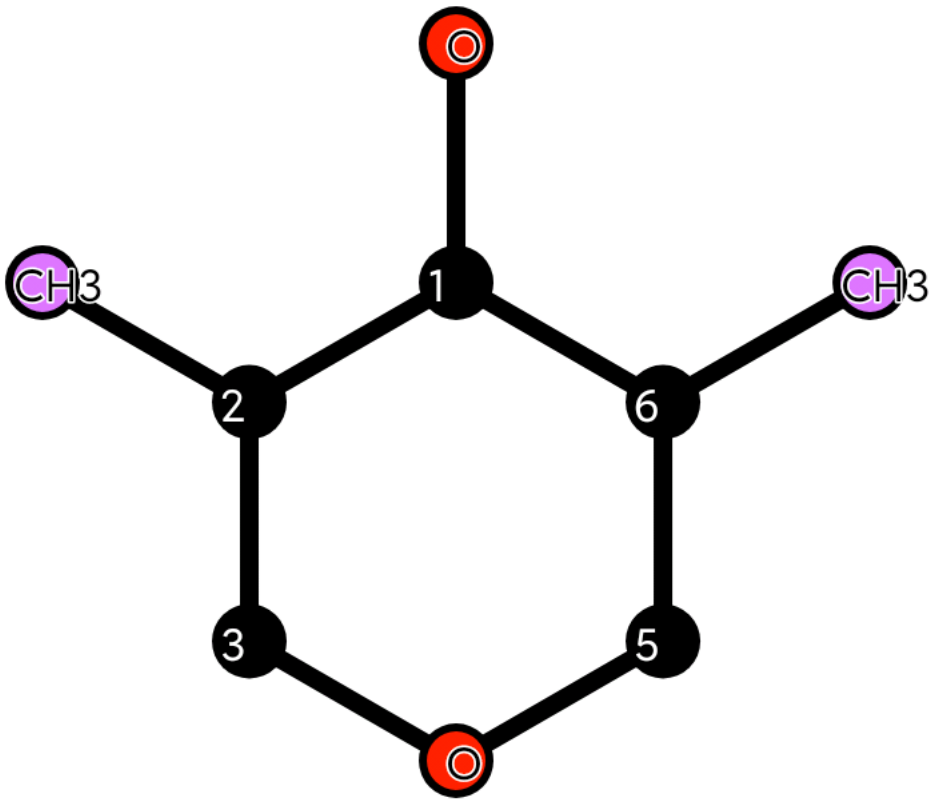
Print calculated values

Report generated by:root, 06.03.2020 - 11:55:31

The following determinant is calculated:

-x	1.0	0.0	0.0	0.0	1.0	1.93	0.0	0.0
1.0	-x	1.0	0.0	0.0	0.0	0.0	0.18	0.0
0.0	1.0	-x	0.19	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.19	-x+2.06	0.19	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.19	-x	1.0	0.0	0.0	0.0
1.0	0.0	0.0	0.0	1.0	-x	0.0	0.0	0.18
1.93	0.0	0.0	0.0	0.0	0.0	-x+1.18	0.0	0.0
0.0	0.18	0.0	0.0	0.0	0.0	0.0	-x+0.88	0.0
0.0	0.0	0.0	0.0	0.0	0.18	0.0	0.0	-x+0.88

It is about this molecule:

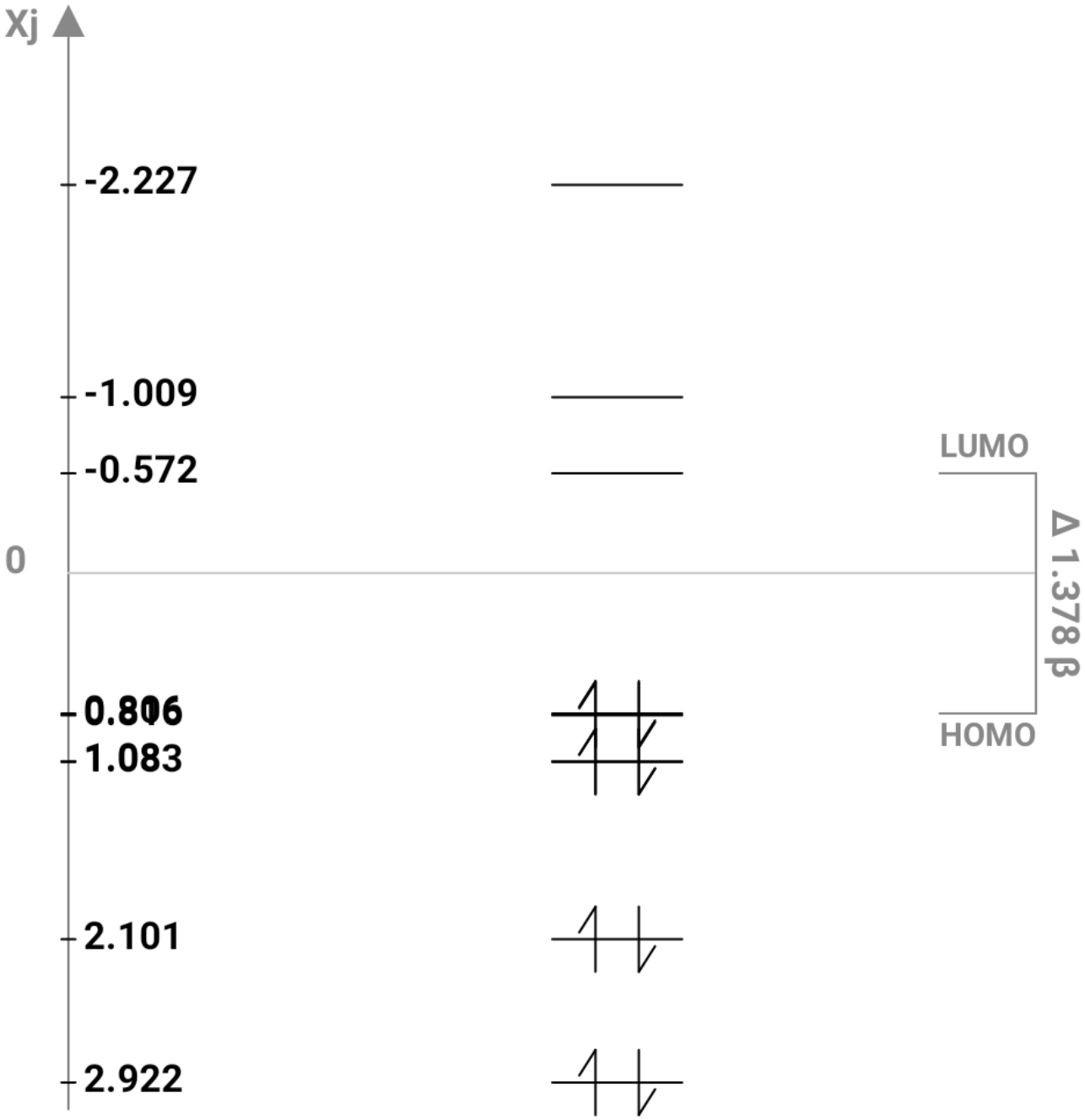


HMO-Energies

x1 = 2.922; x2 = 2.101; x3 = 1.083; x4 = 1.08; x5 = 0.816; x6 = 0.806; x7 = -0.572; x8 = -1.009; x9 = -2.227;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 9α + 17.616β -

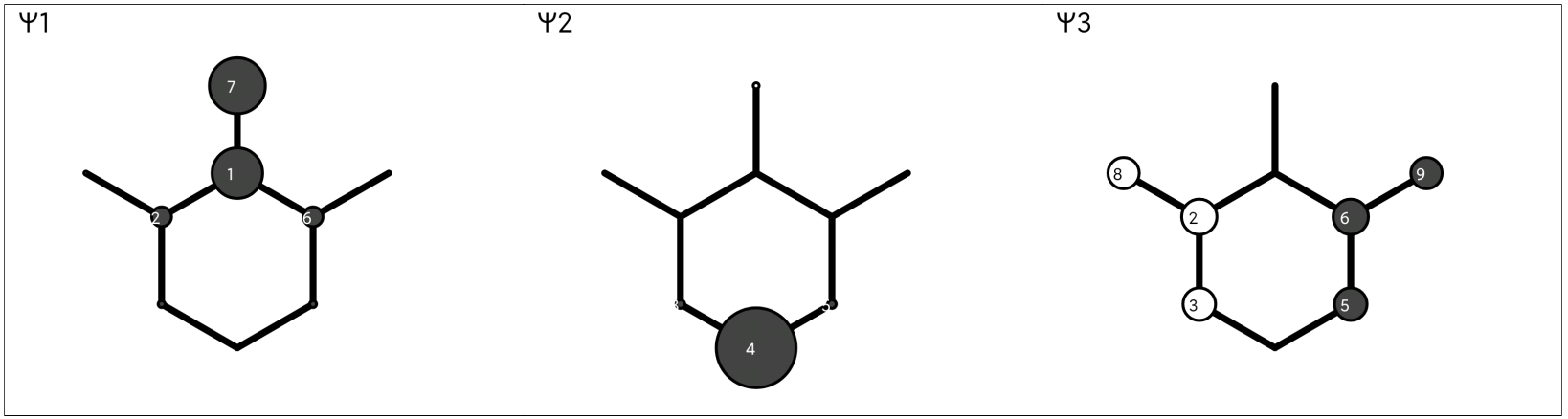
this corresponds to one πelectron: 1.468β

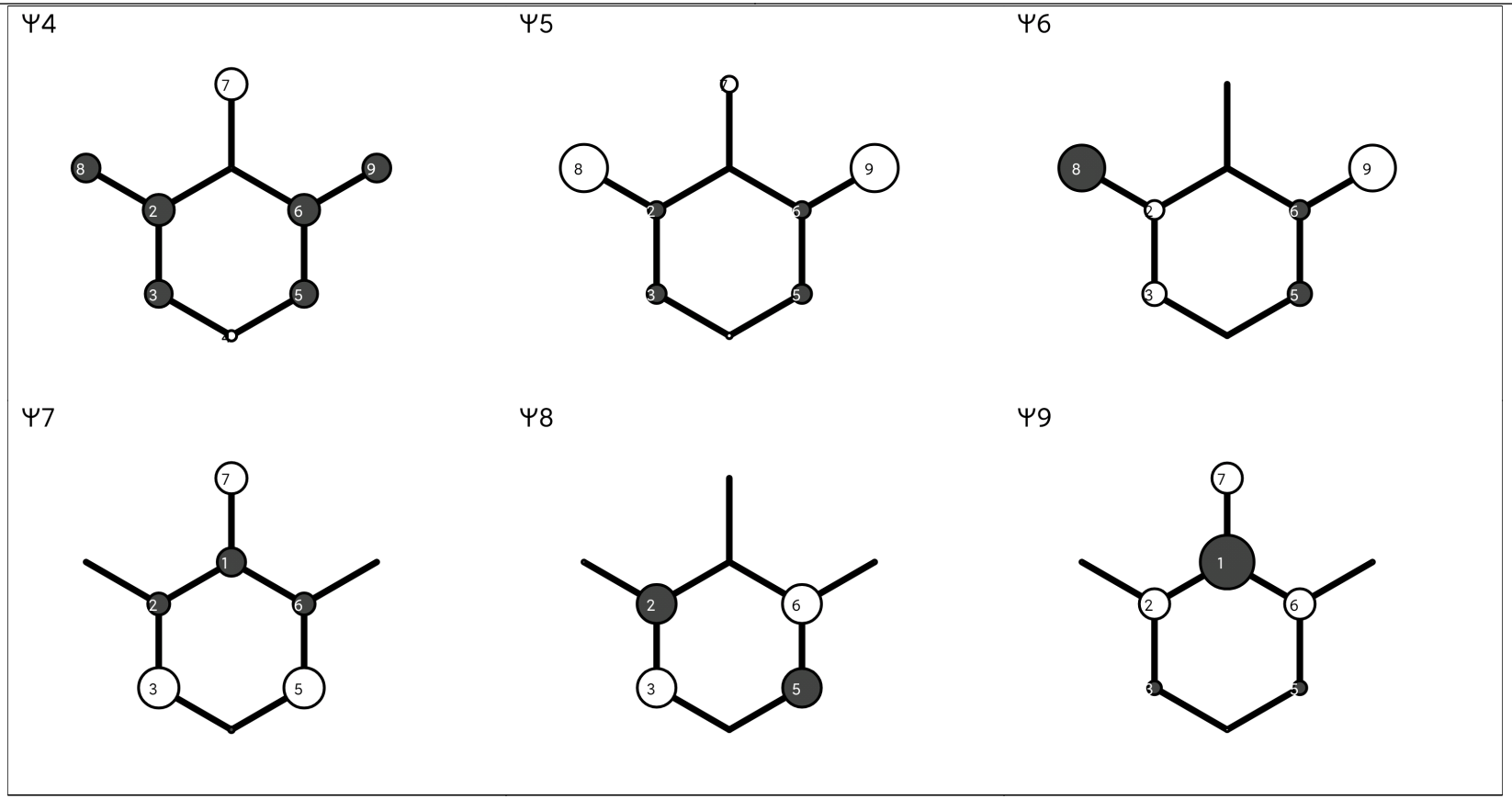
2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9
	x1= 2.922	x2= 2.101	x3= 1.083	x4= 1.08	x5= 0.816	x6= 0.806	x7= -0.572	x8= -1.009	x9= -2.227
1	-0.623	0.035	0.0	-0.021	-0.039	0.0	-0.364	0.0	-0.69
2	-0.244	-0.034	0.435	-0.4	-0.215	0.244	-0.283	-0.501	0.391
3	-0.086	-0.105	0.402	-0.347	-0.246	0.303	0.519	0.497	-0.177
4	-0.038	-0.984	0.0	0.134	0.075	0.0	-0.075	0.0	0.016
5	-0.086	-0.105	-0.402	-0.347	-0.246	-0.303	0.519	-0.497	-0.177
6	-0.244	-0.034	-0.435	-0.4	-0.215	-0.244	-0.283	0.501	0.391
7	-0.69	0.073	0.0	0.403	0.206	0.0	0.401	0.0	0.391
8	-0.021	-0.005	0.386	-0.36	0.607	-0.591	0.035	0.048	-0.023
9	-0.021	-0.005	-0.386	-0.36	0.607	0.591	0.035	-0.048	-0.023

2.2. Molecule orbital presentation:



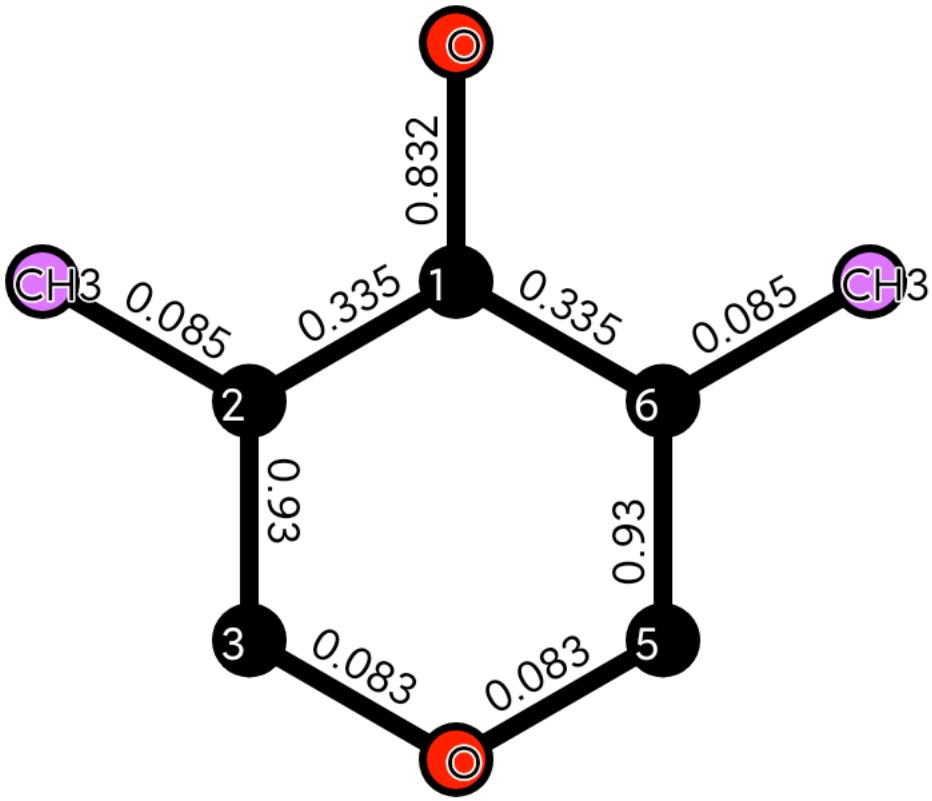

Ψ4
Ψ5
Ψ6
Ψ7
Ψ8
Ψ9

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9
1	0.782								
2	0.335	1.032							
3	0.133	0.93	0.905						
4	-0.033	-0.055	0.083	1.988					
5	0.133	-0.066	-0.108	0.083	0.905				
6	0.335	0.036	-0.066	-0.055	0.93	1.032			
7	0.832	-0.08	-0.278	0.048	-0.278	-0.08	1.373		
8	-0.006	0.085	-0.092	0.006	0.003	-0.01	-0.01	1.992	
9	-0.006	-0.01	0.003	0.006	-0.092	0.085	-0.01	0.001	1.992

3.2. Presentation of bond order:

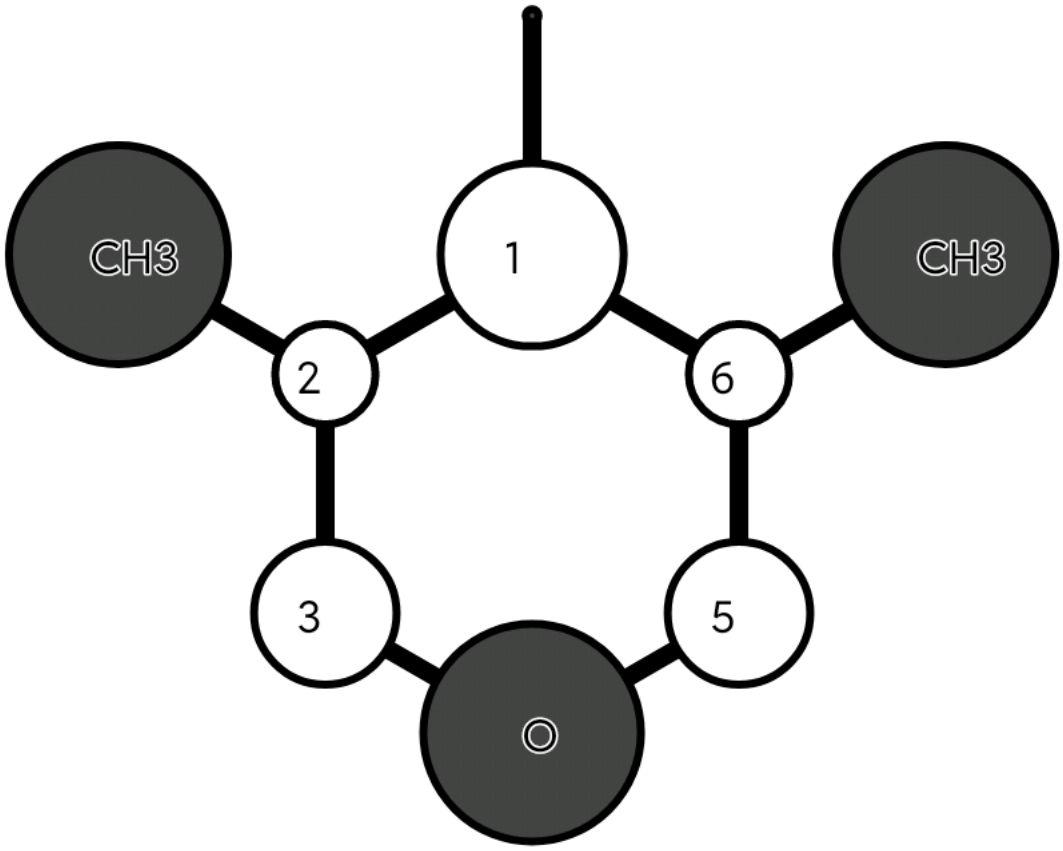


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9
1	0.551								
2		0.302							
3			0.429						
4				-0.655					
5					0.429				
6						0.302			
7							-0.039		
8								-0.659	
9									-0.659

4.2. Presentation of molecule:

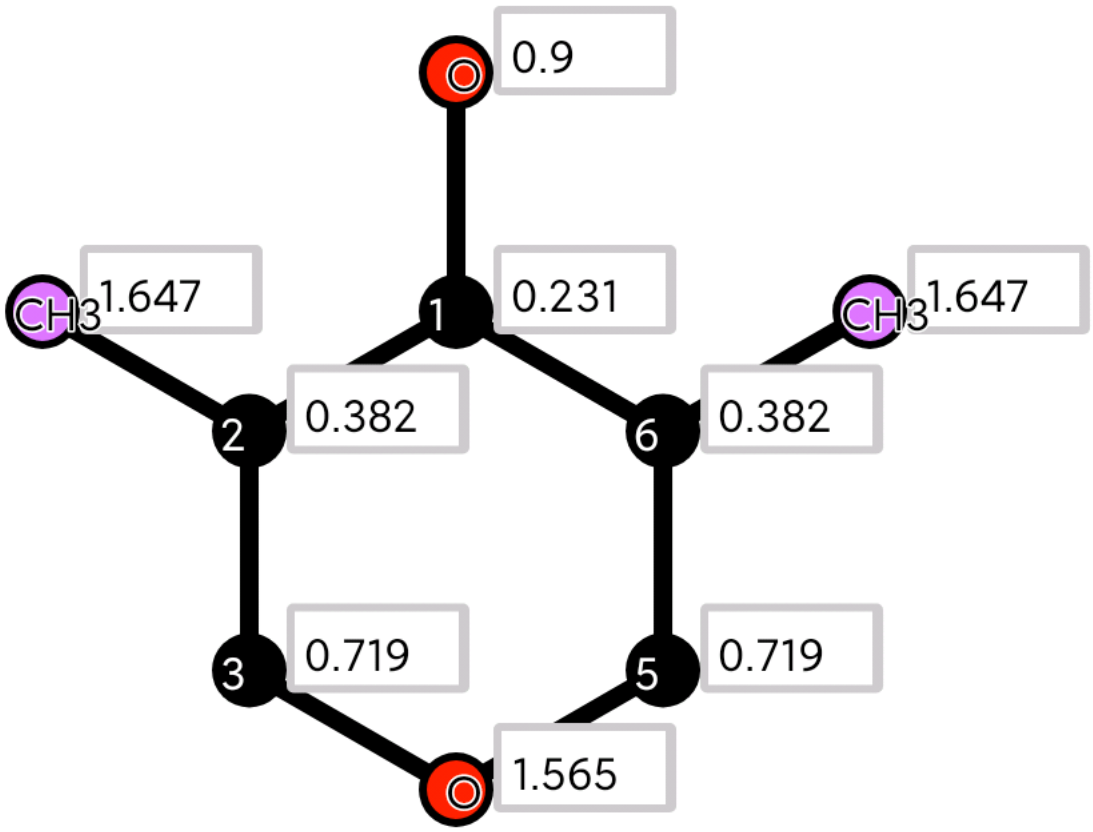


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9
0.231	0.382	0.719	1.565	0.719	0.382	0.9	1.647	1.647

5.2. Presentation of molecule:

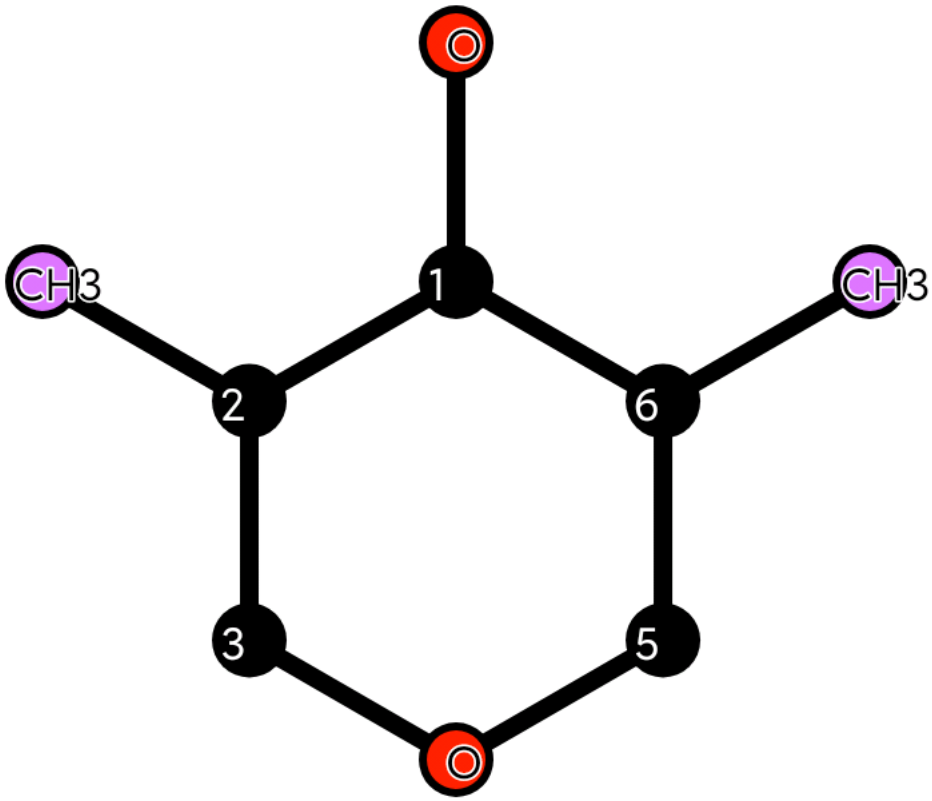


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9
1	0.205								
2	-0.015	0.433							
3	-0.012	-0.434	0.548						
4	-0.001	-0.003	0.0	0.009					
5	-0.012	-0.001	-0.016	0.0	0.548				
6	-0.015	0.002	-0.001	-0.003	-0.434	0.433			
7	-0.151	0.018	-0.075	-0.003	-0.075	0.018	0.268		
8	0.0	0.0	-0.01	0.0	0.0	0.0	0.0	0.009	
9	0.0	0.0	0.0	0.0	-0.01	0.0	0.0	0.0	0.009

6.2. Presentation of molecule:

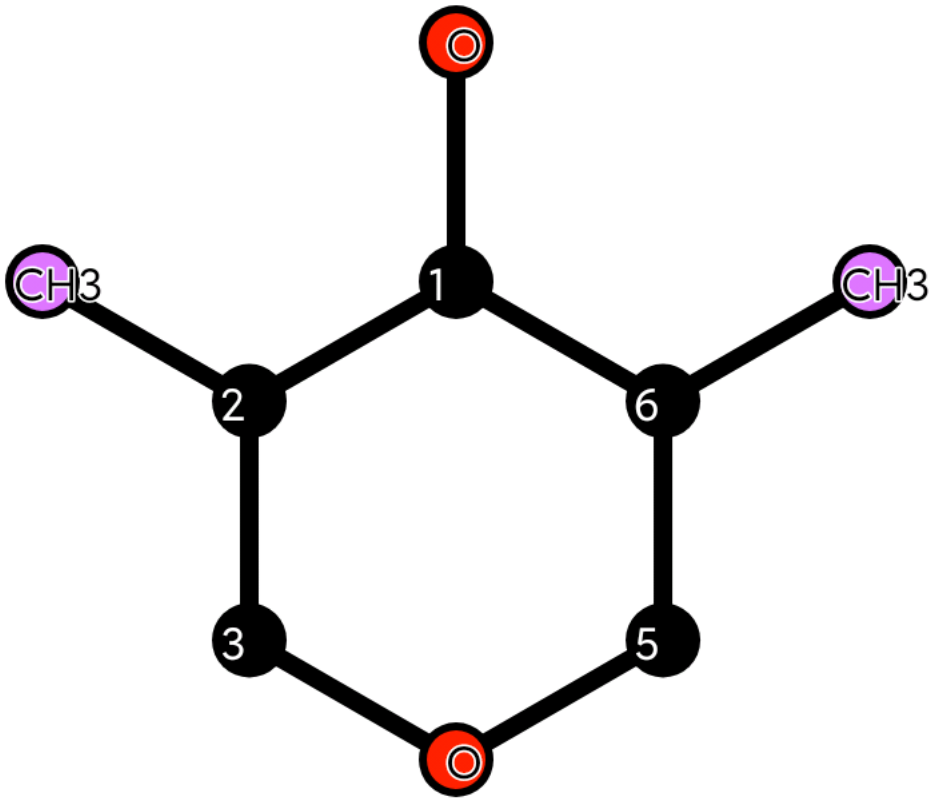


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9
1 2	0.029	0.023	-0.094	-0.002	0.009	-0.006	0.039	0.001	0.0
1 6	0.029	-0.006	0.009	-0.002	-0.094	0.023	0.039	0.0	0.001
1 7	0.031	-0.002	0.037	0.002	0.037	-0.002	-0.102	0.0	0.0
2 3	-0.015	-0.028	0.061	0.002	-0.007	0.003	-0.021	0.004	0.0
2 8	-0.001	-0.02	0.068	0.0	0.0	0.0	-0.003	-0.045	0.0
3 4	0.004	0.035	-0.023	-0.031	0.002	-0.002	0.015	0.001	0.0
4 5	0.004	-0.002	0.002	-0.031	-0.023	0.035	0.015	0.0	0.001
5 6	-0.015	0.003	-0.007	0.002	0.061	-0.028	-0.021	0.0	0.004
6 9	-0.001	0.0	0.0	0.0	0.068	-0.02	-0.003	0.0	-0.045

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	1 7	2 3	2 8	3 4	4 5	5 6	6 9
1 2	0.303								
1 6	-0.028	0.303							
1 7	-0.108	-0.108	0.129						
2 3	-0.12	0.005	0.045	0.06					
2 8	-0.017	0.002	0.004	-0.034	0.475				
3 4	0.03	0.008	-0.016	-0.037	-0.011	0.382			
4 5	0.008	0.03	-0.016	-0.005	0.0	0.058	0.382		
5 6	0.005	-0.12	0.045	0.0	-0.001	-0.005	-0.037	0.06	
6 9	0.002	-0.017	0.004	-0.001	0.0	0.0	-0.011	-0.034	0.475

8.2. Presentation of molecule: