
2
3
4
5
6
7
8
9
10
0.603
0.516
0.577
0.723
0.557
0.551
0.731

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.079										
2		0.091									
3			0.079								
4				0.093							
5					0.074						
6						0.093					
7							0.02				
8								0.149			
9									0.059		
10										0.096	
11											-0.832

4.2. Presentation of molecule:

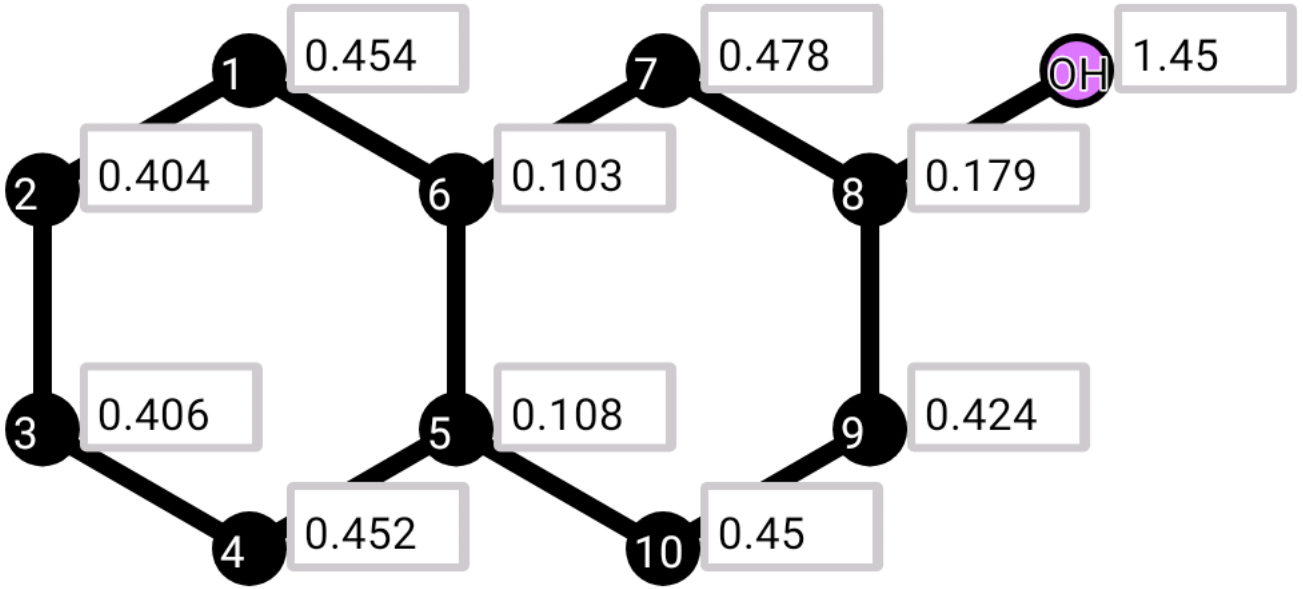

OH

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11
0.454	0.404	0.406	0.452	0.108	0.103	0.478	0.179	0.424	0.45	1.45

5.2. Presentation of molecule:

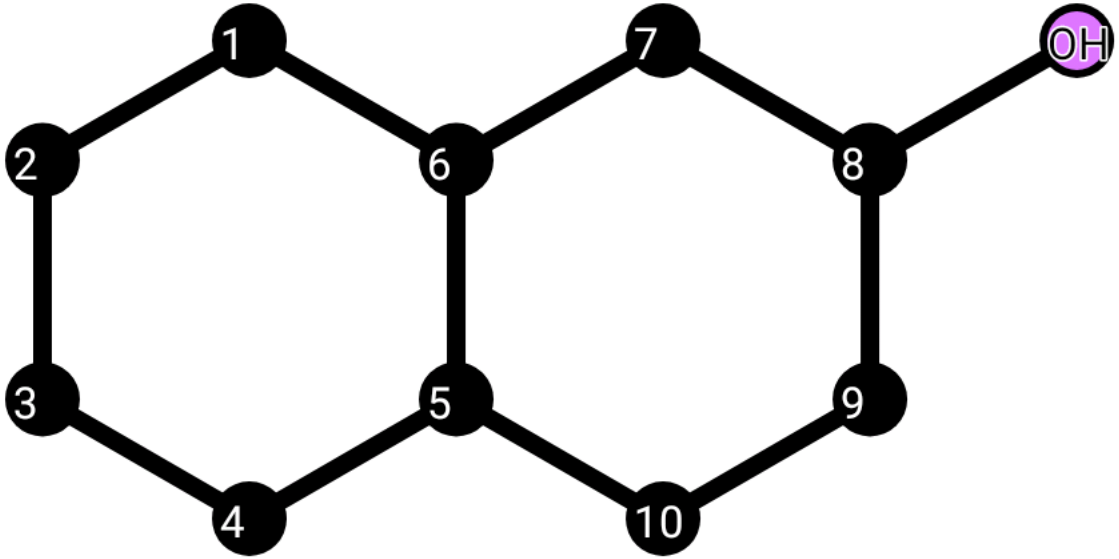


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.444										
2	-0.213	0.405									
3	0.018	-0.11	0.406								
4	-0.138	0.018	-0.212	0.442							
5	0.003	-0.049	0.007	-0.09	0.332						
6	-0.088	0.007	-0.048	0.003	-0.076	0.329					
7	0.028	-0.032	0.006	-0.022	0.003	-0.091	0.454				
8	-0.03	0.0	-0.031	0.006	-0.045	0.006	-0.196	0.368			
9	0.005	-0.033	0.0	-0.033	0.008	-0.047	0.011	-0.098	0.415		
10	-0.023	0.006	-0.031	0.026	-0.087	0.004	-0.135	0.016	-0.218	0.44	
11	-0.005	0.0	-0.005	0.001	-0.007	0.0	-0.026	0.004	-0.01	0.001	0.046

6.2. Presentation of molecule:


1
2
3
4
5
6
7
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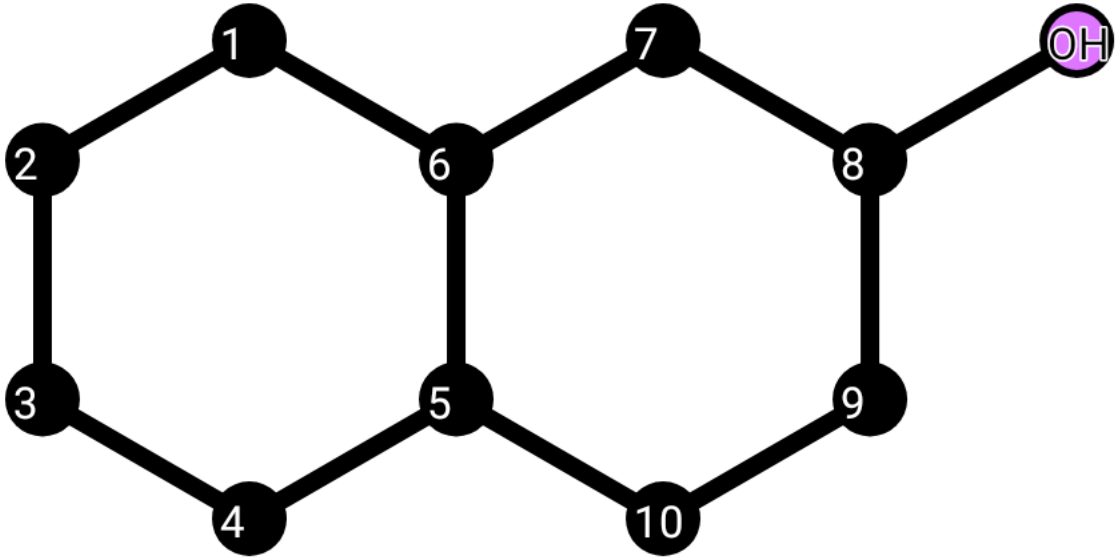
9
10
OH

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1 2	-0.007	0.0	0.004	0.001	0.004	0.0	-0.007	0.0	0.004	0.001	0.0
1 6	-0.003	0.0	-0.003	0.001	-0.004	0.001	0.01	0.002	-0.005	0.0	0.001
2 3	0.007	0.0	-0.004	-0.001	-0.004	0.0	0.007	0.0	-0.004	-0.001	0.0
3 4	-0.006	0.0	-0.006	0.002	0.005	0.001	-0.005	0.002	0.004	0.002	0.001
4 5	0.007	0.0	0.008	-0.001	-0.006	-0.001	0.006	-0.003	-0.005	-0.002	-0.002
5 6	-0.004	0.0	-0.004	0.0	-0.004	0.002	0.011	0.003	-0.005	0.0	0.002
5 10	-0.003	0.0	-0.003	0.0	-0.003	0.001	-0.015	0.005	0.012	0.004	0.003
6 7	0.008	0.0	0.008	-0.001	0.01	-0.002	-0.025	-0.006	0.012	0.0	-0.004
7 8	-0.004	0.0	-0.006	0.002	-0.008	-0.002	-0.017	0.029	-0.017	0.006	0.018
8 9	-0.005	0.0	-0.004	-0.001	-0.004	0.002	-0.026	0.023	0.004	-0.004	0.015
8 11	0.013	0.0	0.013	-0.002	0.018	-0.002	0.073	-0.057	0.033	-0.005	-0.083
9 10	0.004	0.0	0.004	-0.001	0.006	0.0	0.021	-0.008	-0.019	-0.003	-0.005

7.2. Presentation of molecule: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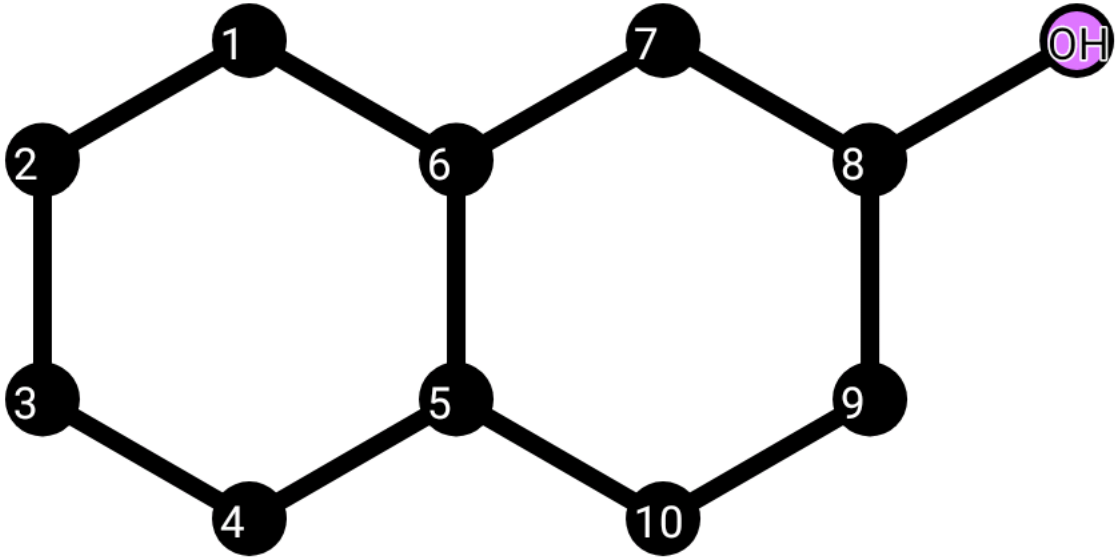
OH

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	8 9	8 11	9 10
1 2	0.21											
1 6	-0.181	0.289										
2 3	-0.21	0.111	0.296									
3 4	0.124	-0.073	-0.209	0.211								
4 5	-0.074	0.095	0.111	-0.183	0.289							
5 6	0.066	-0.107	-0.041	0.066	-0.109	0.255						
5 10	0.025	-0.025	-0.045	0.06	-0.145	-0.108	0.291					
6 7	0.06	-0.148	-0.045	0.024	-0.024	-0.112	0.094	0.292				
7 8	-0.031	0.058	0.031	-0.018	0.022	0.065	-0.068	-0.177	0.217			
8 9	0.031	-0.042	-0.032	0.032	-0.045	-0.039	0.109	0.104	-0.184	0.295		
8 11	0.0	-0.004	0.0	-0.004	0.006	-0.006	-0.009	0.013	-0.073	-0.063	0.322	
9 10	-0.02	0.024	0.032	-0.033	0.061	0.065	-0.185	-0.072	0.114	-0.203	0.016	0.21

8.2. Presentation of molecule: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OH