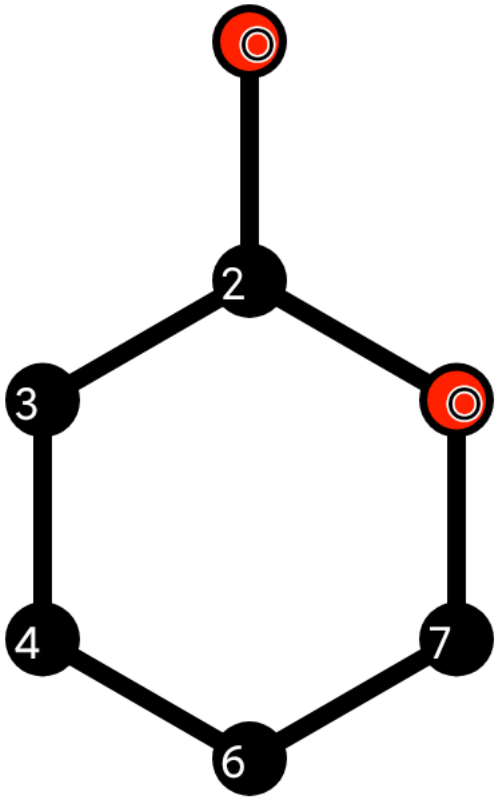
Print calculated values

Report generated by:root, 20.01.2020 - 12:36:13

The following determinant is calculated:

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

It is about this molecule:

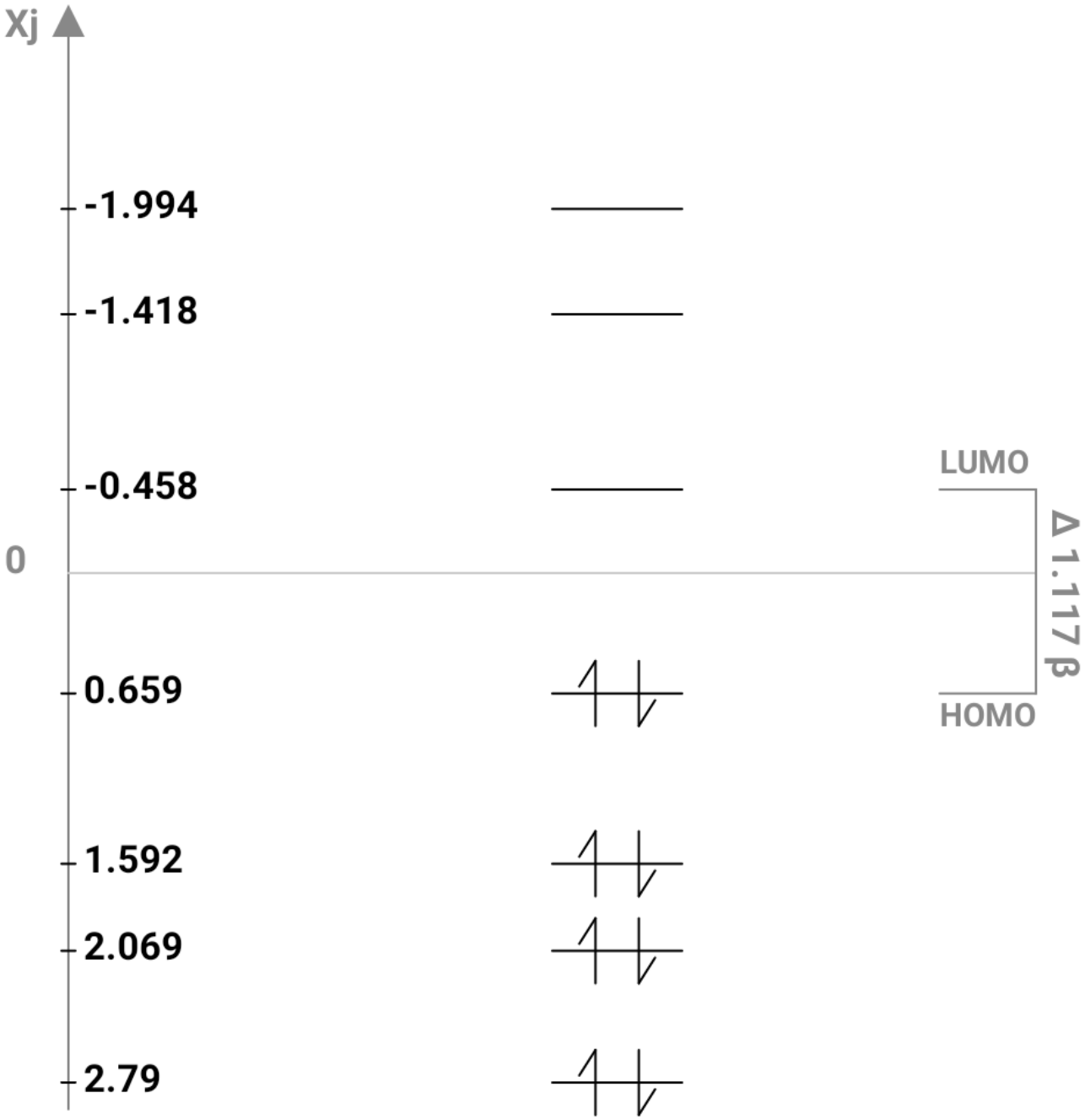


HMO-Energies

x1 = 2.79; x2 = 2.069; x3 = 1.592; x4 = 0.659; x5 = -0.458; x6 = -1.418; x7 = -1.994;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 7α + 14.22β -

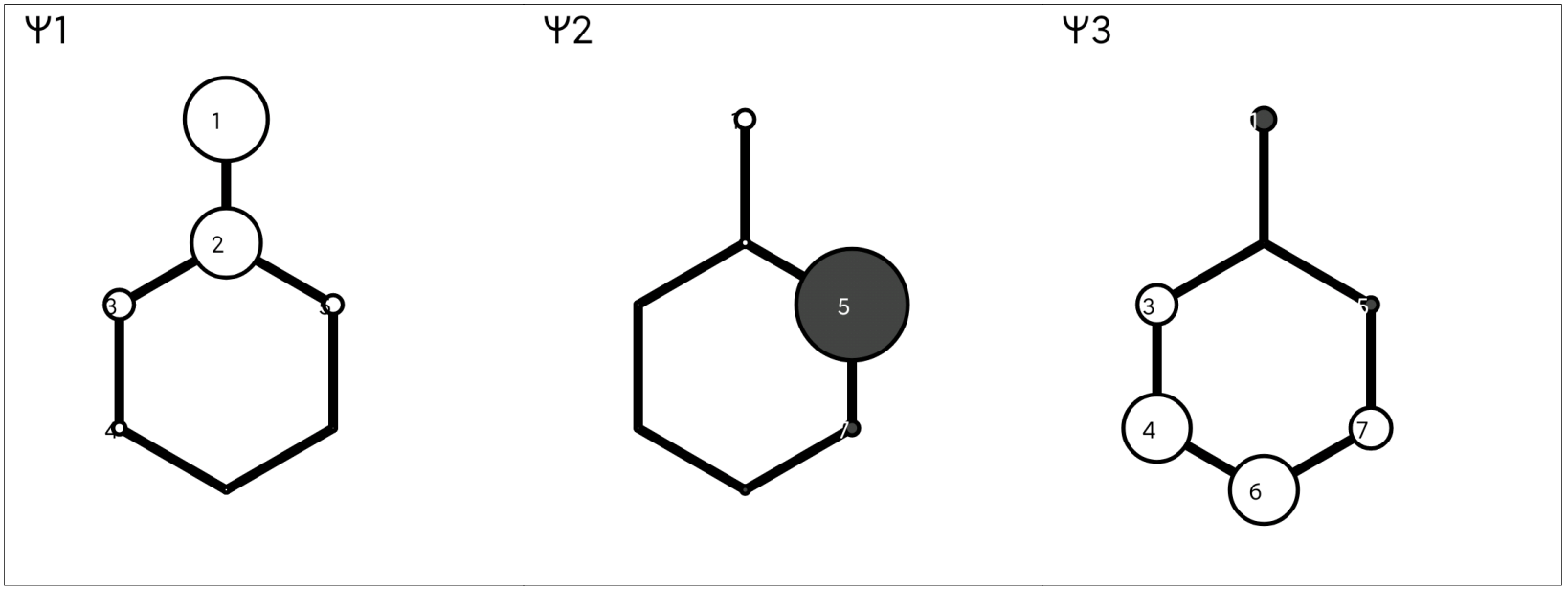
this corresponds to one πelectron: 1.778β

2. Hueckel-coefficient

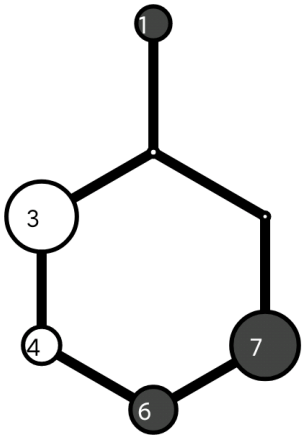
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7
	x1= 2.79	x2= 2.069	x3= 1.592	x4= 0.659	x5= -0.458	x6= -1.418	x7= -1.994
1	0.725	0.163	-0.2	-0.285	-0.297	-0.312	-0.375
2	0.605	0.075	-0.043	0.077	0.252	0.42	0.617
3	0.256	0.026	0.342	0.589	0.469	0.007	-0.5
4	0.11	-0.021	0.587	0.311	-0.467	-0.429	0.379
5	0.165	-0.973	-0.128	0.066	-0.063	0.0	-0.035
6	0.05	-0.07	0.593	-0.384	-0.255	0.602	-0.256
7	0.029	-0.123	0.357	-0.564	0.584	-0.424	0.132

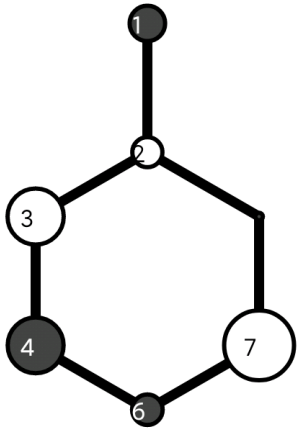
2.2. Molecule orbital presentation:



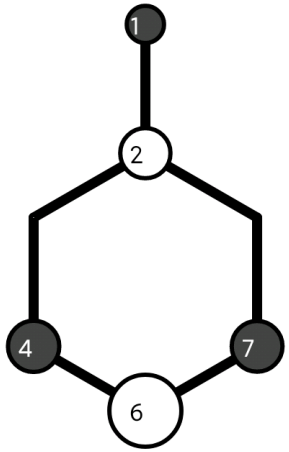
Ψ4



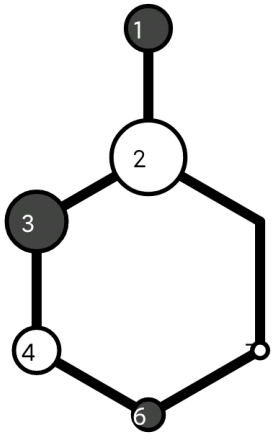
Ψ5



Ψ6



Ψ7

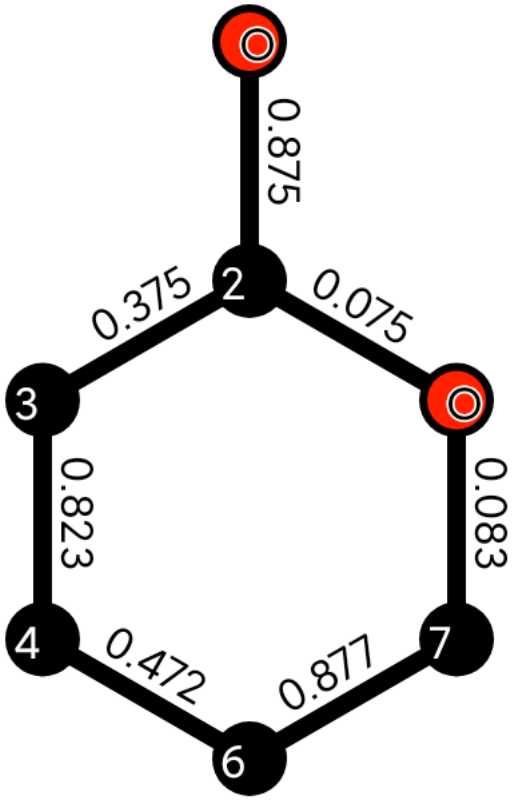


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7
1	1.348						
2	0.875	0.758					
3	-0.093	0.375	1.06				
4	-0.26	0.127	0.823	0.908			
5	-0.064	0.075	0.024	-0.032	1.99		
6	0.031	-0.06	-0.024	0.472	-0.051	1.014	
7	0.181	-0.101	-0.411	0.081	0.083	0.877	0.923

3.2. Presentation of bond order:

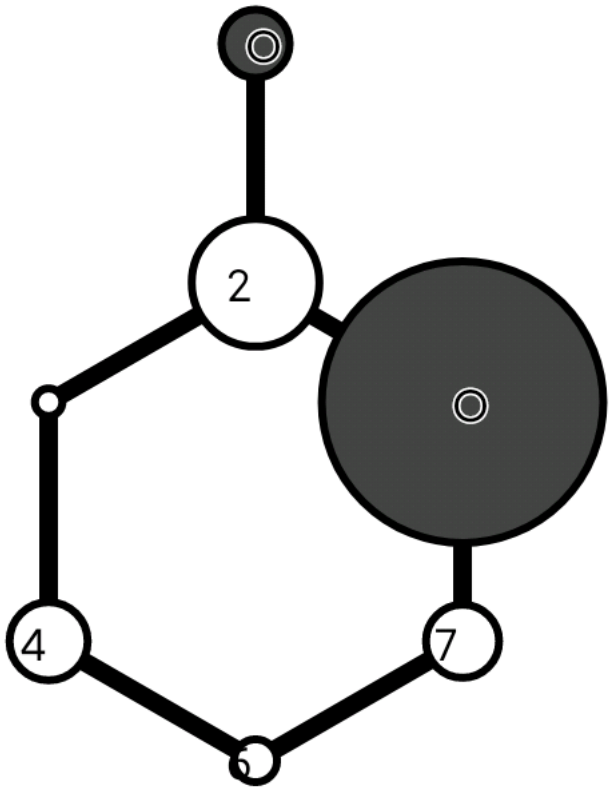


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7
1	-0.205						
2		0.384					
3			0.083				
4				0.235			
5					-0.847		
6						0.129	
7							0.22

4.2. Presentation of molecule:

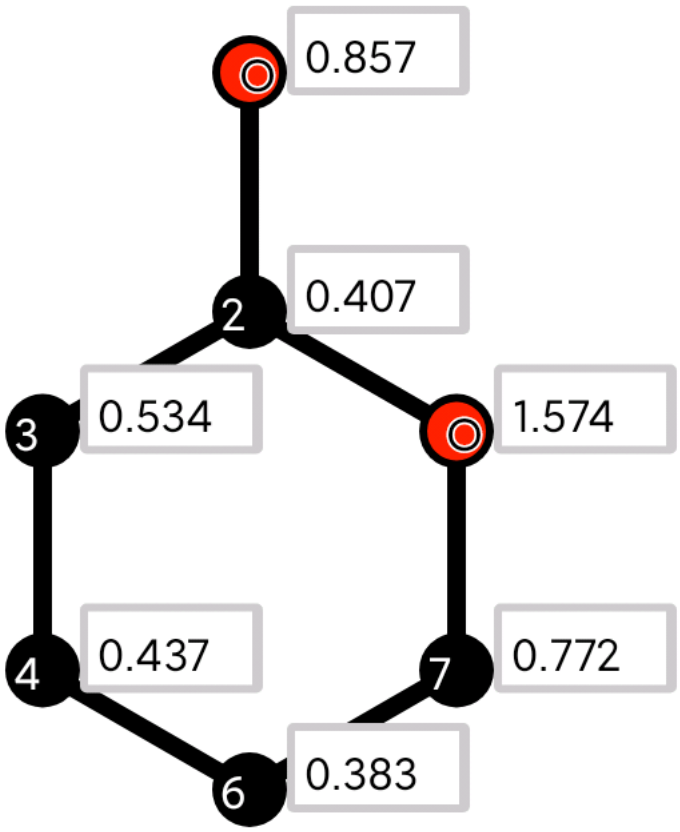


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7
0.857	0.407	0.534	0.437	1.574	0.383	0.772

5.2. Presentation of molecule:

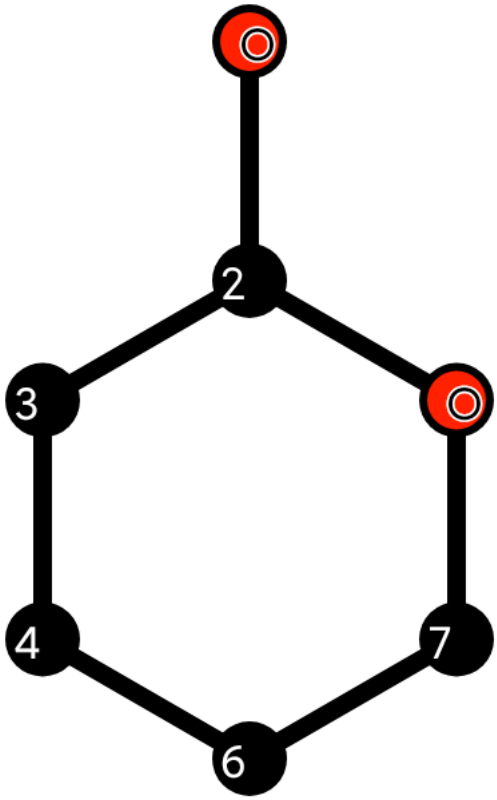


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7
1	0.254						
2	-0.172	0.218					
3	0.038	-0.017	0.519				
4	-0.068	-0.012	-0.338	0.424			
5	-0.003	-0.001	-0.002	0.0	0.007		
6	0.005	-0.001	0.034	-0.052	-0.002	0.396	
7	-0.055	-0.015	-0.234	0.046	0.001	-0.38	0.637

6.2. Presentation of molecule:

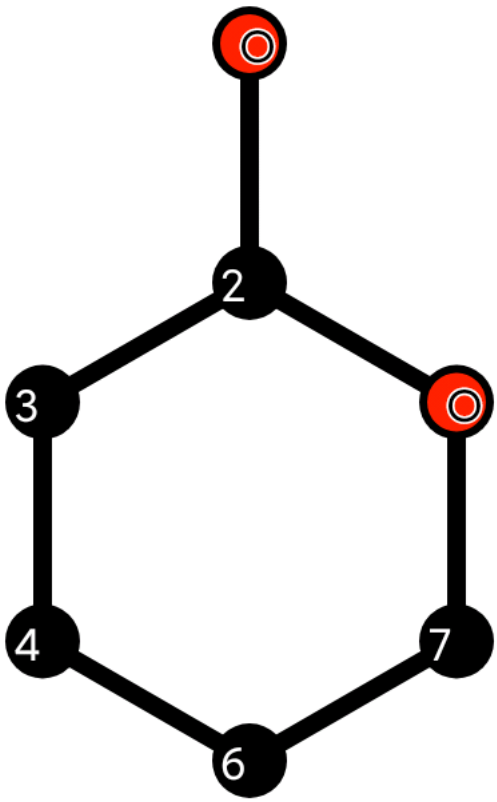


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7
1 2	-0.095	0.039	-0.009	0.035	0.002	-0.002	0.03
2 3	0.052	0.044	0.043	-0.079	-0.001	0.006	-0.064
2 5	0.023	0.001	-0.002	0.002	-0.023	-0.002	0.001
3 4	-0.025	-0.02	-0.054	0.049	0.001	0.0	0.049
4 6	0.011	0.008	0.024	0.017	-0.002	0.004	-0.062
5 7	0.012	0.003	0.019	-0.003	-0.031	0.03	-0.031
6 7	-0.008	-0.006	-0.019	-0.013	0.002	-0.012	0.056

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	2 3	2 5	3 4	4 6	5 7	6 7
1 2	0.11						
2 3	-0.145	0.339					
2 5	-0.028	-0.002	0.337				
3 4	0.056	-0.137	0.0	0.145			
4 6	-0.022	0.047	0.006	-0.185	0.367		
5 7	-0.014	0.021	0.053	-0.016	0.026	0.385	
6 7	0.016	-0.031	-0.004	0.099	-0.201	-0.036	0.114

8.2. Presentation of molecule: