Print calculated values

Report generated by:root, 18.02.2020 - 15:30:10

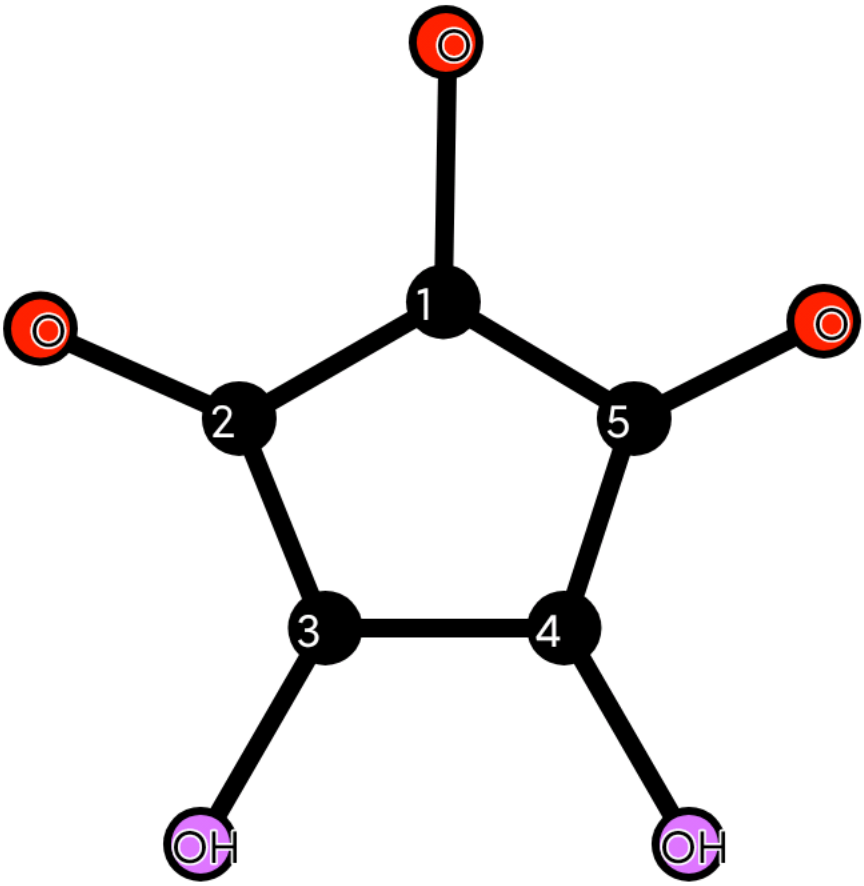
The following determinant is calculated:

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

It is about this molecule:

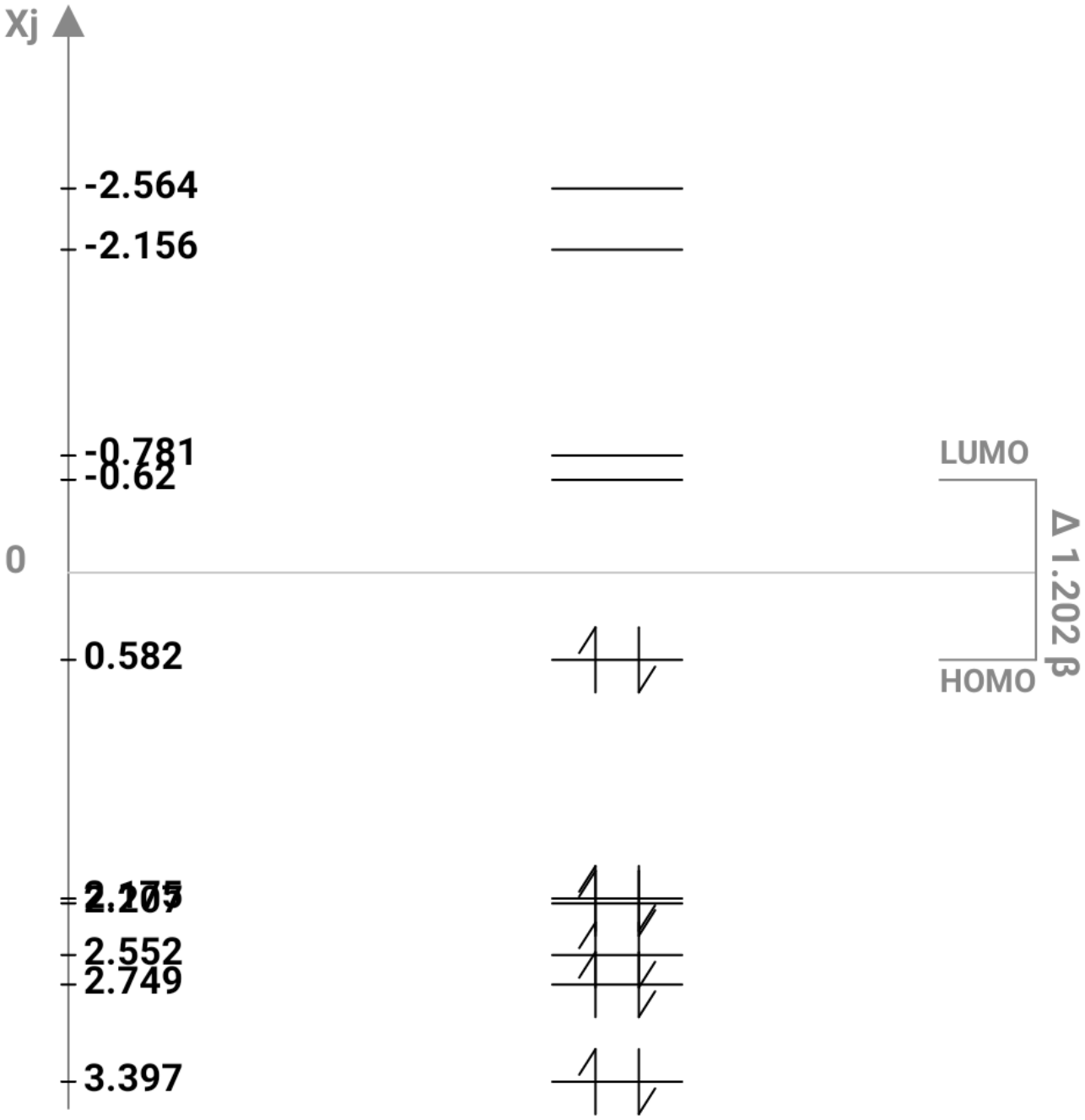
HMO-Energies

x1 = 3.397; x2 = 2.749; x3 = 2.552; x4 = 2.207; x5 = 2.175; x6 = 0.582; x7 = -0.62; x8 = -0.781; x9 = -2.156; x10 = -2.564;


O
1
O
2
5
O
3
4
OH
OH

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 10α + 27.324β -

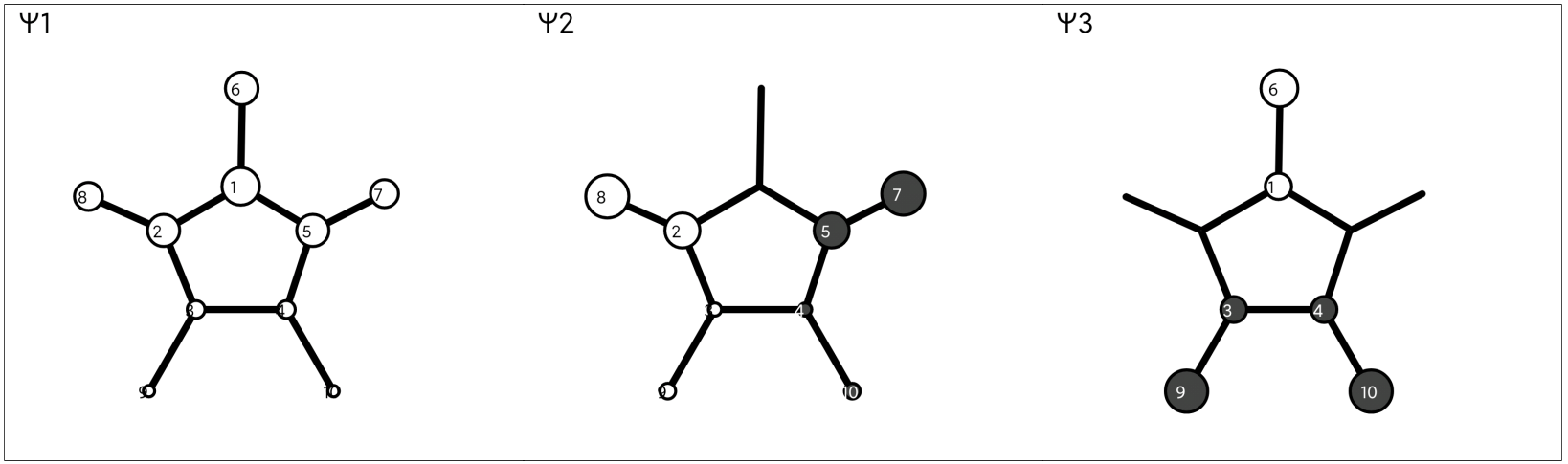
this corresponds to one πelectron: 2.277β

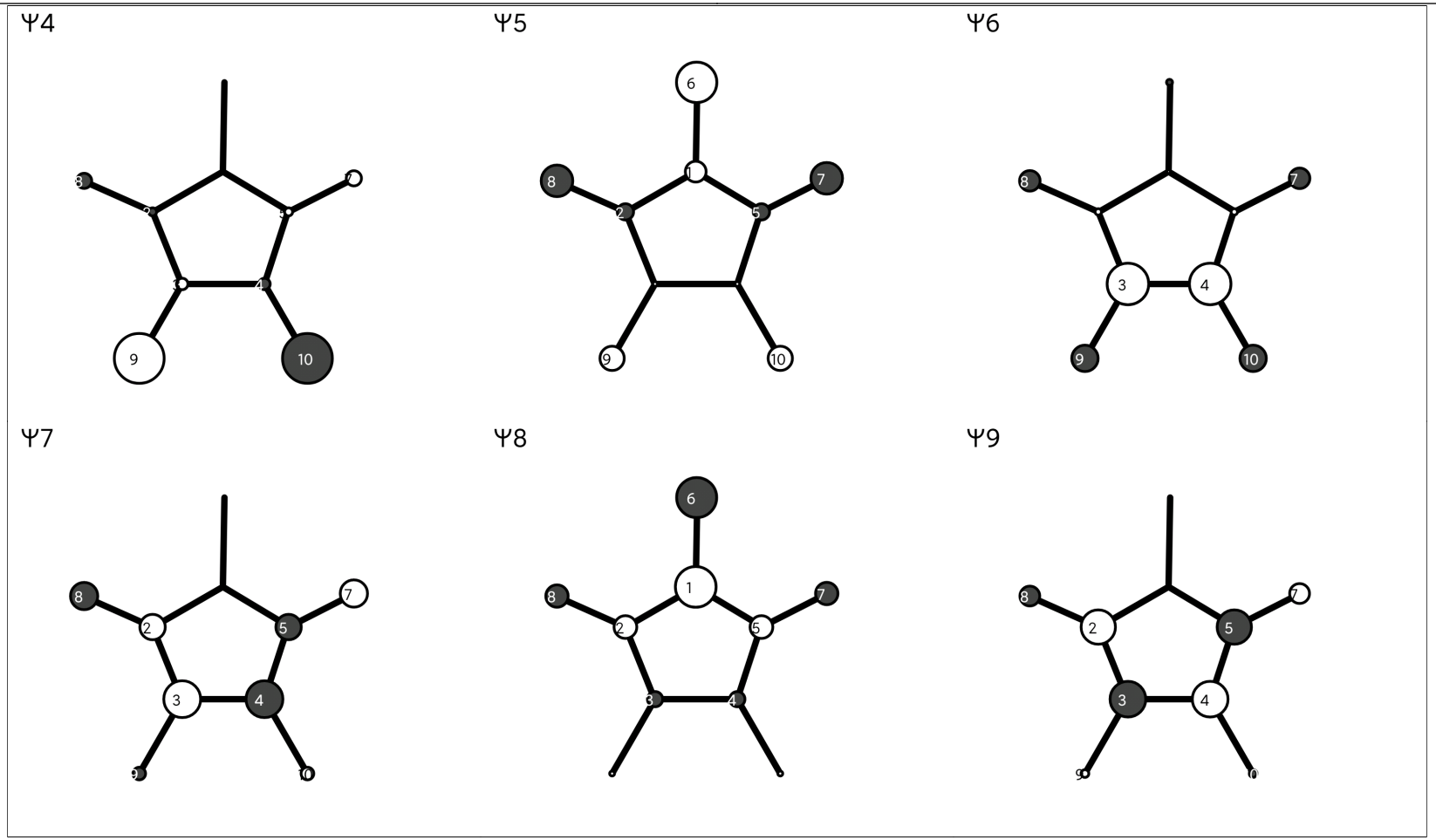
2. Hueckel-coefficient

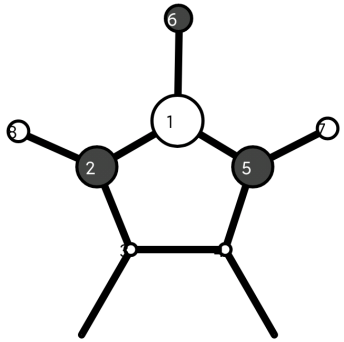
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10
	x1= 3.397	x2= 2.749	x3= 2.552	x4= 2.207	x5= 2.175	x6= 0.582	x7= -0.62	x8= -0.781	x9= -2.156	x10= -2.564
1	0.448	0.0	0.314	0.0	0.273	0.025	0.0	0.534	0.0	0.584
2	0.385	0.418	-0.026	-0.106	-0.214	0.084	0.333	0.298	0.45	-0.458
3	0.212	0.157	-0.31	0.15	0.062	0.545	0.483	-0.2	-0.468	0.135
4	0.212	-0.157	-0.31	-0.15	0.062	0.545	-0.483	-0.2	0.468	0.135
5	0.385	-0.418	-0.026	0.106	-0.214	0.084	-0.333	0.298	-0.45	-0.458
6	0.39	0.0	0.442	0.0	0.529	-0.079	0.0	-0.525	0.0	-0.301
7	0.335	-0.515	-0.036	0.199	-0.414	-0.27	0.357	-0.294	0.26	0.236
8	0.335	0.515	-0.036	-0.199	-0.414	-0.27	-0.357	-0.294	-0.26	0.236
9	0.136	0.188	-0.505	0.653	0.319	-0.346	-0.166	0.065	0.101	-0.027
10	0.136	-0.188	-0.505	-0.653	0.319	-0.346	0.166	0.065	-0.101	-0.027

2.2. Molecule orbital presentation:




Ψ4
Ψ5
Ψ6
Ψ7
Ψ8
Ψ9

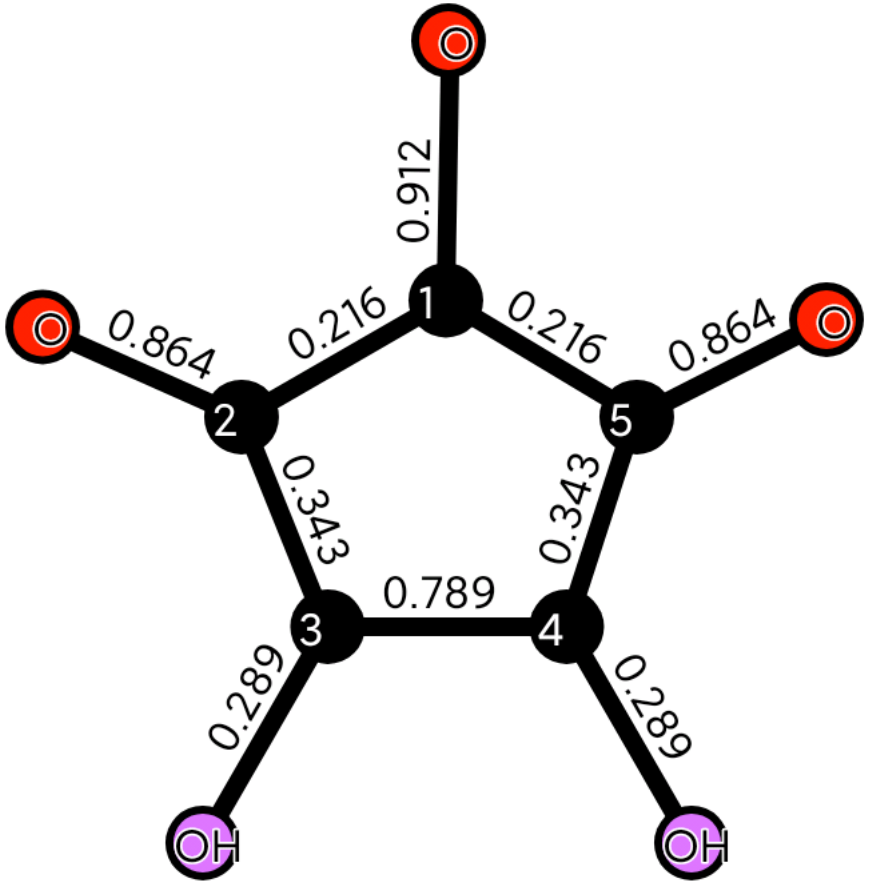
Ψ10 		

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.749									
2	0.216	0.775								
3	0.056	0.343	0.978							
4	0.056	0.144	0.789	0.978						
5	0.216	0.03	0.144	0.343	0.775					
6	0.912	0.038	-0.129	-0.129	0.038	1.267				
7	0.038	-0.081	-0.283	-0.08	0.864	-0.166	1.325			
8	0.038	0.864	-0.08	-0.283	-0.081	-0.166	0.107	1.325		
9	-0.038	-0.044	0.289	-0.222	-0.082	0.052	0.117	-0.015	1.914	
10	-0.038	-0.082	-0.222	0.289	-0.044	0.052	-0.015	0.117	0.066	1.914

3.2. Presentation of bond order:

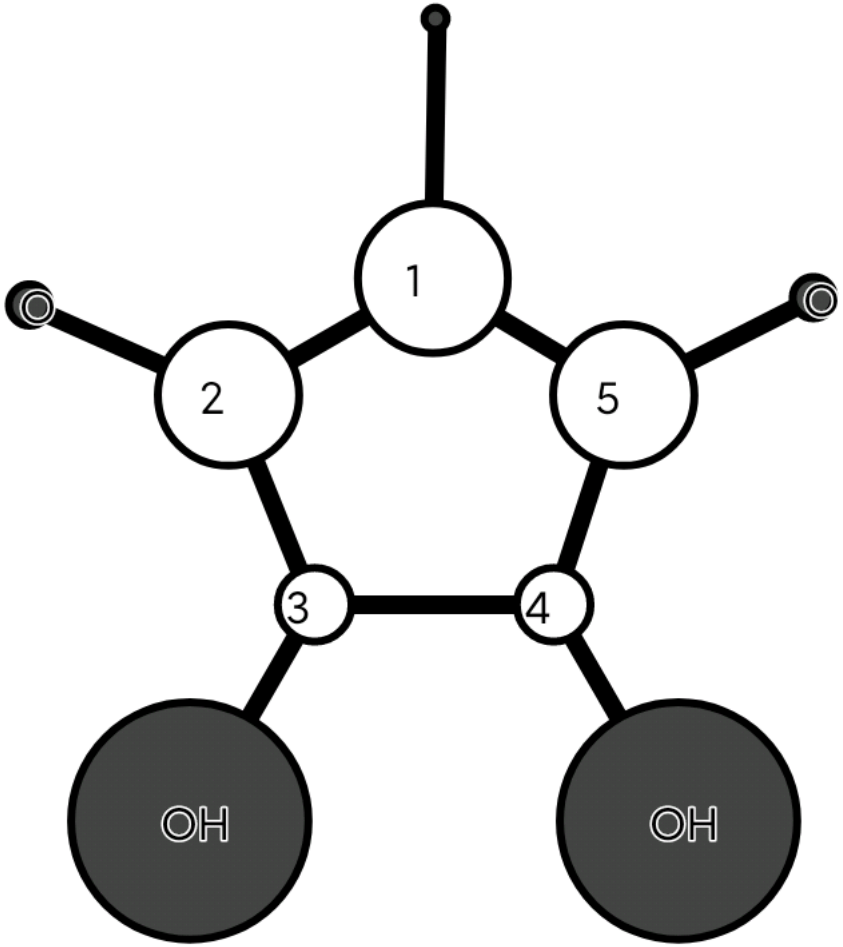

O
0.912
O
0.864
0.216
1
0.216
0.864
O
2
5
0.343
0.343
0.789
3
4
0.289
0.289
OH
OH

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.451									
2		0.425								
3			0.222							
4				0.222						
5					0.425					
6						-0.067				
7							-0.125			
8								-0.125		
9									-0.714	
10										-0.714

4.2. Presentation of molecule:

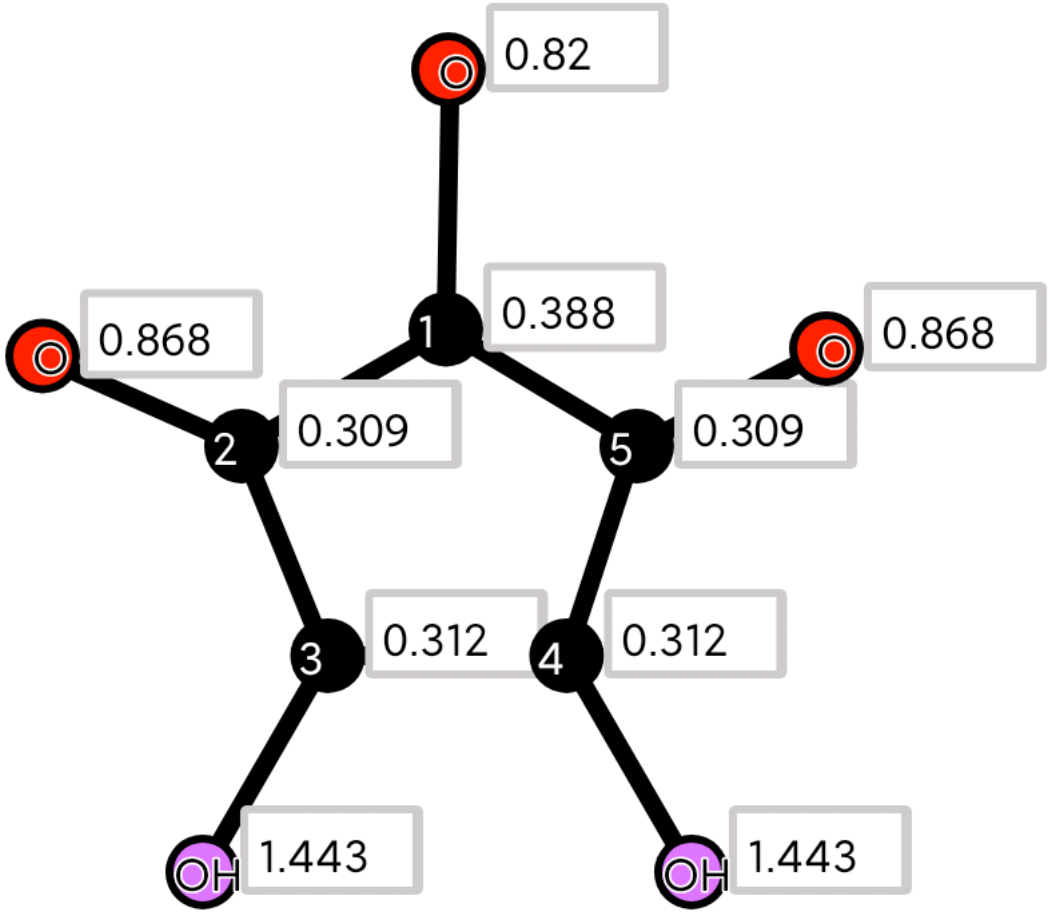

1
2
5
3
4
OH
OH

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10
0.388	0.309	0.312	0.312	0.309	0.82	0.868	0.868	1.443	1.443

5.2. Presentation of molecule:

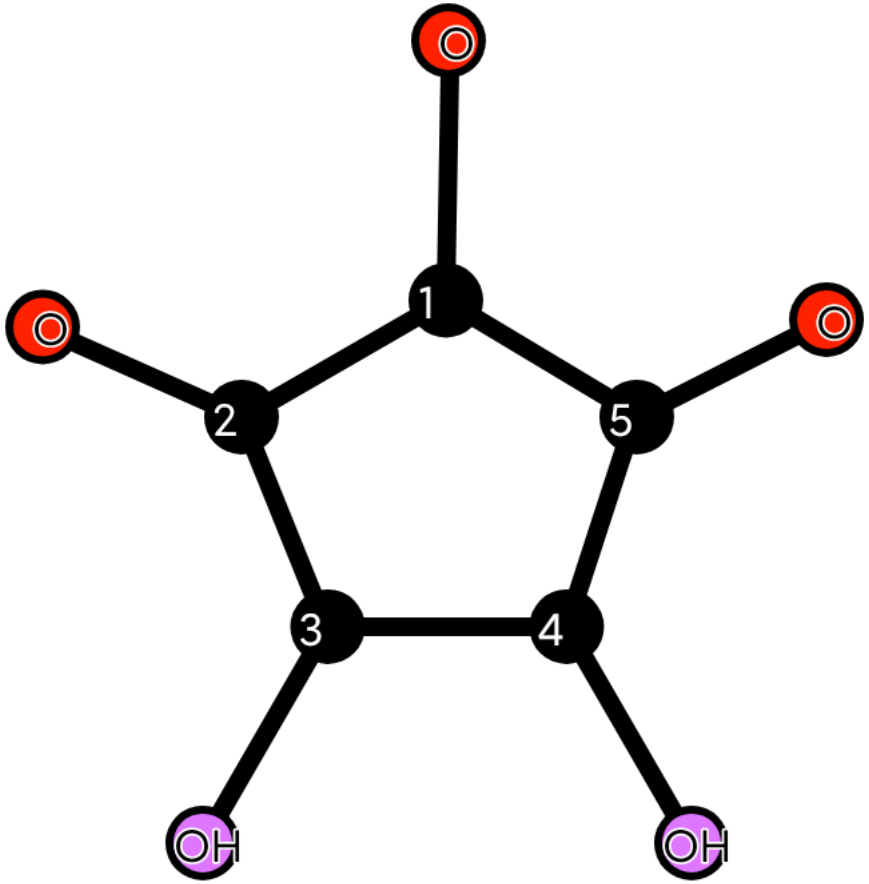

0.82
0.868
1
0.388
0.868
2
0.309
5
0.309
3
0.312
4
0.312
OH
1.443
OH
1.443

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.212									
2	-0.004	0.214								
3	-0.002	-0.013	0.468							
4	-0.002	-0.023	-0.321	0.468						
5	-0.004	0.0	-0.023	-0.013	0.214					
6	-0.207	0.005	-0.014	-0.014	0.005	0.26				
7	0.005	-0.005	-0.091	0.027	-0.168	-0.014	0.274			
8	0.005	-0.168	0.027	-0.091	-0.005	-0.014	-0.014	0.274		
9	-0.001	0.002	0.017	-0.047	-0.007	-0.003	-0.017	0.005	0.058	
10	-0.001	-0.007	-0.047	0.017	0.002	-0.003	0.005	-0.017	-0.006	0.058

6.2. Presentation of molecule:

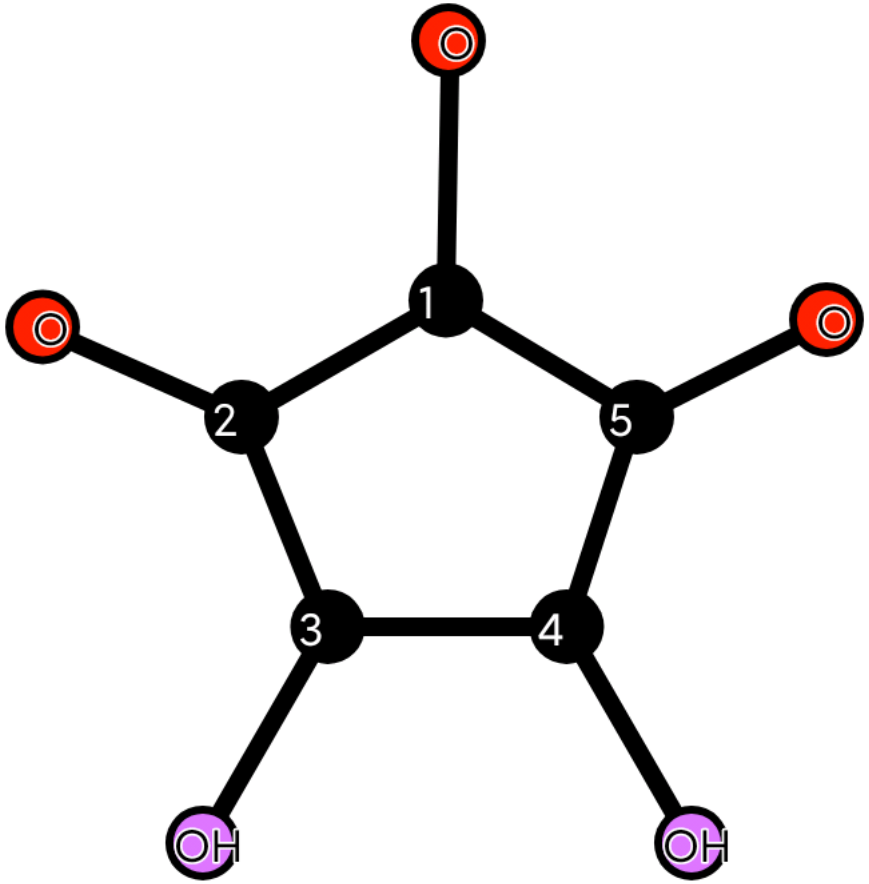

O
O
1
O
2
5
3
4
OH
OH

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1 2	0.019	0.018	-0.009	-0.008	-0.001	-0.01	0.003	-0.007	-0.001	-0.003
1 5	0.019	-0.001	-0.008	-0.009	0.018	-0.01	-0.007	0.003	-0.003	-0.001
1 6	0.051	-0.004	0.007	0.007	-0.004	-0.065	0.001	0.001	0.002	0.002
2 3	-0.002	0.04	0.044	-0.103	-0.004	0.006	-0.022	0.051	0.012	-0.021
2 8	-0.004	0.032	-0.008	0.051	0.002	0.001	0.009	-0.093	-0.004	0.012
3 4	-0.002	-0.02	0.027	0.027	-0.02	-0.014	-0.023	-0.023	0.024	0.024
3 9	0.002	0.0	-0.096	0.126	0.013	0.007	0.041	-0.012	-0.097	0.018
4 5	-0.002	-0.004	-0.103	0.044	0.04	0.006	0.051	-0.022	-0.021	0.012
4 10	0.002	0.013	0.126	-0.096	0.0	0.007	-0.012	0.041	0.018	-0.097
5 7	-0.004	0.002	0.051	-0.008	0.032	0.001	-0.093	0.009	0.012	-0.004

7.2. Presentation of molecule:

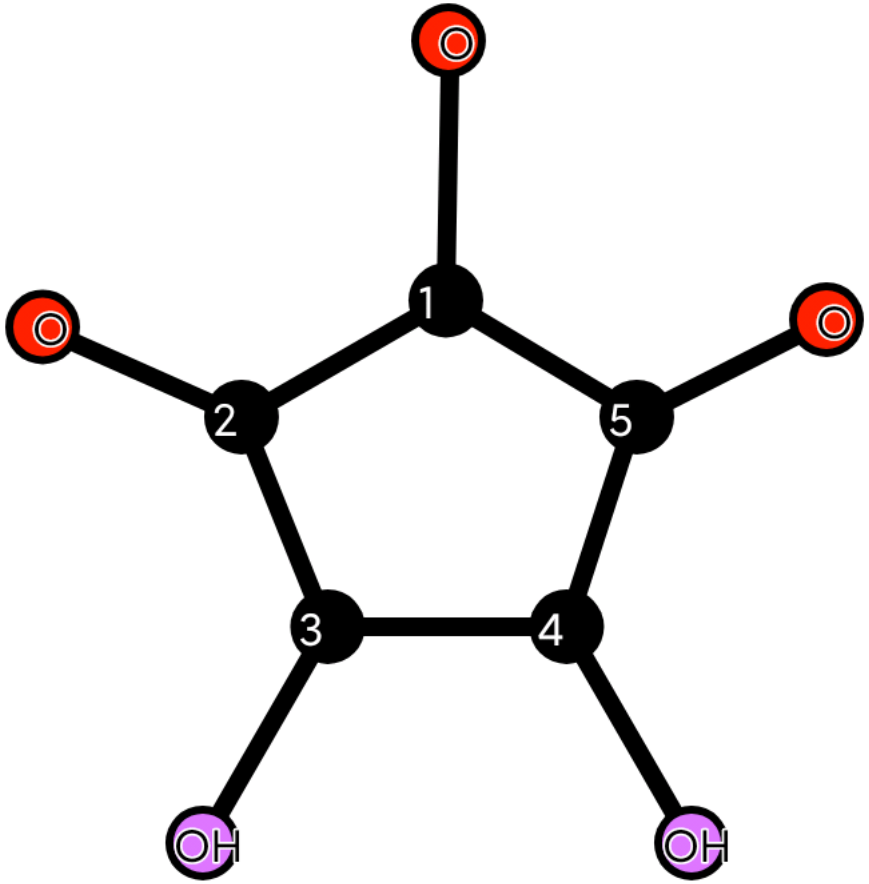

O
O
O
1
2
5
3
4
OH
OH

8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 5	1 6	2 3	2 8	3 4	3 9	4 5	4 10	5 7
1 2	0.209									
1 5	-0.008	0.209								
1 6	-0.043	-0.043	0.058							
2 3	-0.007	-0.003	0.0	0.318						
2 8	-0.044	0.001	0.01	-0.132	0.111					
3 4	-0.017	-0.017	0.015	-0.105	0.052	0.147				
3 9	0.008	0.01	-0.008	-0.061	0.015	-0.088	0.355			
4 5	-0.003	-0.007	0.0	-0.048	0.023	-0.105	0.097	0.318		
4 10	0.01	0.008	-0.008	0.097	-0.05	-0.088	-0.095	-0.061	0.355	
5 7	0.001	-0.044	0.01	0.023	-0.011	0.052	-0.05	-0.132	0.015	0.111

8.2. Presentation of molecule:


O
1
O
O
2
5
3
4
OH
OH