Print calculated values

Report generated by:root, 18.02.2020 - 15:31:58

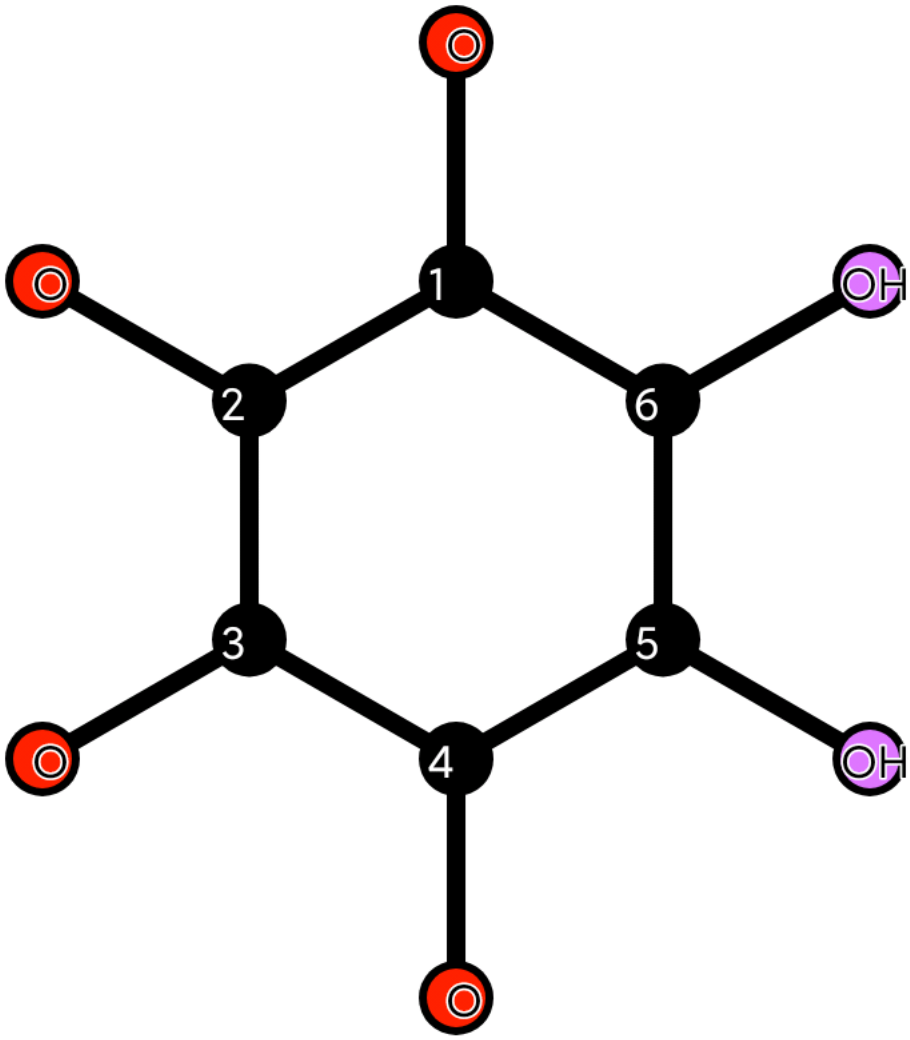
The following determinant is calculated:

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

It is about this molecule:

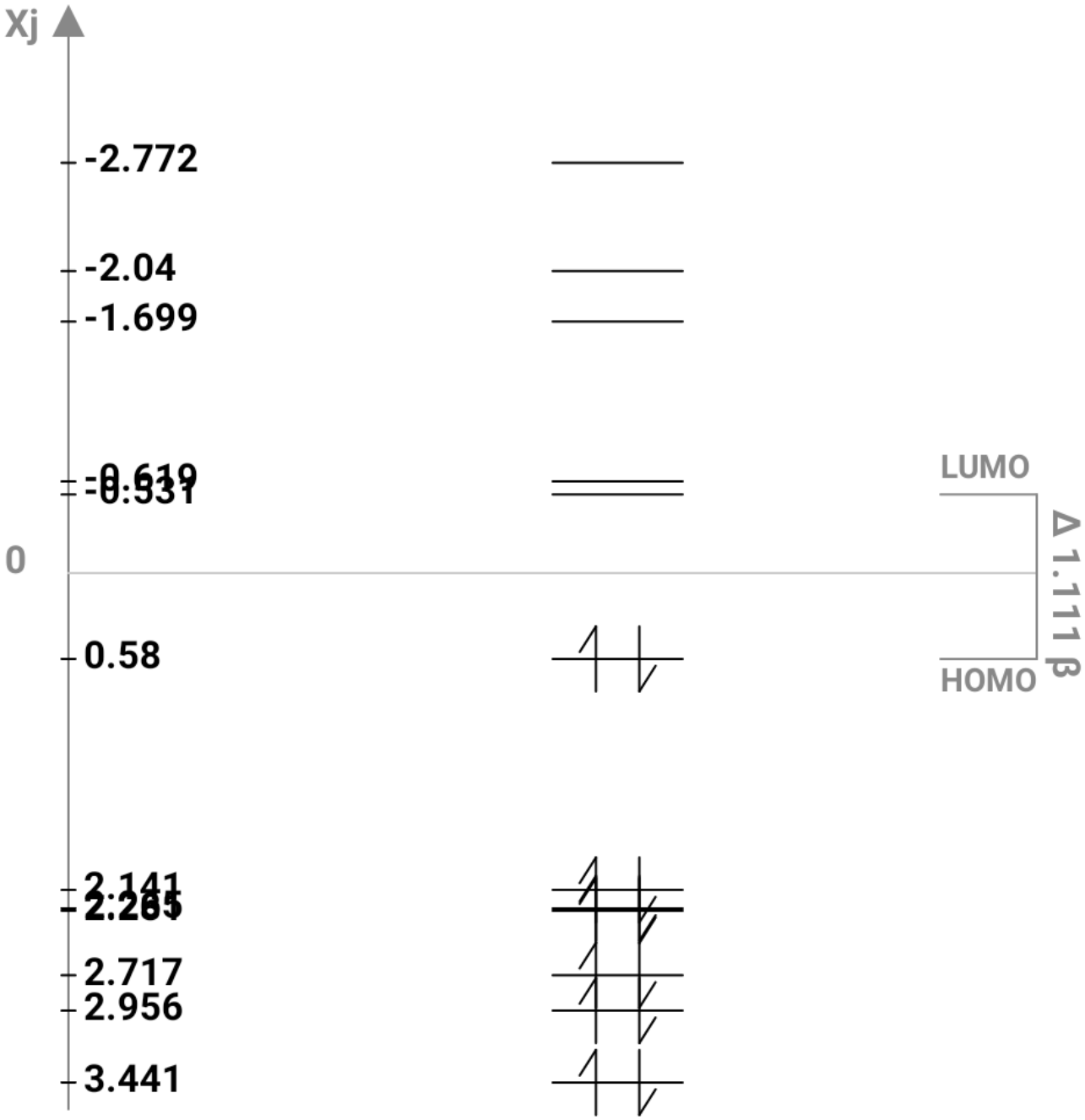
HMO-Energies

x1 = 3.441; x2 = 2.956; x3 = 2.717; x4 = 2.281; x5 = 2.265; x6 = 2.141; x7 = 0.58; x8 = -0.531;
x9 = -0.619; x10 = -1.699; x11 = -2.04; x12 = -2.772;


1
2
3
4
5
6
OH
OH

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 12α + 32.762β -

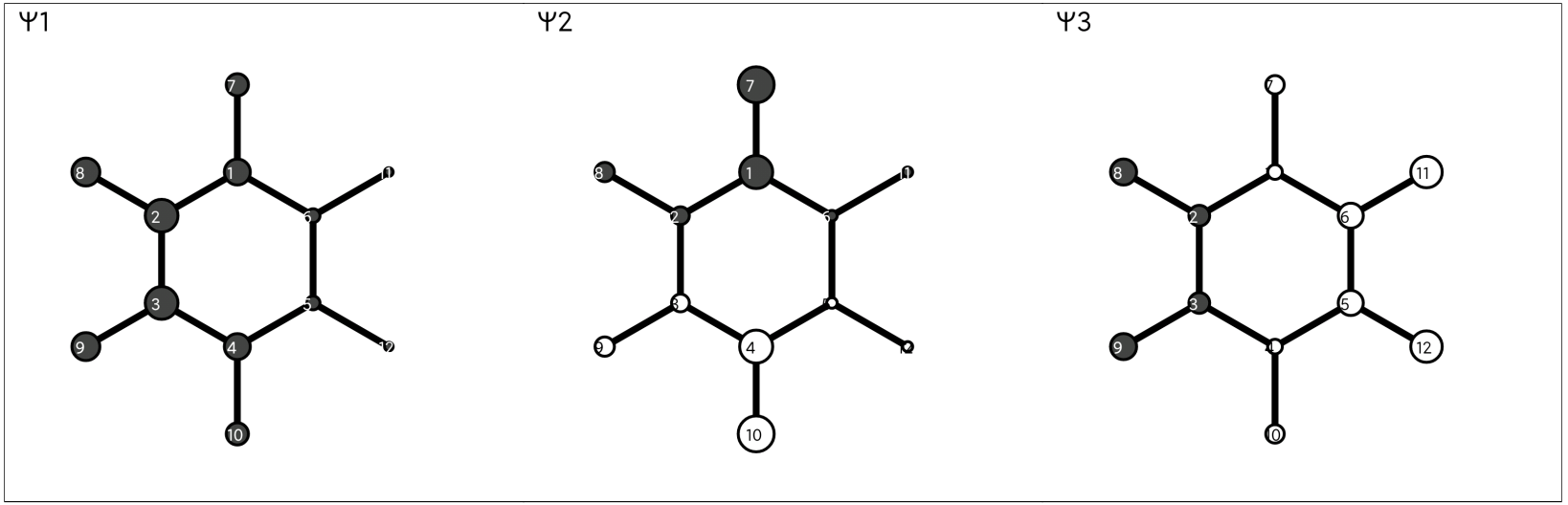
this corresponds to one πelectron: 2.34β

2. Hueckel-coefficient

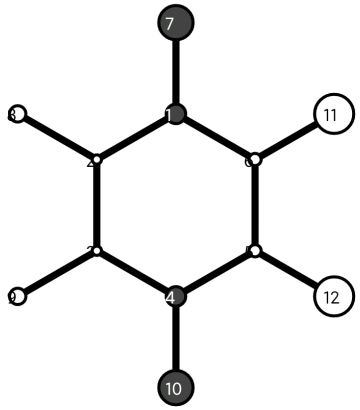
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11	Psi 12
	x1= 3.441	x2= 2.956	x3= 2.717	x4= 2.281	x5= 2.265	x6= 2.141	x7= 0.58	x8= -0.531	x9= -0.619	x10= -1.699	x11= -2.04	x12= -2.772
1	-0.32	-0.408	0.181	-0.231	-0.034	-0.157	-0.083	0.337	-0.193	0.222	0.517	-0.381
2	-0.404	-0.219	-0.256	0.11	0.201	0.212	-0.014	0.127	-0.429	0.373	-0.274	0.459
3	-0.404	0.219	-0.256	0.11	-0.201	-0.212	-0.014	-0.127	-0.429	-0.373	-0.274	-0.459
4	-0.32	0.408	0.181	-0.231	0.034	0.157	-0.083	-0.337	-0.193	-0.222	0.517	0.381
5	-0.171	0.131	0.309	0.144	0.162	-0.06	-0.547	-0.427	0.148	0.463	-0.182	-0.238
6	-0.171	-0.131	0.309	0.144	-0.162	0.06	-0.547	0.427	0.148	-0.463	-0.182	0.238
7	-0.274	-0.443	0.228	-0.404	-0.06	-0.315	0.266	-0.38	0.208	-0.149	-0.31	0.186
8	-0.345	-0.238	-0.322	0.192	0.357	0.427	0.046	-0.144	0.46	-0.25	0.164	-0.224
9	-0.345	0.238	-0.322	0.192	-0.357	-0.427	0.046	0.144	0.46	0.25	0.164	0.224
10	-0.274	0.443	0.228	-0.404	0.06	0.315	0.266	0.38	0.208	0.149	-0.31	-0.186
11	-0.107	-0.123	0.388	0.462	-0.549	0.382	0.347	-0.152	-0.051	0.113	0.041	-0.045
12	-0.107	0.123	0.388	0.462	0.549	-0.382	0.347	0.152	-0.051	-0.113	0.041	0.045

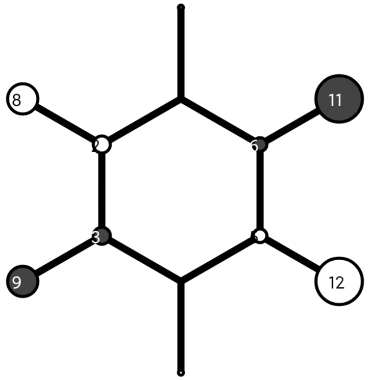
2.2. Molecule orbital presentation:



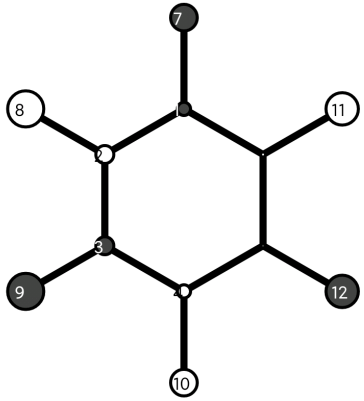
Ψ4



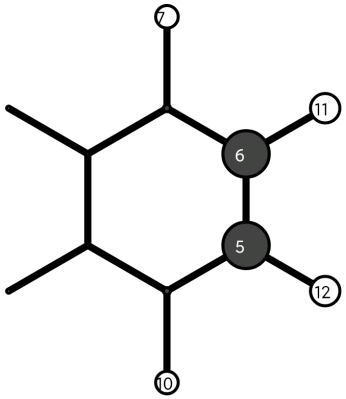
Ψ5



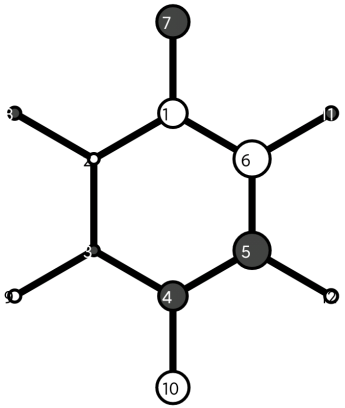
Ψ6



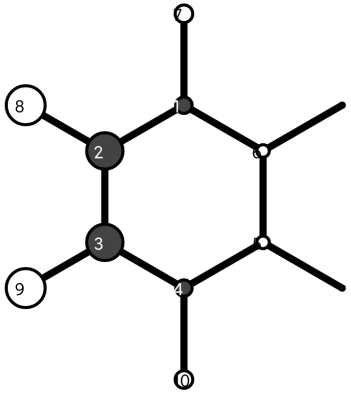
Ψ7

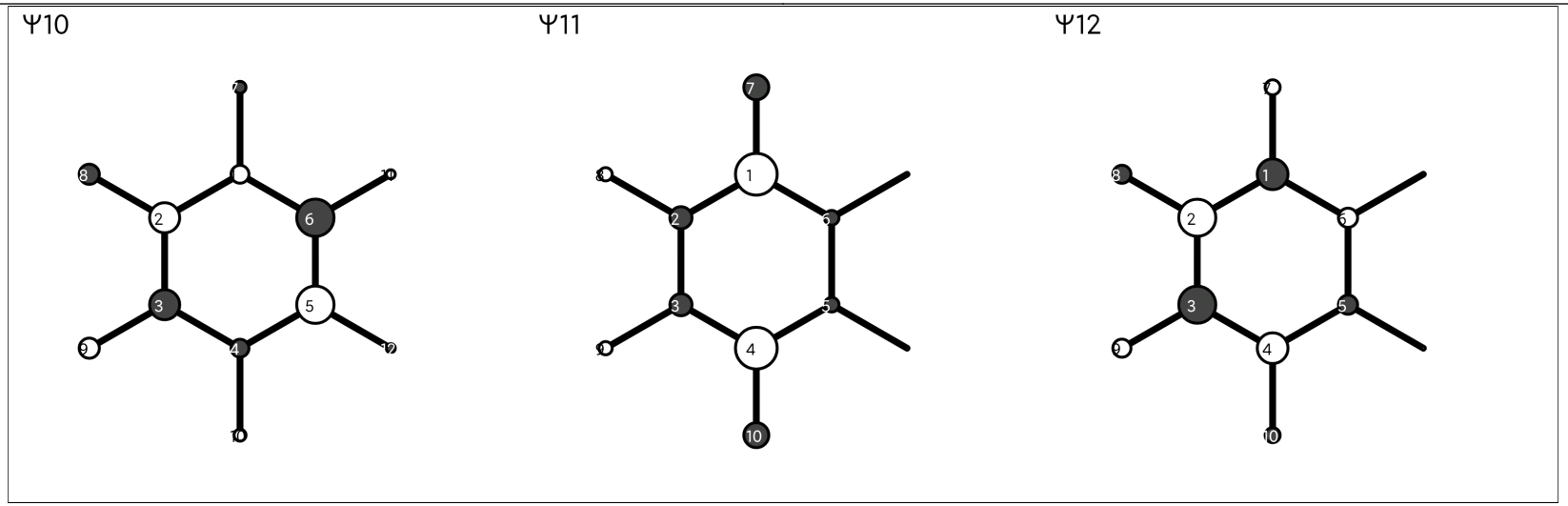


Ψ8



Ψ9



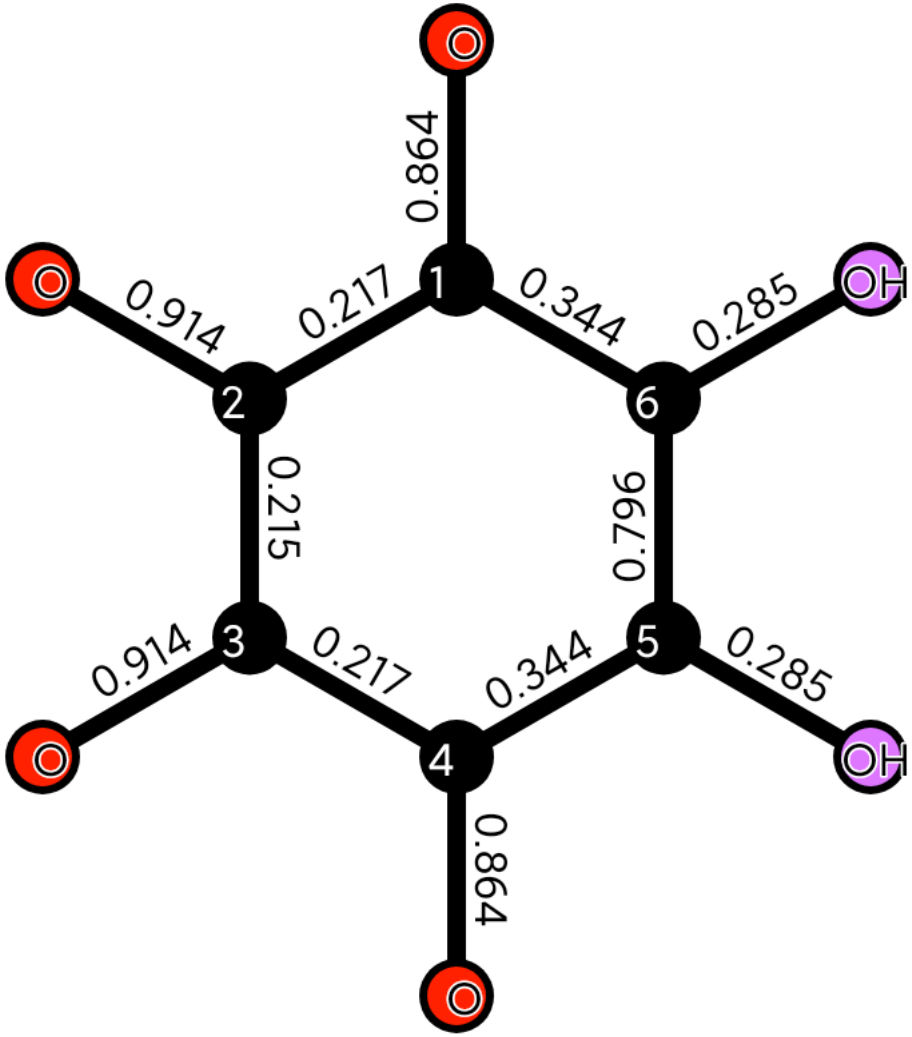

Ψ10
Ψ11
Ψ12

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12
1	0.775											
2	0.217	0.749										
3	0.019	0.215	0.749									
4	0.007	0.019	0.217	0.775								
5	0.146	0.009	0.045	0.344	0.984							
6	0.344	0.045	0.009	0.146	0.796	0.984						
7	0.864	0.045	-0.029	-0.064	-0.272	-0.076	1.32					
8	0.045	0.914	0.055	-0.029	-0.074	-0.078	-0.189	1.256				
9	-0.029	0.055	0.914	0.045	-0.078	-0.074	0.011	-0.21	1.256			
10	-0.064	-0.029	0.045	0.864	-0.076	-0.272	0.124	0.011	-0.189	1.32		
11	-0.043	-0.025	-0.017	-0.08	-0.226	0.285	-0.019	0.026	0.041	0.111	1.916	
12	-0.08	-0.017	-0.025	-0.043	0.285	-0.226	0.111	0.041	0.026	-0.019	0.067	1.916

3.2. Presentation of bond order:

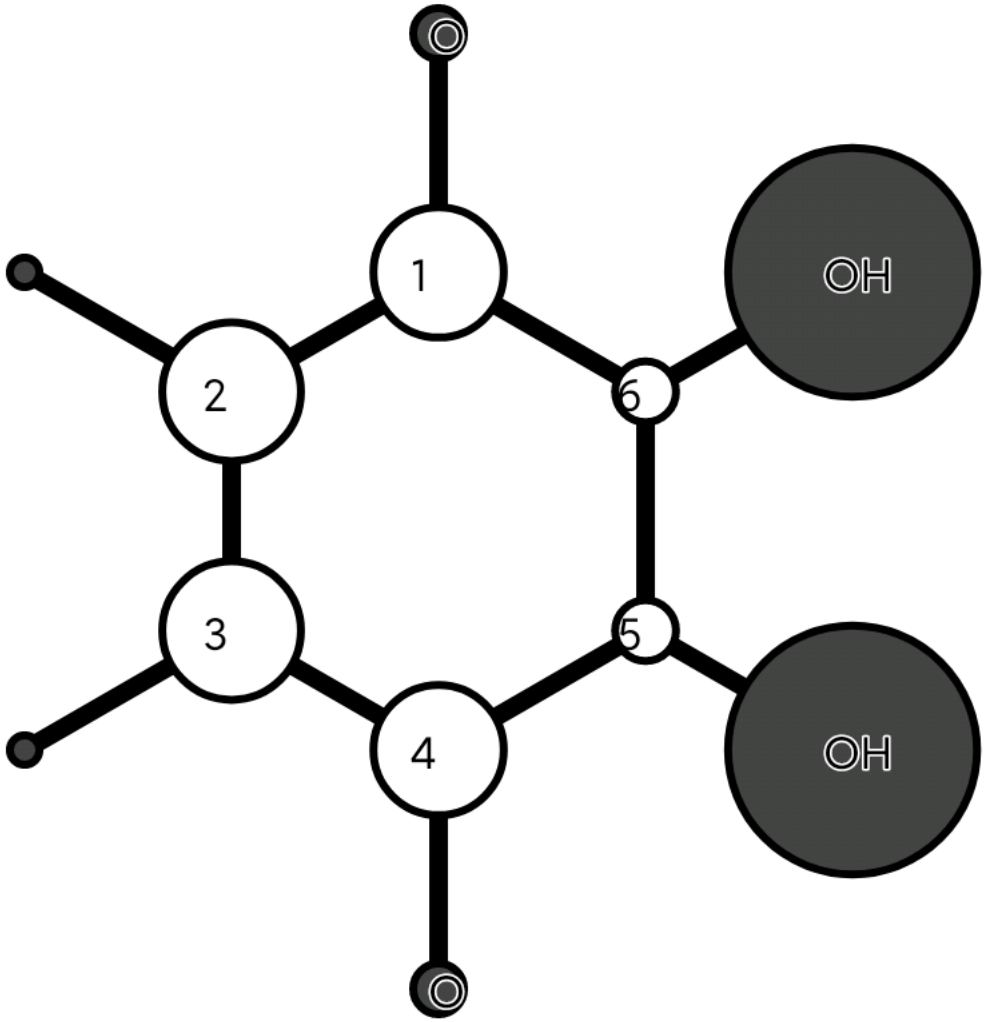

0.864
0.914
0.217
1
0.344
0.285
OH
2
6
0.215
0.796
0.914
3
0.217
0.344
5
0.285
OH
4
0.864

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12
1	0.392											
2		0.417										
3			0.417									
4				0.392								
5					0.183							
6						0.183						
7							-0.153					
8								-0.089				
9									-0.089			
10										-0.153		
11											-0.749	
12												-0.749

4.2. Presentation of molecule:

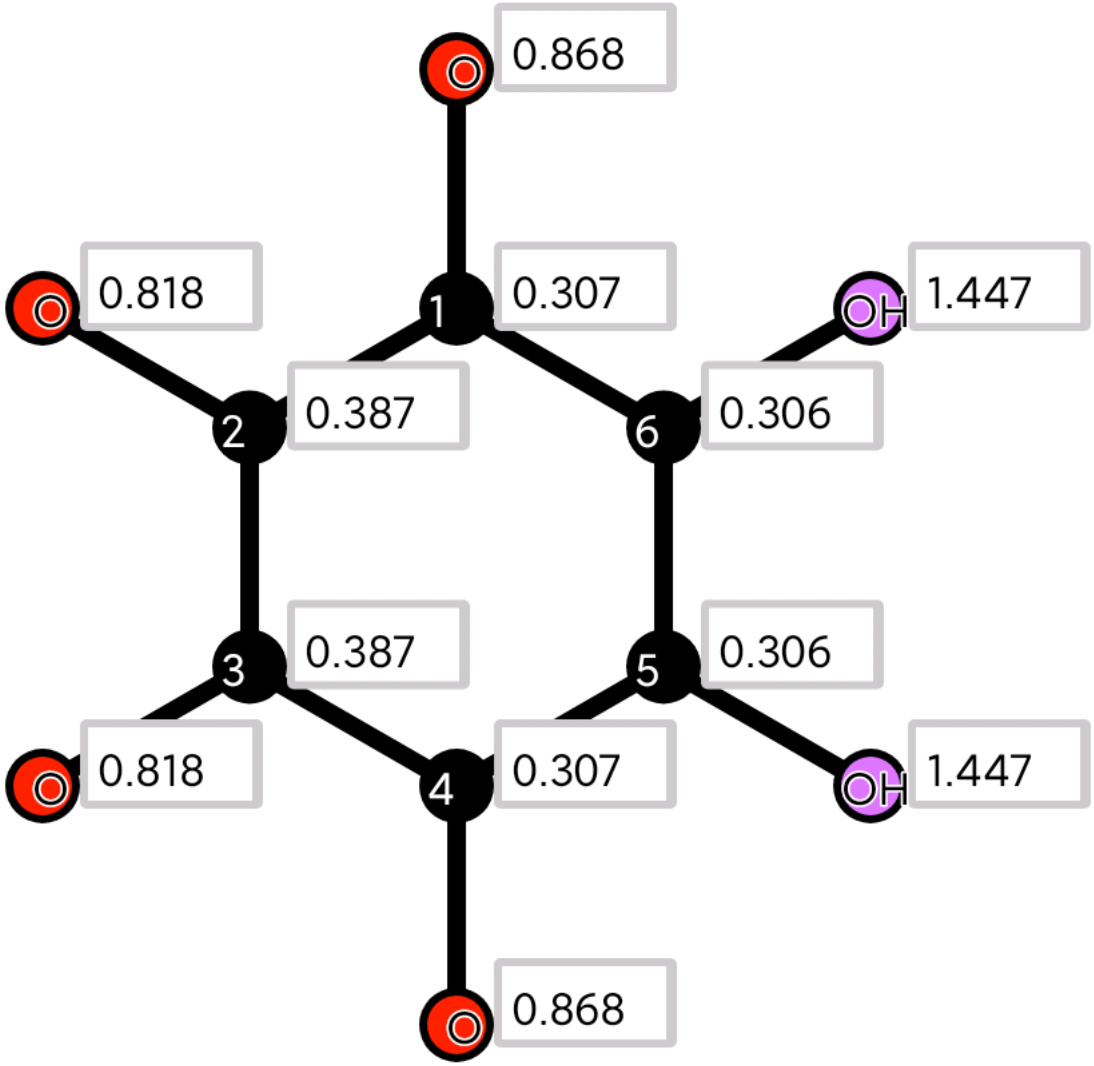

1
2
3
4
5
6
OH
OH

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11	12
0.307	0.387	0.387	0.307	0.306	0.306	0.868	0.818	0.818	0.868	1.447	1.447

5.2. Presentation of molecule:

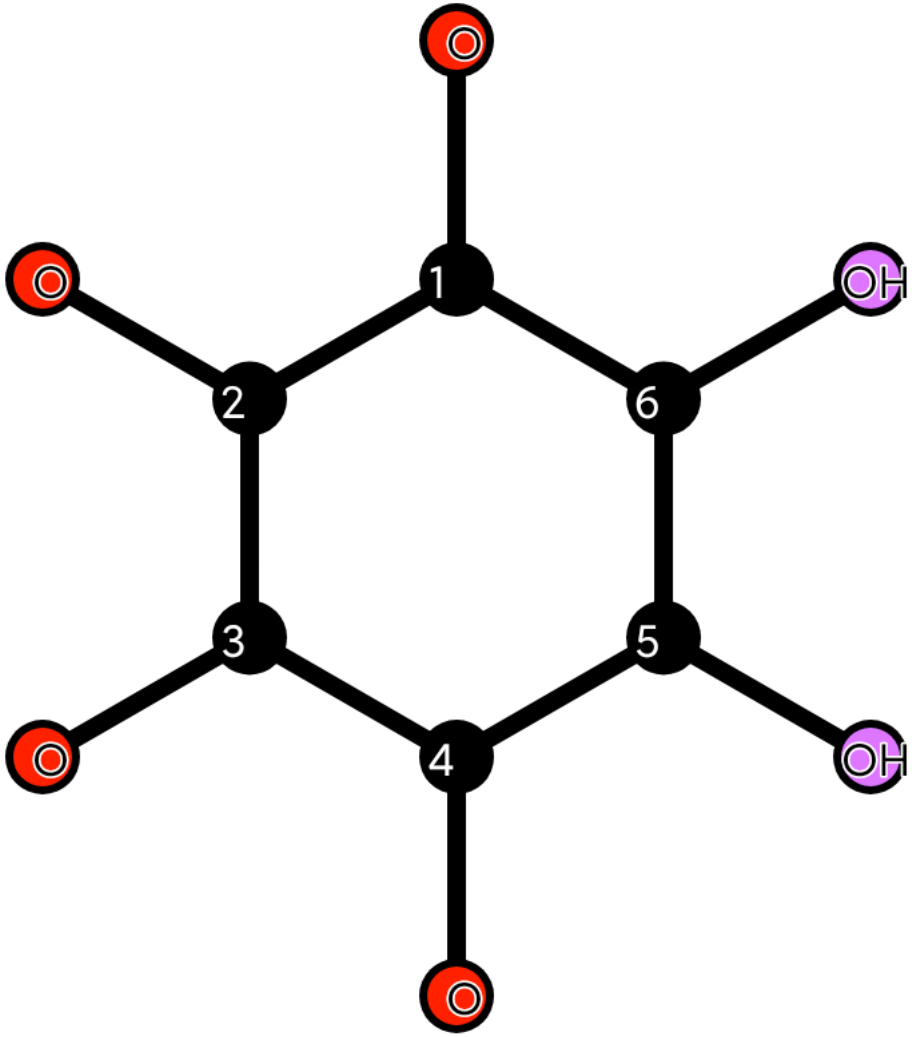

0.868
0.818
0.307
1.447
OH
1
2
0.387
6
0.306
3
0.387
5
0.306
0.818
4
0.307
OH
1.447
0.868

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12
1	0.214											
2	-0.004	0.211										
3	0.0	-0.004	0.211									
4	-0.001	0.0	-0.004	0.214								
5	-0.023	-0.001	-0.001	-0.012	0.466							
6	-0.012	-0.001	-0.001	-0.023	-0.331	0.466						
7	-0.169	0.005	0.0	-0.005	-0.088	0.032	0.278					
8	0.005	-0.21	0.004	0.0	-0.007	-0.004	-0.02	0.263				
9	0.0	0.004	-0.21	0.005	-0.004	-0.007	0.0	-0.028	0.263			
10	-0.005	0.0	0.005	-0.169	0.032	-0.088	-0.021	0.0	-0.02	0.278		
11	0.002	0.0	0.0	-0.007	-0.049	0.018	0.006	0.0	-0.002	-0.017	0.057	
12	-0.007	0.0	0.0	0.002	0.018	-0.049	-0.017	-0.002	0.0	0.006	-0.007	0.057

6.2. Presentation of molecule:

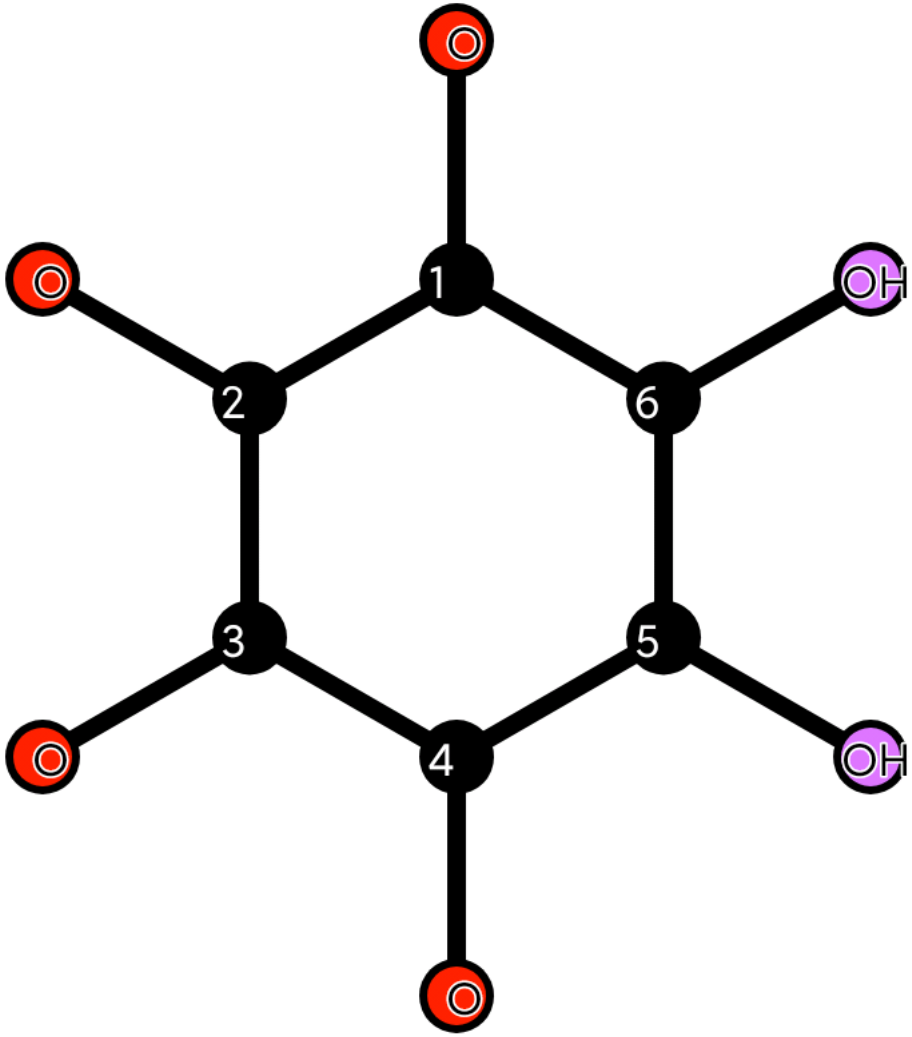

O
O
1
OH
2
6
3
5
O
4
OH
O

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12
1 2	0.018	0.018	-0.001	0.0	-0.005	-0.005	-0.01	-0.014	0.001	-0.001	-0.001	-0.002
1 6	0.04	-0.001	0.0	-0.004	-0.102	0.045	0.051	0.005	-0.001	-0.024	0.012	-0.021
1 7	0.032	-0.004	0.0	0.002	0.049	-0.01	-0.092	0.003	0.0	0.012	-0.004	0.011
2 3	-0.001	0.019	0.019	-0.001	-0.001	-0.001	0.001	-0.018	-0.018	0.001	0.0	0.0
2 8	-0.004	0.051	-0.004	0.0	0.003	0.002	0.003	-0.06	0.007	0.0	0.0	0.001
3 4	0.0	-0.001	0.018	0.018	-0.005	-0.005	-0.001	0.001	-0.014	-0.01	-0.002	-0.001
3 9	0.0	-0.004	0.051	-0.004	0.002	0.003	0.0	0.007	-0.06	0.003	0.001	0.0
4 5	-0.004	0.0	-0.001	0.04	0.045	-0.102	-0.024	-0.001	0.005	0.051	-0.021	0.012
4 10	0.002	0.0	-0.004	0.032	-0.01	0.049	0.012	0.0	0.003	-0.092	0.011	-0.004
5 6	-0.019	-0.001	-0.001	-0.019	0.022	0.022	-0.019	-0.006	-0.006	-0.019	0.023	0.023
5 12	0.013	0.001	0.001	-0.001	-0.096	0.13	0.039	0.004	0.001	-0.014	0.018	-0.096
6 11	-0.001	0.001	0.001	0.013	0.13	-0.096	-0.014	0.001	0.004	0.039	-0.096	0.018

7.2. Presentation of molecule:

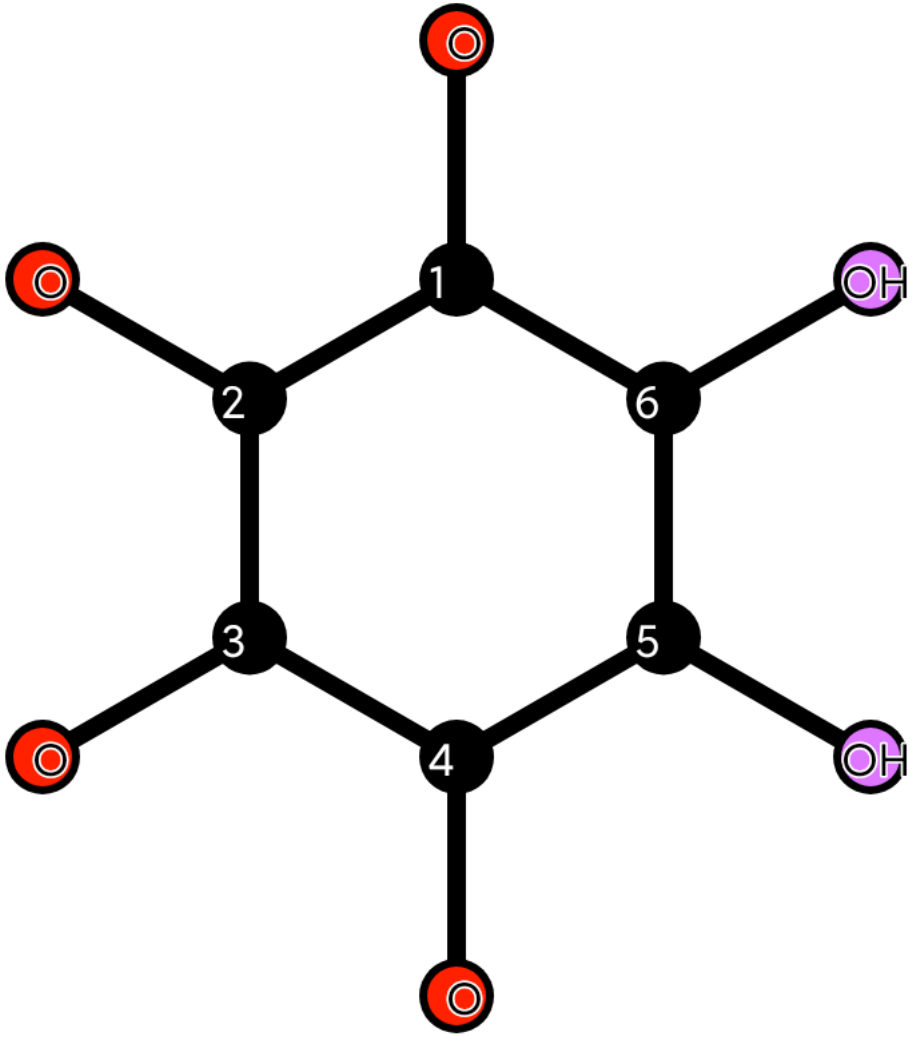

O
O
1
OH
2
6
3
5
O
4
OH
O

8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	1 7	2 3	2 8	3 4	3 9	4 5	4 10	5 6	5 12	6 11
1 2	0.209											
1 6	-0.006	0.32										
1 7	-0.044	-0.134	0.111									
2 3	-0.007	0.0	0.001	0.207								
2 8	-0.042	-0.001	0.01	-0.04	0.054							
3 4	0.0	-0.002	0.001	-0.007	0.001	0.209						
3 9	0.001	0.001	0.0	-0.04	0.008	-0.042	0.054					
4 5	-0.002	-0.046	0.023	0.0	0.001	-0.006	-0.001	0.32				
4 10	0.001	0.023	-0.011	0.001	0.0	-0.044	0.01	-0.134	0.111			
5 6	-0.009	-0.101	0.048	-0.002	0.005	-0.009	0.005	-0.101	0.048	0.135		
5 12	0.006	0.096	-0.048	0.001	-0.003	0.004	-0.002	-0.063	0.017	-0.084	0.352	
6 11	0.004	-0.063	0.017	0.001	-0.002	0.006	-0.003	0.096	-0.048	-0.084	-0.098	0.352

8.2. Presentation of molecule:


O
O
1
OH
2
6
3
5
O
4
OH
O