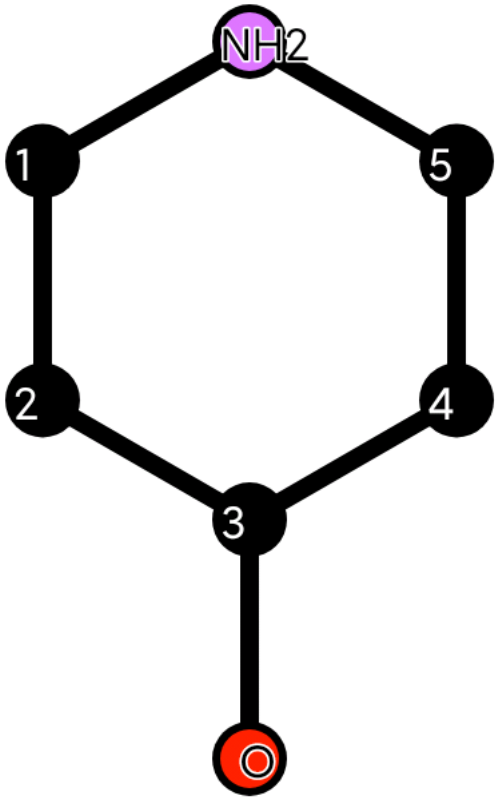
Print calculated values

Report generated by:root, 26.03.2020 - 17:40:55

The following determinant is calculated:

-x	1.0	0.0	0.0	0.0	1.3	0.0
1.0	-x	1.0	0.0	0.0	0.0	0.0
0.0	1.0	-x	1.0	0.0	0.0	1.93
0.0	0.0	1.0	-x	1.0	0.0	0.0
0.0	0.0	0.0	1.0	-x	1.3	0.0
1.3	0.0	0.0	0.0	1.3	-x+1.47	0.0
0.0	0.0	1.93	0.0	0.0	0.0	-x+1.18

It is about this molecule:

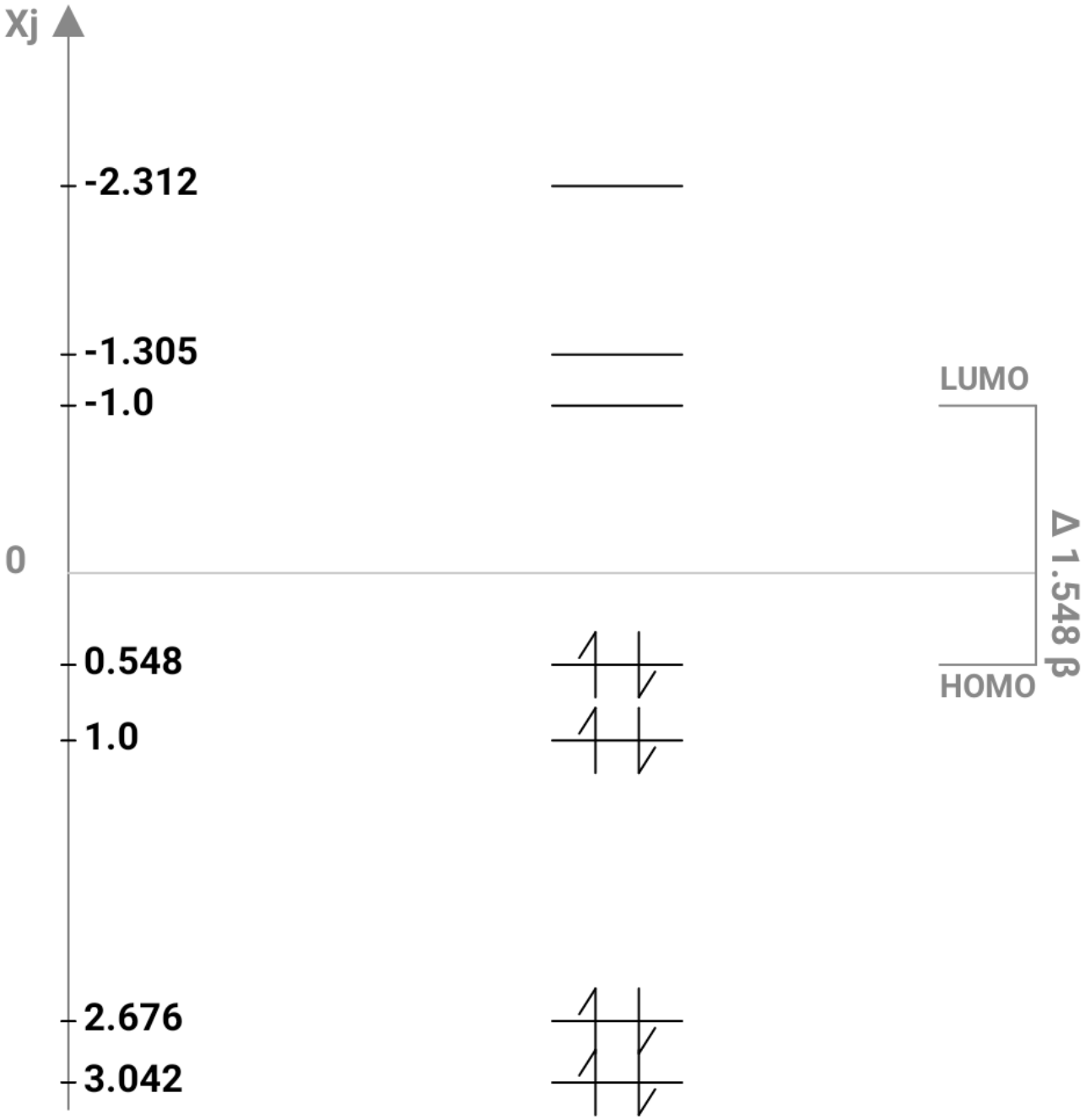


HMO-Energies

x1 = 3.042; x2 = 2.676; x3 = 1.0; x4 = 0.548; x5 = -1.0; x6 = -1.305; x7 = -2.312;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 7α + 14.532β -

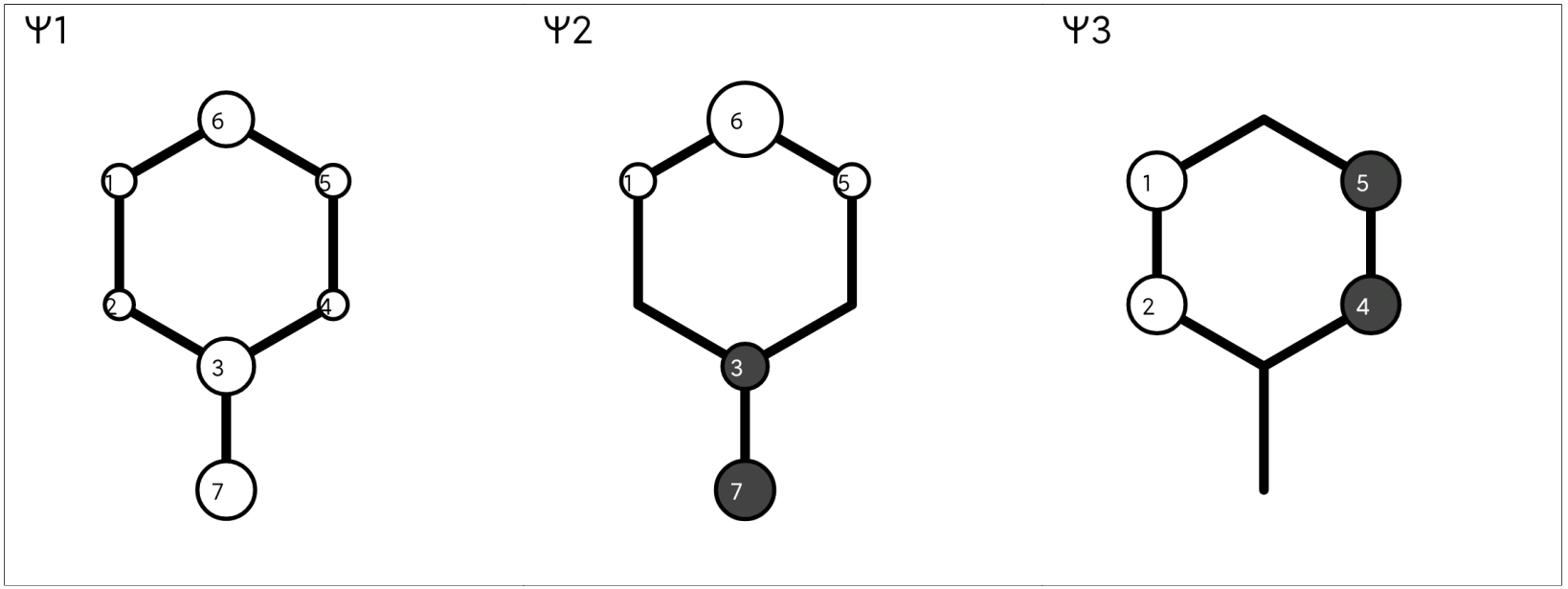
this corresponds to one πelectron: 1.817β

2. Hueckel-coefficient

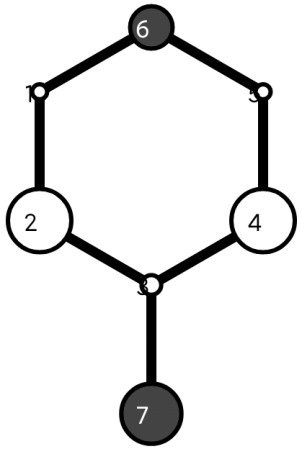
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7
	x1= 3.042	x2= 2.676	x3= 1.0	x4= 0.548	x5= -1.0	x6= -1.305	x7= -2.312
1	0.284	0.296	0.5	0.126	-0.5	-0.491	-0.275
2	0.253	-0.037	0.5	0.53	0.5	0.042	0.389
3	0.486	-0.395	0.0	0.165	0.0	0.435	-0.625
4	0.253	-0.037	-0.5	0.53	-0.5	0.042	0.389
5	0.284	0.296	-0.5	0.126	0.5	-0.491	-0.275
6	0.47	0.638	0.0	-0.355	0.0	0.46	0.189
7	0.504	-0.509	0.0	-0.503	0.0	-0.338	0.346

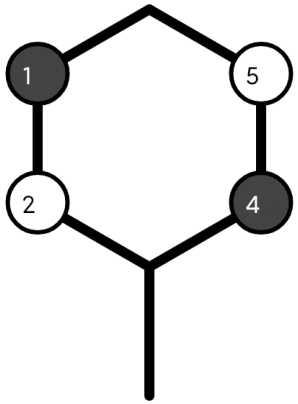
2.2. Molecule orbital presentation:



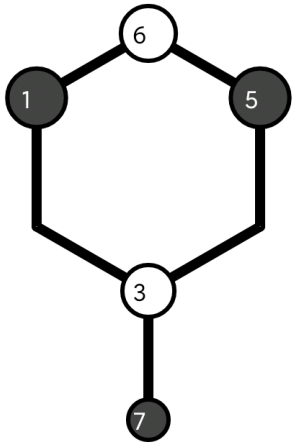
Ψ4



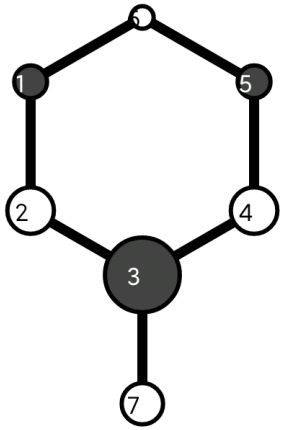
Ψ5



Ψ6



Ψ7

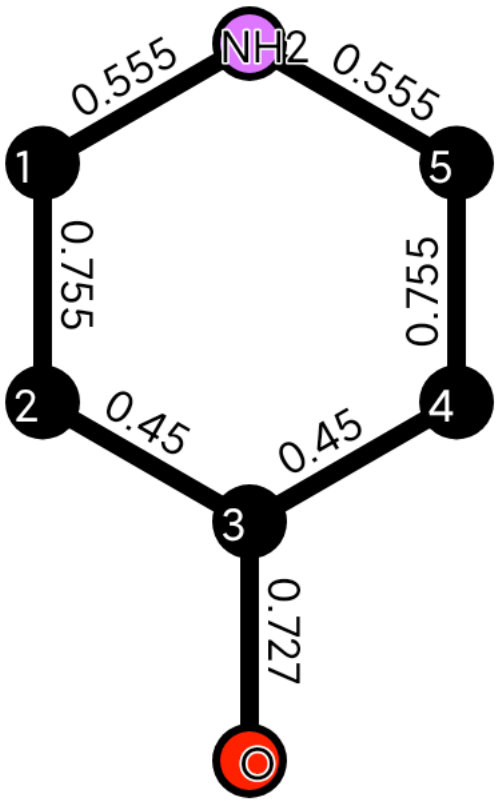


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7
1	0.868						
2	0.755	1.193					
3	0.084	0.45	0.839				
4	-0.245	0.193	0.45	1.193			
5	-0.132	-0.245	0.084	0.755	0.868		
6	0.555	-0.186	-0.164	-0.186	0.555	1.506	
7	-0.142	-0.24	0.727	-0.24	-0.142	0.18	1.532

3.2. Presentation of bond order:

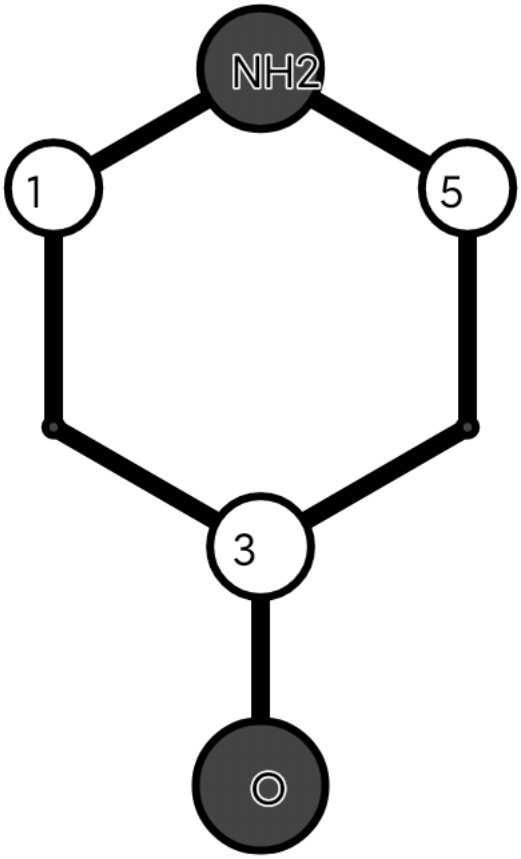


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7
1	0.275						
2		-0.05					
3			0.304				
4				-0.05			
5					0.275		
6						-0.363	
7							-0.39

4.2. Presentation of molecule:

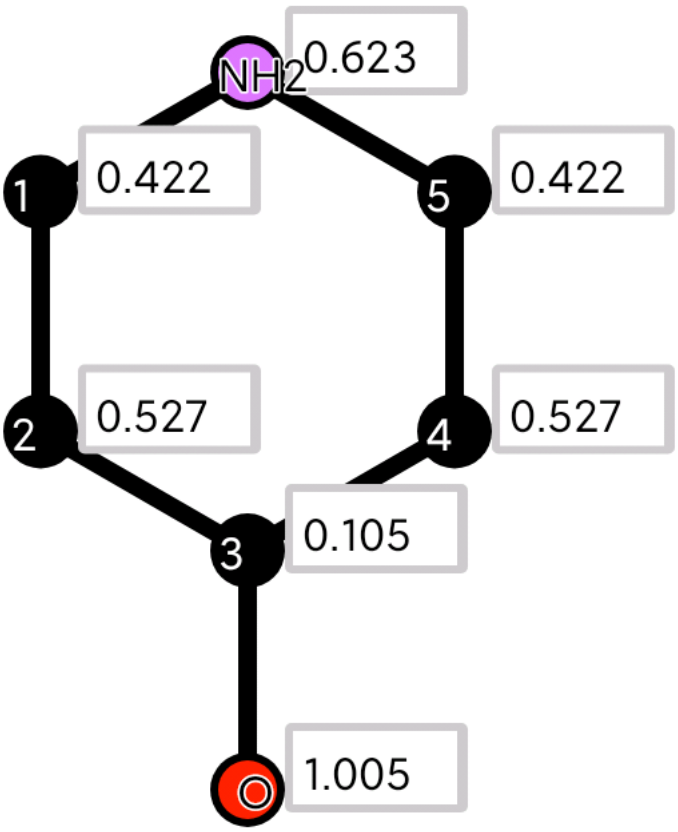


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7
0.422	0.527	0.105	0.527	0.422	0.623	1.005

5.2. Presentation of molecule:

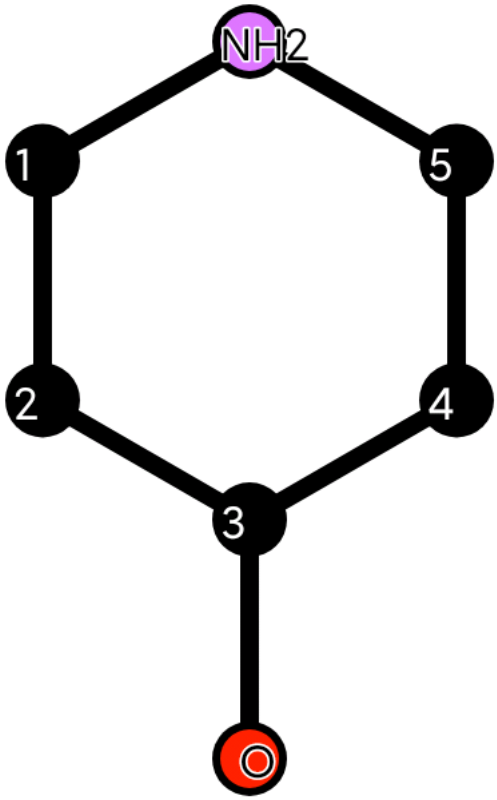


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7
1	0.365						
2	-0.243	0.438					
3	-0.005	-0.049	0.215				
4	-0.045	-0.051	-0.049	0.438			
5	0.003	-0.045	-0.005	-0.243	0.365		
6	-0.058	-0.02	-0.02	-0.02	-0.058	0.21	
7	-0.016	-0.029	-0.086	-0.029	-0.016	-0.032	0.209

6.2. Presentation of molecule:

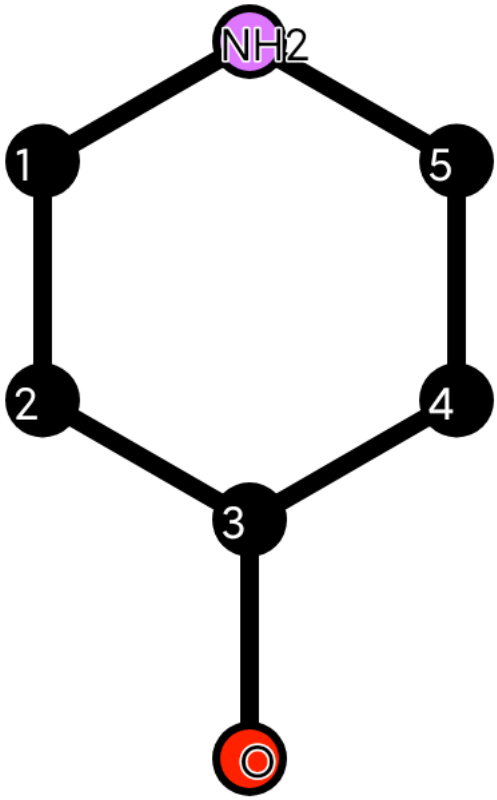


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7
1 2	0.064	-0.087	-0.019	0.047	-0.026	0.05	-0.03
1 6	-0.022	0.085	0.012	-0.044	0.036	-0.091	0.024
2 3	-0.04	-0.018	0.037	-0.043	0.016	-0.026	0.074
3 4	0.016	-0.043	0.037	-0.018	-0.04	-0.026	0.074
3 7	0.011	0.041	0.0	0.041	0.011	0.027	-0.13
4 5	-0.026	0.047	-0.019	-0.087	0.064	0.05	-0.03
5 6	0.036	-0.044	0.012	0.085	-0.022	-0.091	0.024

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	2 3	3 4	3 7	4 5	5 6
1 2	0.203						
1 6	-0.195	0.271					
2 3	-0.151	0.09	0.286				
3 4	0.03	-0.011	-0.033	0.286			
3 7	0.053	-0.037	-0.146	-0.146	0.204		
4 5	-0.024	0.042	0.03	-0.151	0.053	0.203	
5 6	0.042	-0.078	-0.011	0.09	-0.037	-0.195	0.271

8.2. Presentation of molecule: