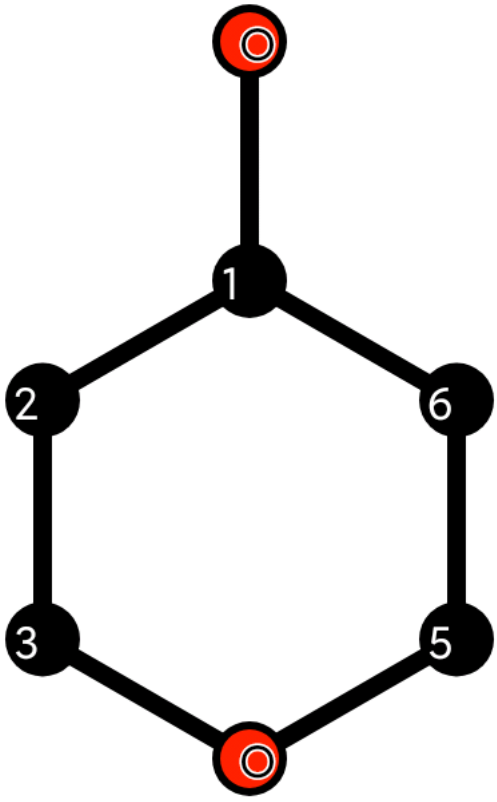
Print calculated values

Report generated by:root, 03.03.2020 - 18:15:24

The following determinant is calculated:

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

It is about this molecule:

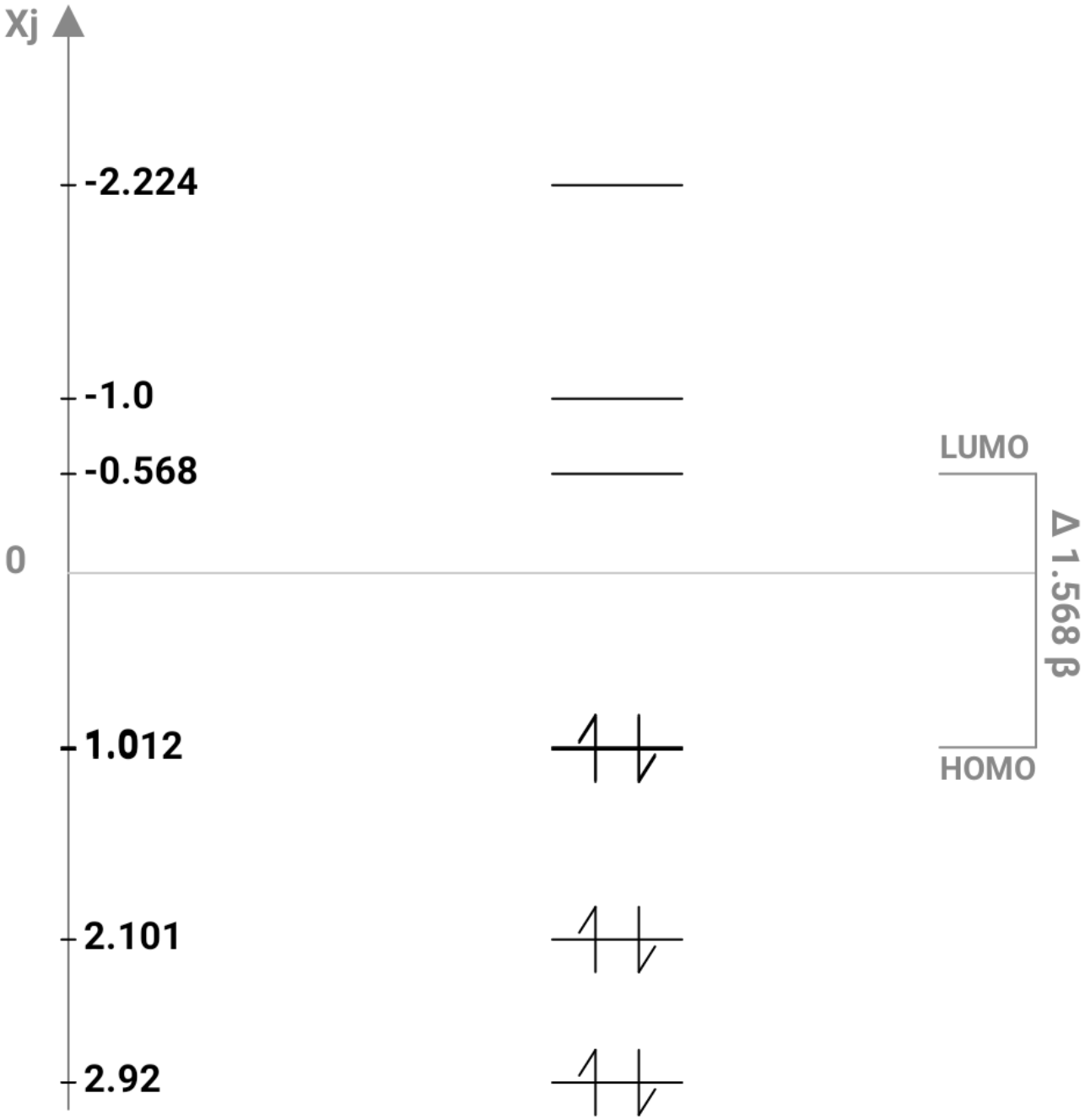


HMO-Energies

x1 = 2.92; x2 = 2.101; x3 = 1.012; x4 = 1.0; x5 = -0.568; x6 = -1.0; x7 = -2.224;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 7α + 14.066β -

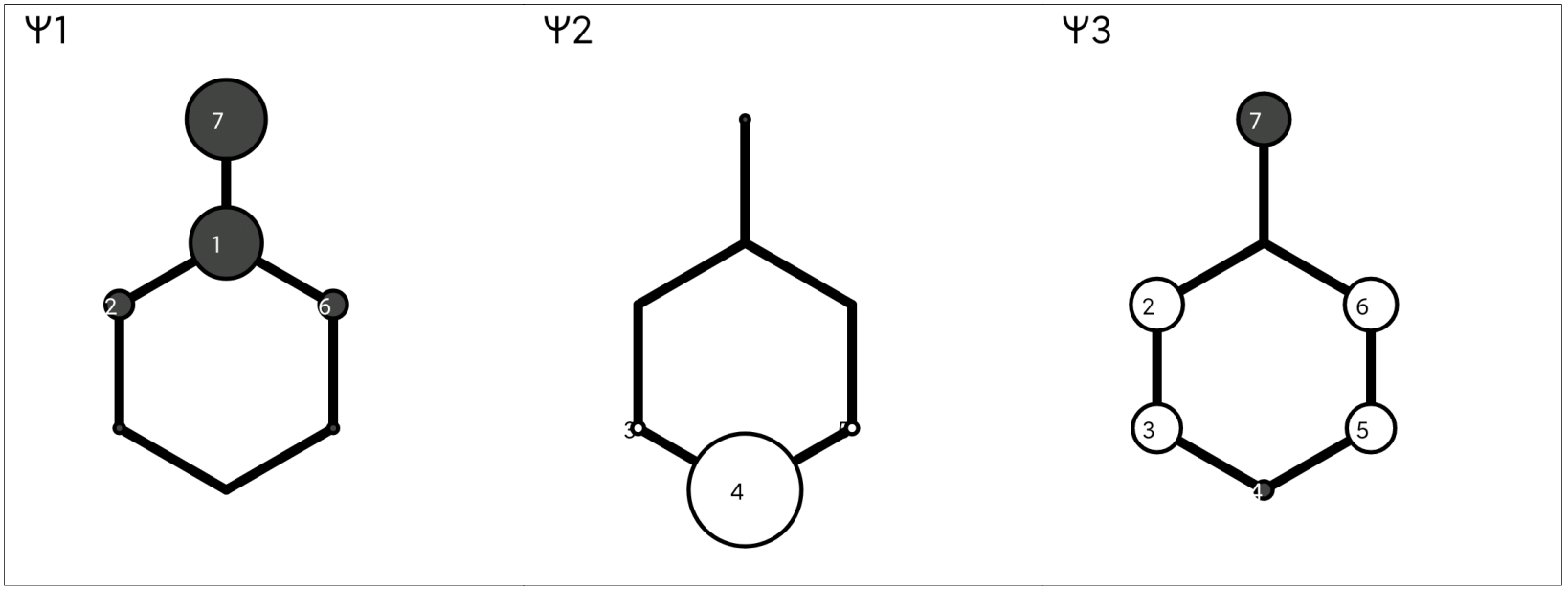
this corresponds to one πelectron: 1.758β

2. Hueckel-coefficient

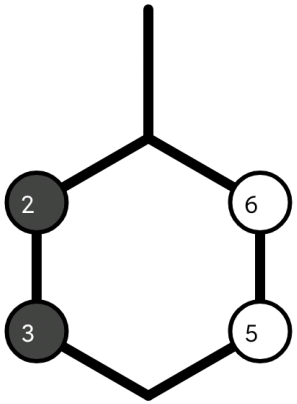
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7
	x1= 2.92	x2= 2.101	x3= 1.012	x4= 1.0	x5= -0.568	x6= -1.0	x7= -2.224
1	-0.623	-0.035	0.039	0.0	0.362	0.0	-0.692
2	-0.243	0.034	0.456	-0.5	0.282	-0.5	0.391
3	-0.086	0.105	0.422	-0.5	-0.522	0.5	-0.177
4	-0.038	0.985	-0.153	0.0	0.075	0.0	0.016
5	-0.086	0.105	0.422	0.5	-0.522	-0.5	-0.177
6	-0.243	0.034	0.456	0.5	0.282	0.5	0.391
7	-0.691	-0.072	-0.452	0.0	-0.399	0.0	0.392

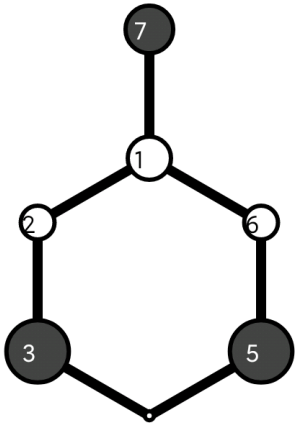
2.2. Molecule orbital presentation:



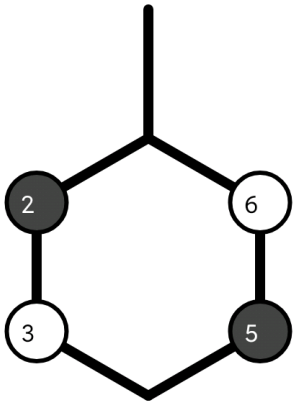
Ψ4



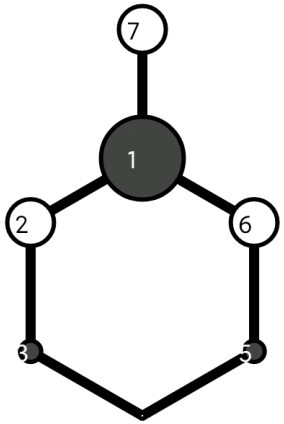
Ψ5



Ψ6



Ψ7

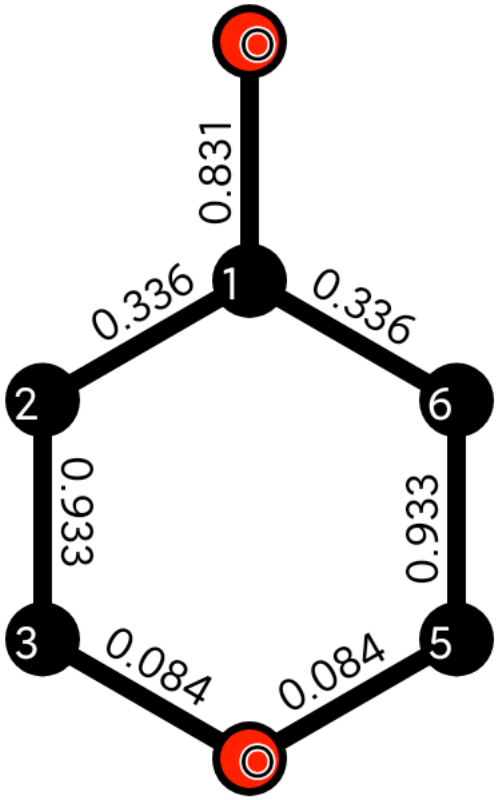


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7
1	0.782						
2	0.336	1.035					
3	0.133	0.933	0.892				
4	-0.033	-0.055	0.084	1.988			
5	0.133	-0.067	-0.108	0.084	0.892		
6	0.336	0.035	-0.067	-0.055	0.933	1.035	
7	0.831	-0.081	-0.278	0.048	-0.278	-0.081	1.374

3.2. Presentation of bond order:

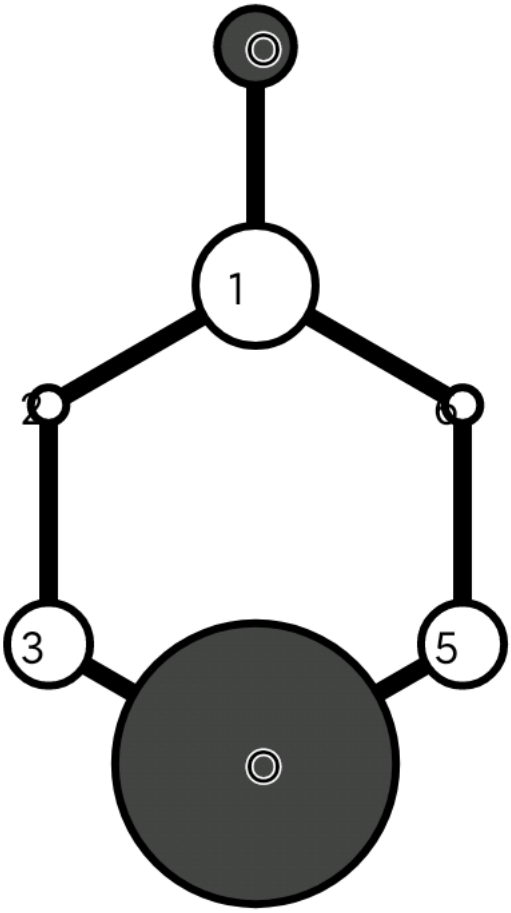


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7
1	0.361						
2		0.107					
3			0.25				
4				-0.845			
5					0.25		
6						0.107	
7							-0.231

4.2. Presentation of molecule:

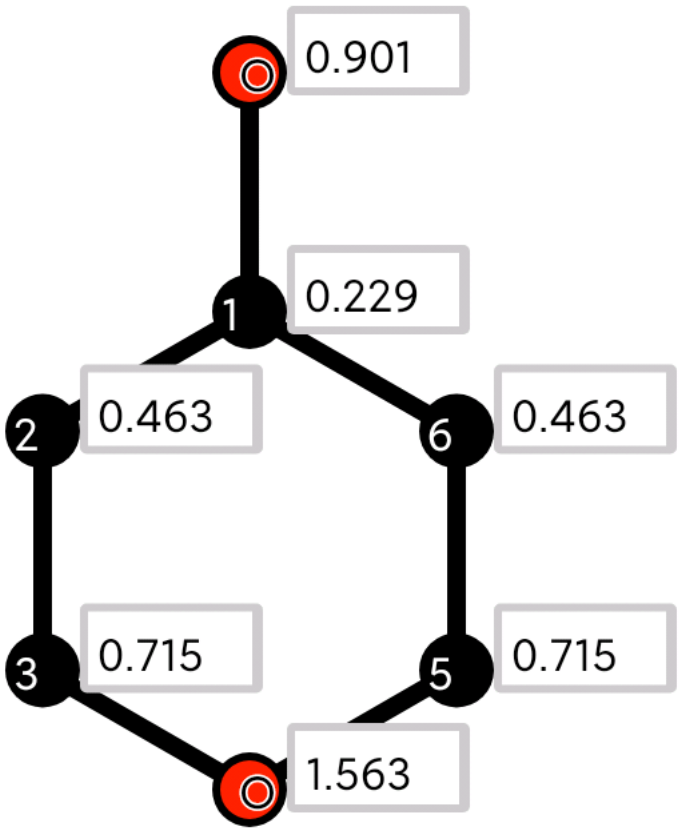


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7
0.229	0.463	0.715	1.563	0.715	0.463	0.901

5.2. Presentation of molecule:

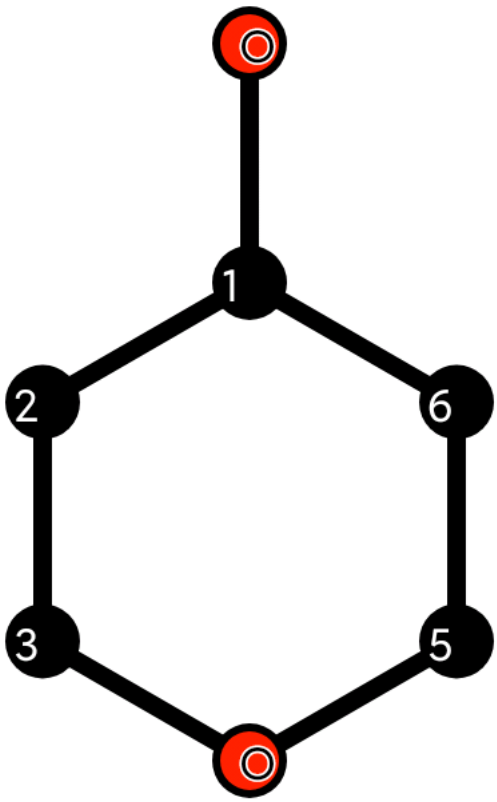


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7
1	0.205						
2	-0.015	0.436					
3	-0.011	-0.436	0.539				
4	-0.001	-0.003	0.0	0.009			
5	-0.011	-0.001	-0.015	0.0	0.539		
6	-0.015	0.002	-0.001	-0.003	-0.436	0.436	
7	-0.151	0.018	-0.075	-0.003	-0.075	0.018	0.267

6.2. Presentation of molecule:

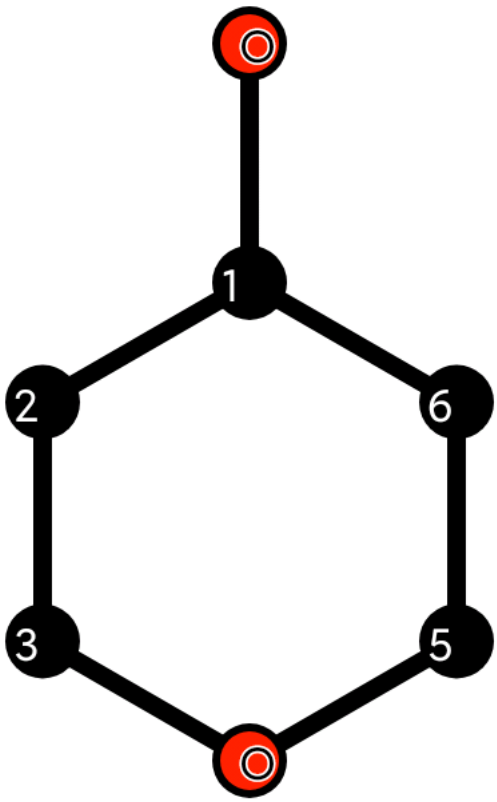


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7
1 2	0.029	0.023	-0.094	-0.002	0.009	-0.006	0.04
1 6	0.029	-0.006	0.009	-0.002	-0.094	0.023	0.04
1 7	0.031	-0.002	0.036	0.002	0.036	-0.002	-0.102
2 3	-0.015	-0.031	0.069	0.002	-0.007	0.003	-0.021
3 4	0.003	0.035	-0.022	-0.031	0.002	-0.002	0.015
4 5	0.003	-0.002	0.002	-0.031	-0.022	0.035	0.015
5 6	-0.015	0.003	-0.007	0.002	0.069	-0.031	-0.021

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	1 7	2 3	3 4	4 5	5 6
1 2	0.303						
1 6	-0.029	0.303					
1 7	-0.108	-0.108	0.129				
2 3	-0.122	0.005	0.045	0.059			
3 4	0.029	0.007	-0.016	-0.039	0.386		
4 5	0.007	0.029	-0.016	-0.005	0.058	0.386	
5 6	0.005	-0.122	0.045	-0.001	-0.005	-0.039	0.059

8.2. Presentation of molecule: