Print calculated values

Report generated by:root, 31.03.2020 - 14:42:25

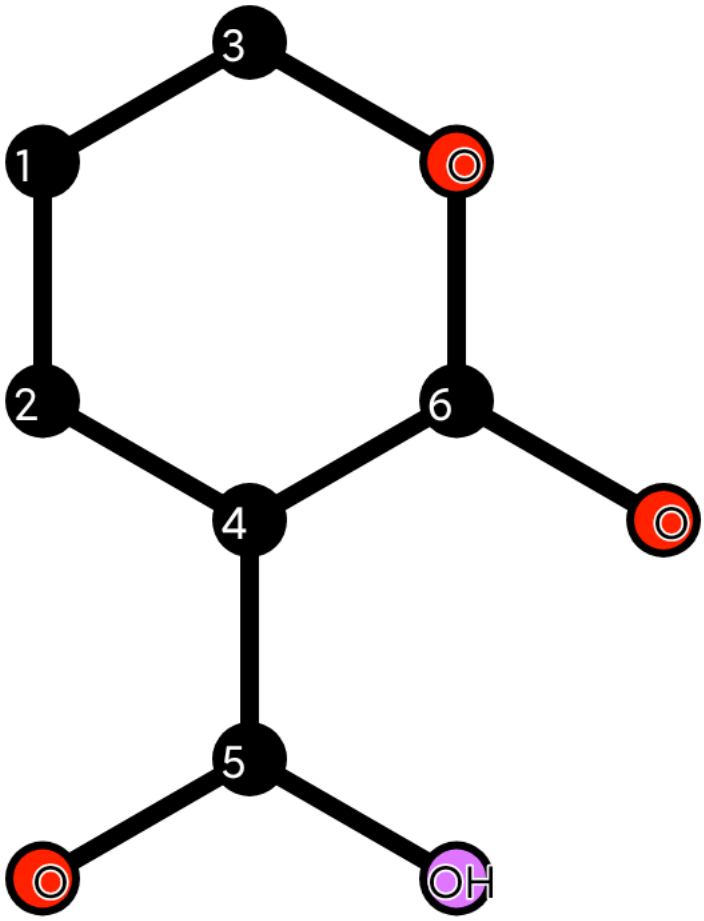
The following determinant is calculated:

-x	1.0	1.0	0.0	0.0	0.0	0.0	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
1.0	0.0	-x	0.0	0.0	0.0	0.0	0.0	0.19	0.0
0.0	1.0	0.0	-x	1.0	1.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	1.0	-x	0.0	1.93	0.0	0.0	0.9
0.0	0.0	0.0	1.0	0.0	-x	0.0	1.93	0.19	0.0
0.0	0.0	0.0	0.0	1.93	0.0	-x+1.18	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	1.93	0.0	-x+1.18	0.0	0.0
0.0	0.0	0.19	0.0	0.0	0.19	0.0	0.0	-x+2.06	0.0
0.0	0.0	0.0	0.0	0.9	0.0	0.0	0.0	0.0	-x+2.0

It is about this molecule:

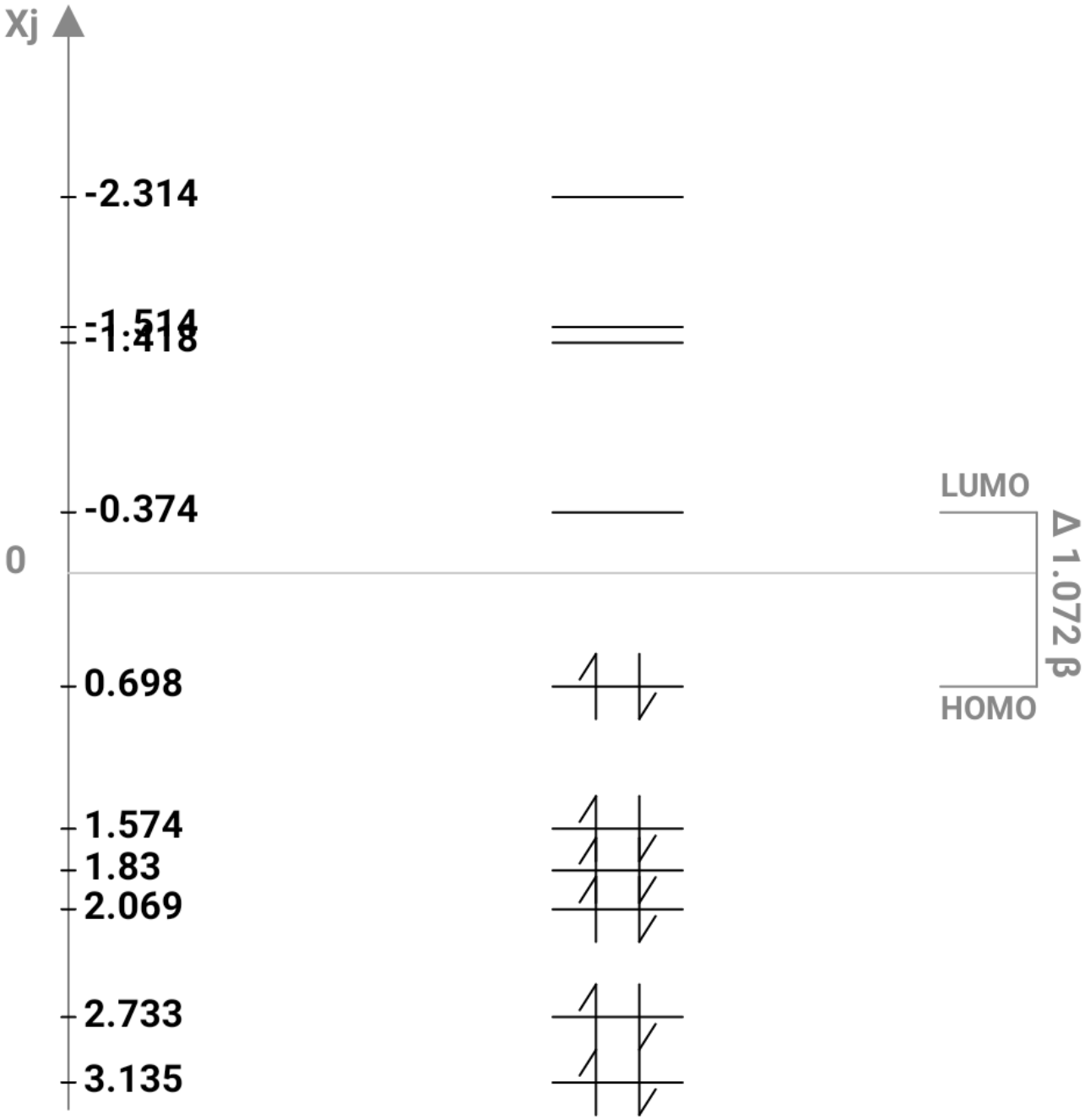
HMO-Energies

x1 = 3.135; x2 = 2.733; x3 = 2.069; x4 = 1.83; x5 = 1.574; x6 = 0.698; x7 = -0.374; x8 = -1.418; x9 = -1.514; x10 = -2.314;


3
1
O
2
6
4
O
5
O
OH

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 10α + 24.078β -

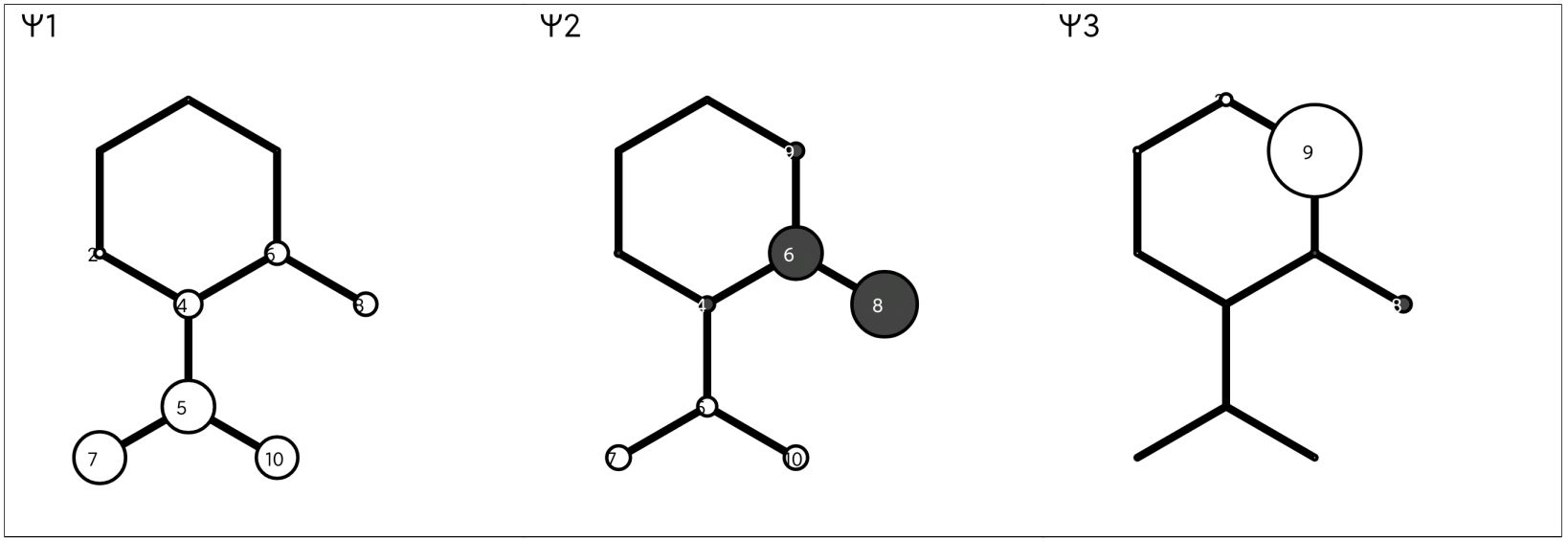
this corresponds to one πelectron: 2.007β

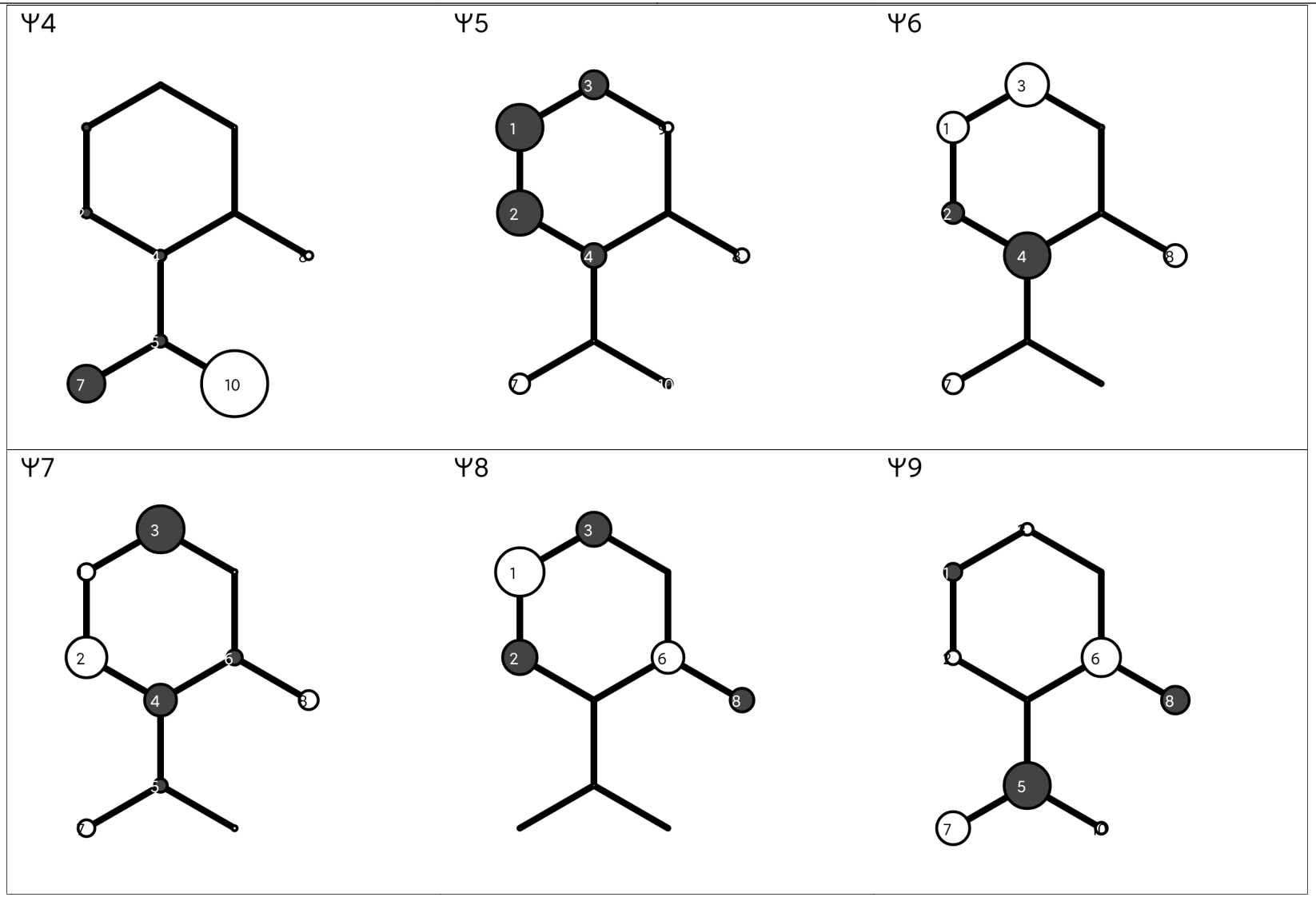
2. Hueckel-coefficient

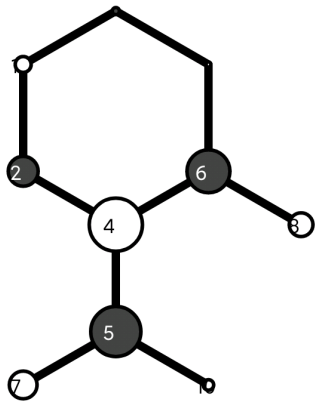
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10
	x1= 3.135	x2= 2.733	x3= 2.069	x4= 1.83	x5= 1.574	x6= 0.698	x7= -0.374	x8= -1.418	x9= -1.514	x10= -2.314
1	0.037	-0.034	0.07	-0.1	-0.584	0.388	0.21	0.611	-0.219	0.161
2	0.103	-0.069	0.022	-0.13	-0.563	-0.268	0.515	-0.435	0.182	-0.301
3	0.015	-0.024	0.123	-0.053	-0.356	0.538	-0.593	-0.431	0.149	-0.071
4	0.285	-0.154	-0.025	-0.138	-0.303	-0.575	-0.403	0.006	-0.058	0.536
5	0.552	0.201	0.002	-0.157	0.051	-0.064	-0.17	0.024	-0.582	-0.506
6	0.239	-0.554	-0.075	0.035	0.035	-0.07	-0.193	0.402	0.486	-0.433
7	0.545	0.249	0.004	-0.467	0.249	0.254	0.212	-0.018	0.417	0.28
8	0.235	-0.688	-0.164	0.103	0.174	0.279	0.24	-0.299	-0.348	0.239
9	0.045	-0.163	0.973	0.015	0.125	-0.065	0.061	0.002	-0.034	0.022
10	0.437	0.246	0.024	0.835	-0.107	0.044	0.065	-0.006	0.149	0.106

2.2. Molecule orbital presentation:




Ψ4
Ψ5
Ψ6
Ψ7
Ψ8
Ψ9

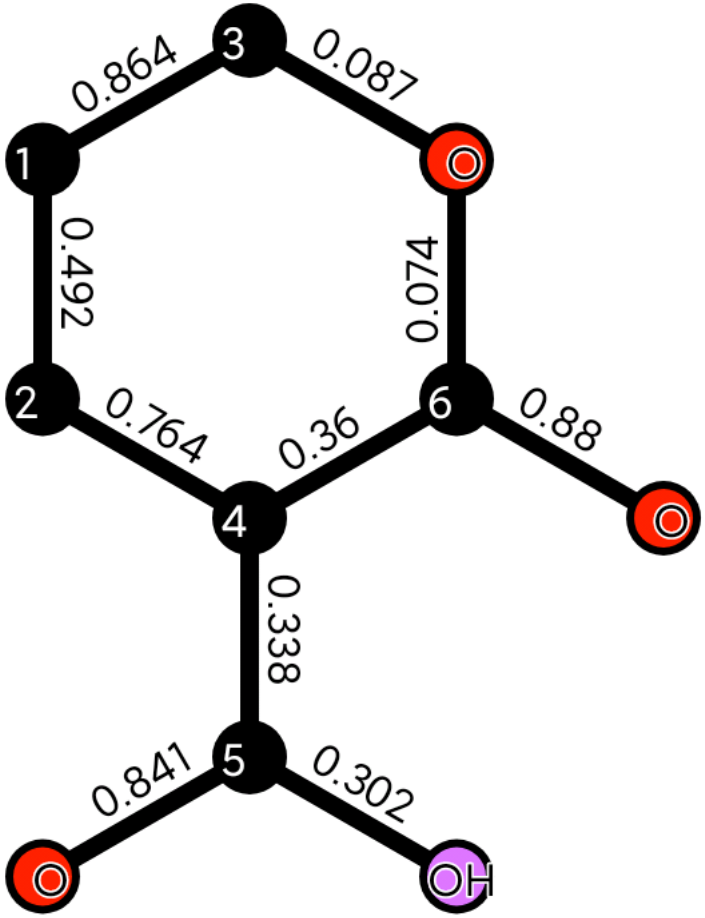
Ψ10 		

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	1.018									
2	0.492	0.844								
3	0.864	0.138	0.87							
4	-0.036	0.764	-0.379	1.094						
5	-0.049	0.104	-0.081	0.338	0.752					
6	-0.058	0.11	-0.089	0.36	0.042	0.753				
7	0.025	-0.217	0.152	-0.081	0.841	-0.067	1.406			
8	0.034	-0.236	0.165	-0.1	-0.067	0.88	0.044	1.349		
9	-0.05	-0.036	0.087	0.022	0.004	0.074	-0.01	-0.063	1.989	
10	0.012	-0.063	0.042	-0.044	0.302	-0.023	-0.211	0.018	-0.002	1.925

3.2. Presentation of bond order:

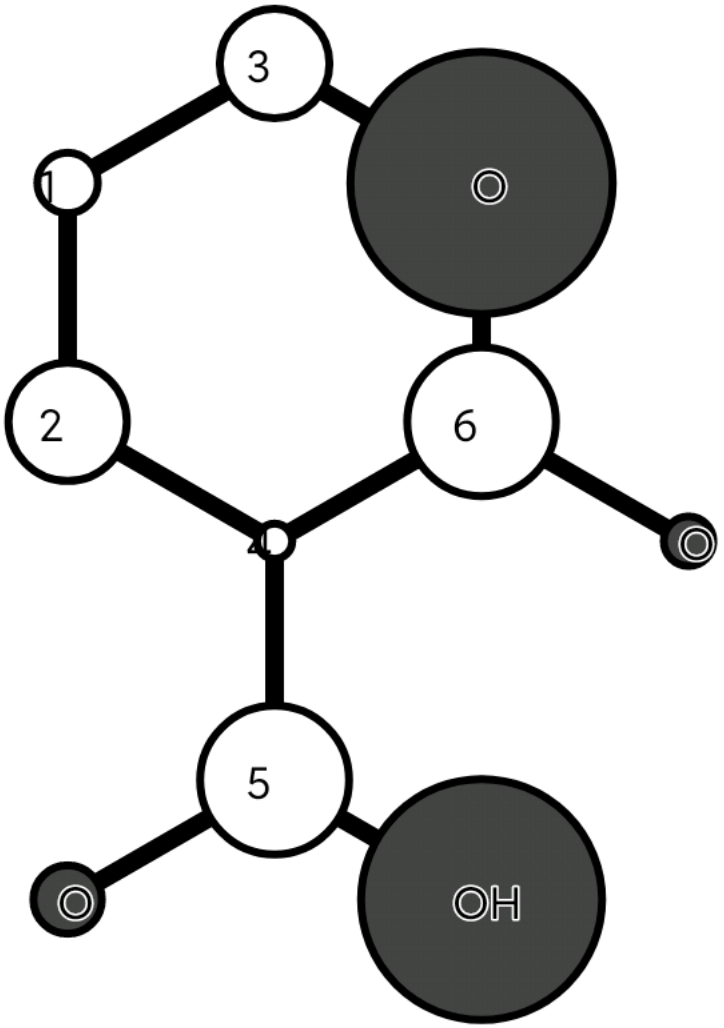

0.864
3
0.087
1
0.492
0.074
2
0.764
0.36
6
0.88
4
0.338
0.841
5
0.302

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.182									
2		0.356								
3			0.33							
4				0.106						
5					0.448					
6						0.447				
7							-0.206			
8								-0.149		
9									-0.789	
10										-0.725

4.2. Presentation of molecule:

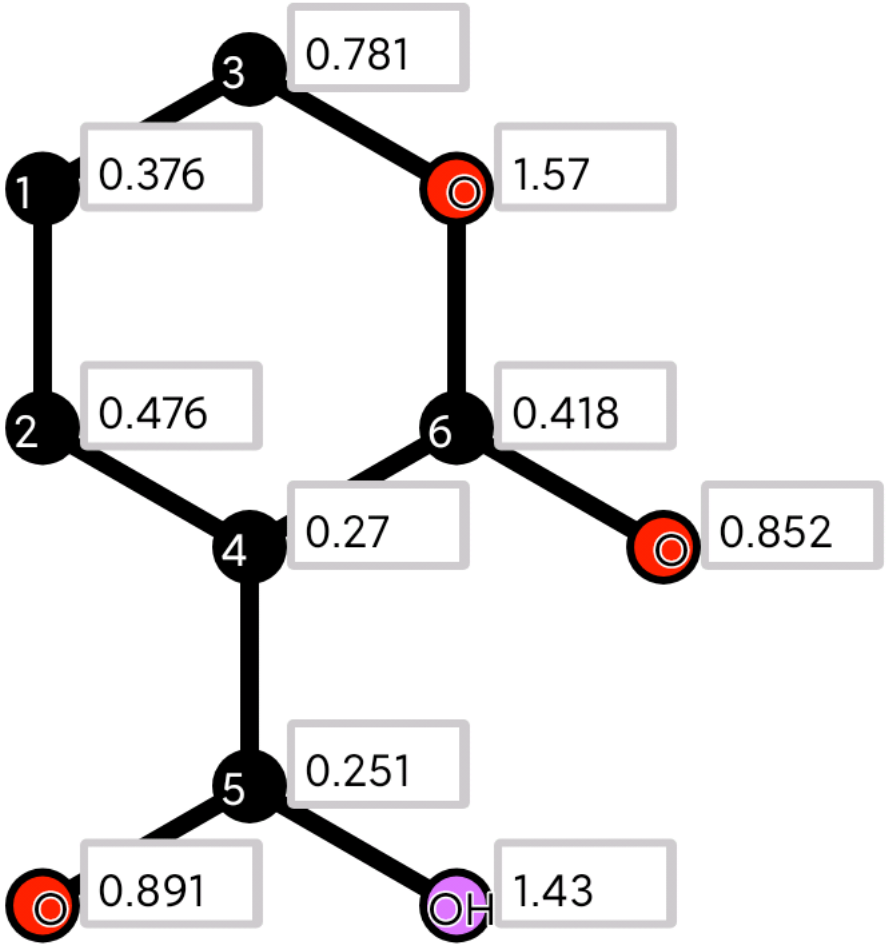

3
O
1
2
6
4
O
5
O
OH

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10
0.376	0.476	0.781	0.27	0.251	0.418	0.891	0.852	1.57	1.43

5.2. Presentation of molecule:

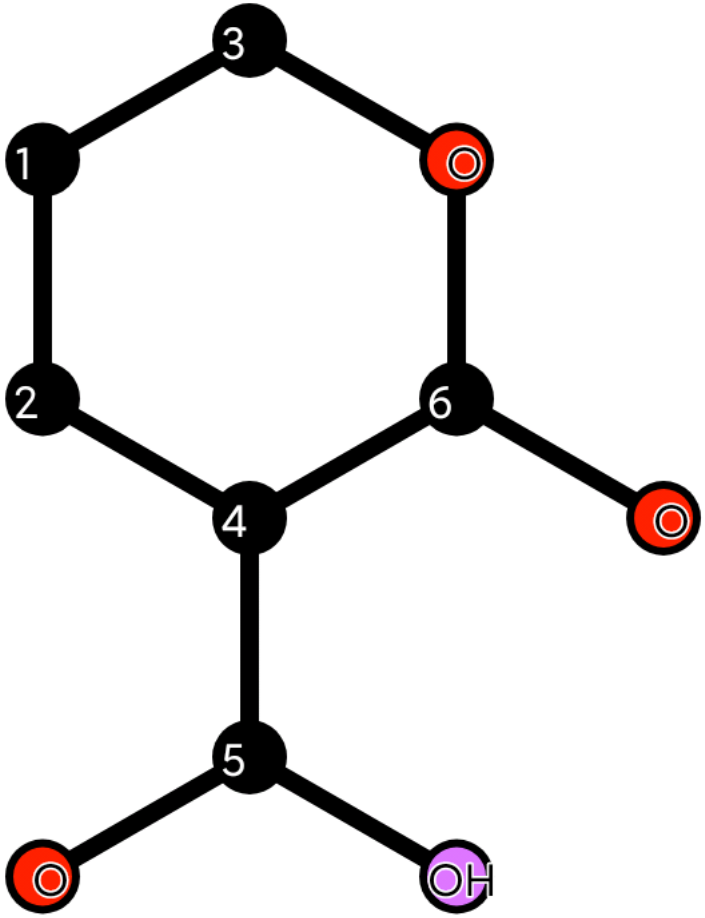

3
0.781
1
0.376
1.57
2
0.476
6
0.418
4
0.27
0.852
5
0.251
0.891
OH
1.43

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.391									
2	-0.057	0.429								
3	-0.363	0.035	0.639							
4	0.026	-0.284	-0.203	0.44						
5	0.0	-0.007	-0.01	-0.014	0.202					
6	-0.001	-0.009	-0.012	-0.017	0.0	0.218				
7	0.003	-0.047	-0.038	0.024	-0.156	-0.002	0.236			
8	0.004	-0.056	-0.046	0.027	-0.002	-0.176	0.003	0.249		
9	-0.002	-0.001	0.001	-0.001	0.0	-0.001	0.0	-0.003	0.008	
10	0.0	-0.003	-0.003	0.002	-0.013	0.0	-0.023	0.0	0.0	0.04

6.2. Presentation of molecule:

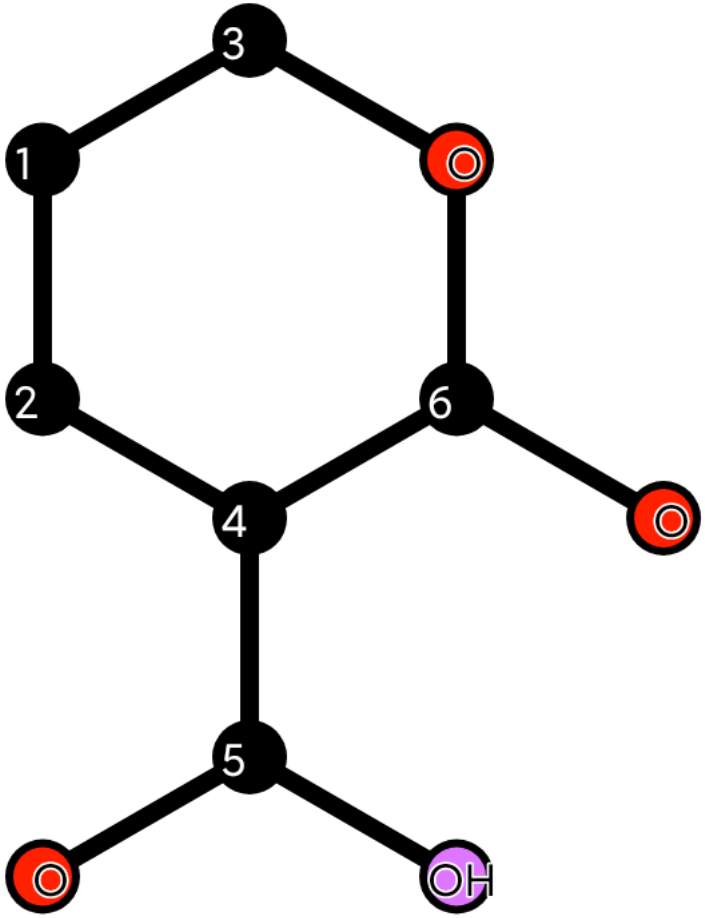

3
1
2
6
4
5

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1 2	0.006	0.033	-0.104	0.033	0.005	0.007	0.008	0.012	-0.002	0.001
1 3	-0.017	-0.026	0.092	-0.026	-0.004	-0.005	-0.006	-0.009	0.002	-0.001
2 4	0.001	0.075	0.078	-0.077	-0.014	-0.016	-0.02	-0.026	0.001	-0.002
3 9	0.029	0.0	-0.03	0.017	0.001	0.003	0.003	0.011	-0.034	0.0
4 5	0.004	-0.057	-0.048	0.027	0.035	-0.005	0.038	0.0	0.0	0.006
4 6	0.003	-0.062	-0.053	0.026	-0.005	0.04	0.001	0.051	-0.001	0.0
5 7	-0.001	0.023	0.02	-0.005	0.043	0.002	-0.102	0.0	0.0	0.02
5 10	0.0	0.005	0.005	0.0	0.001	0.0	0.065	0.0	0.0	-0.077
6 8	-0.001	0.027	0.025	-0.004	0.002	0.042	0.0	-0.093	0.002	0.0
6 9	-0.002	0.002	0.002	-0.002	0.0	0.001	0.0	0.022	-0.023	0.0

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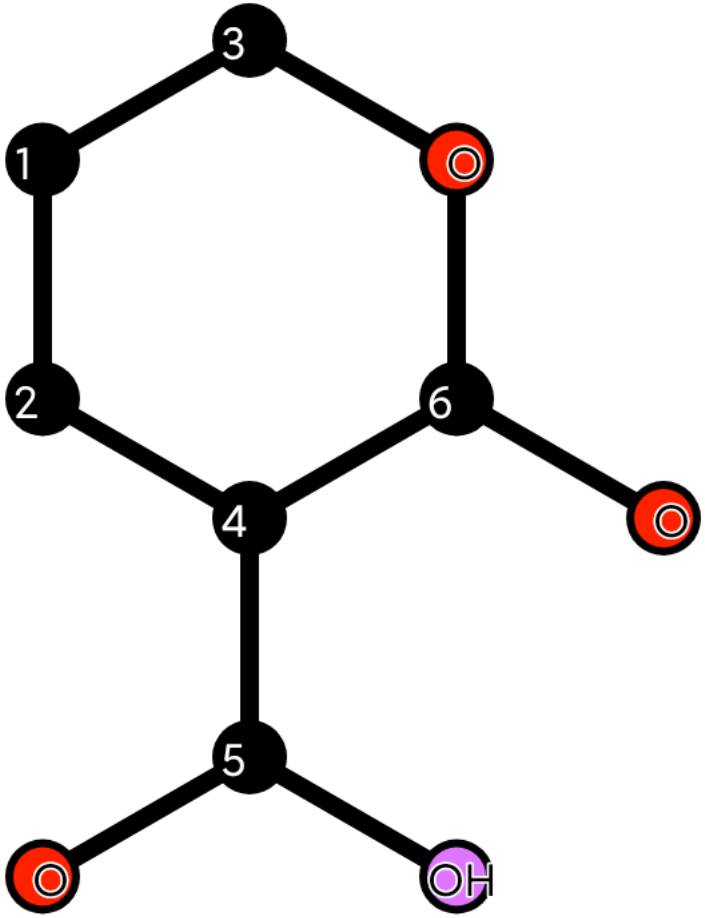
8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3	2 4	3 9	4 5	4 6	5 7	5 10	6 8	6 9
1 2	0.376									
1 3	-0.221	0.137								
2 4	-0.191	0.109	0.194							
3 9	0.033	-0.042	-0.021	0.412						
4 5	0.038	-0.026	-0.113	0.008	0.31					
4 6	0.044	-0.03	-0.125	0.018	-0.031	0.323				
5 7	-0.016	0.011	0.04	-0.003	-0.114	0.008	0.123			
5 10	-0.005	0.003	0.013	-0.001	-0.04	0.004	-0.091	0.311		
6 8	-0.021	0.015	0.051	-0.012	0.01	-0.136	-0.003	-0.001	0.105	
6 9	0.005	-0.003	0.001	0.048	-0.001	-0.002	0.001	0.0	-0.028	0.34

8.2. Presentation of molecule: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