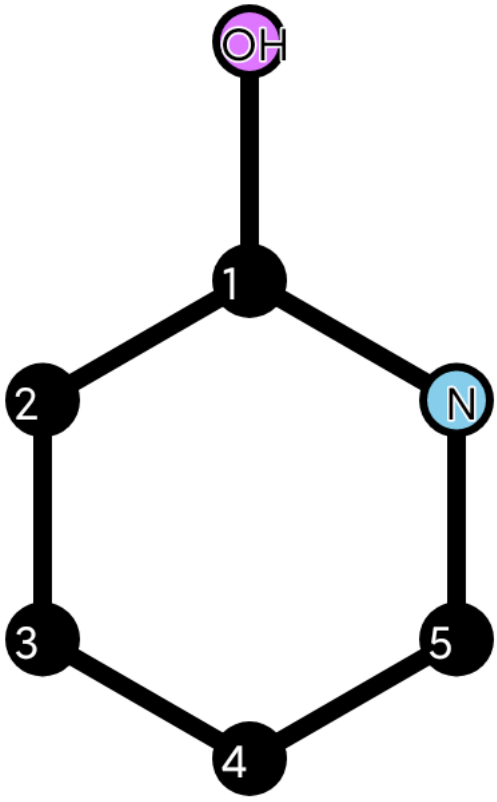
Print calculated values

Report generated by:root, 26.03.2020 - 17:23:55

The following determinant is calculated:

-x	1.0	0.0	0.0	0.0	1.06	0.9
1.0	-x	1.0	0.0	0.0	0.0	0.0
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
0.0	0.0	0.0	1.0	-x	1.06	0.0
1.06	0.0	0.0	0.0	1.06	-x+0.83	0.0
0.9	0.0	0.0	0.0	0.0	0.0	-x+2.0

It is about this molecule:

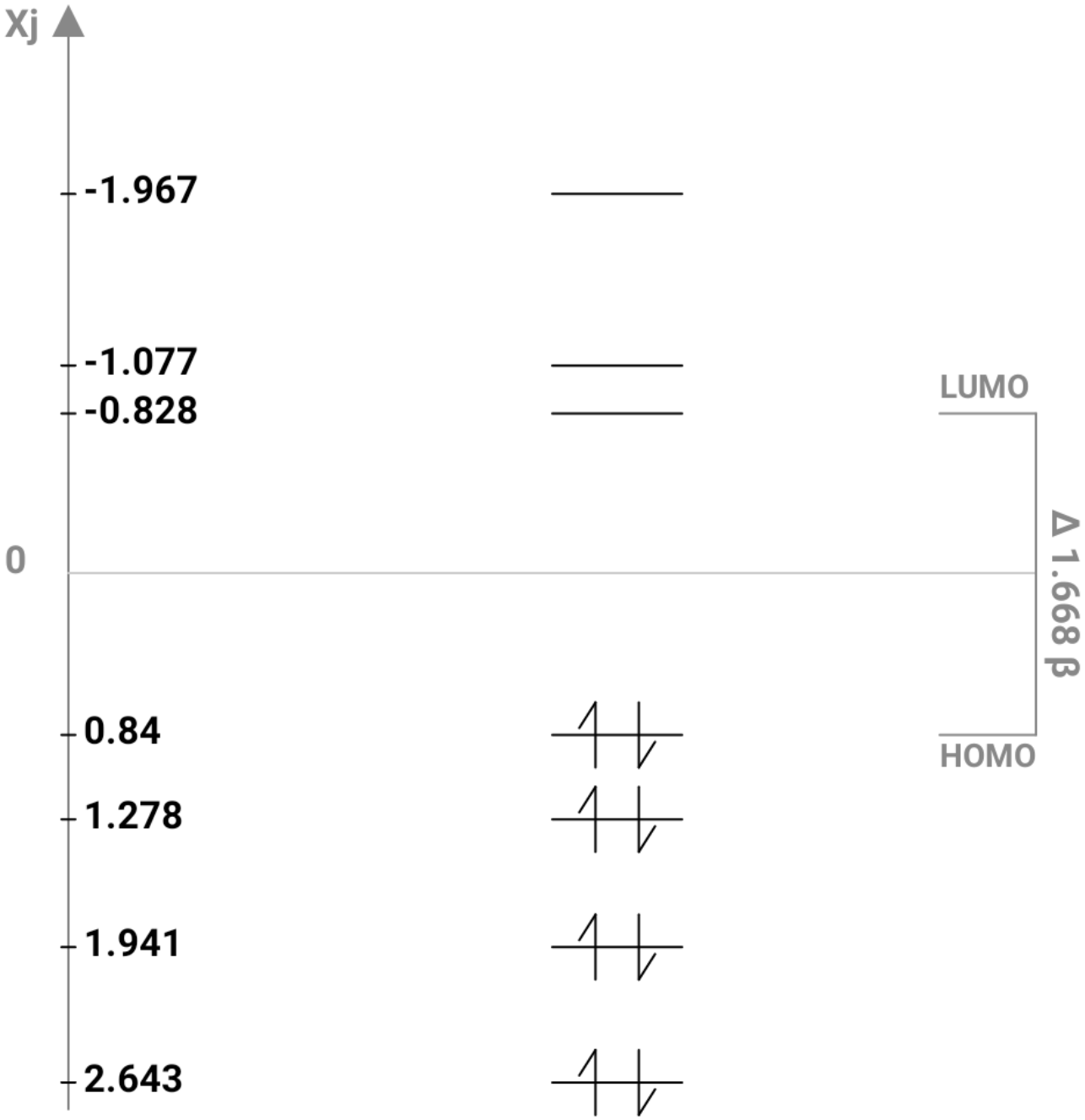


HMO-Energies

x1 = 2.643; x2 = 1.941; x3 = 1.278; x4 = 0.84; x5 = -0.828; x6 = -1.077; x7 = -1.967;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 7α + 13.404β -

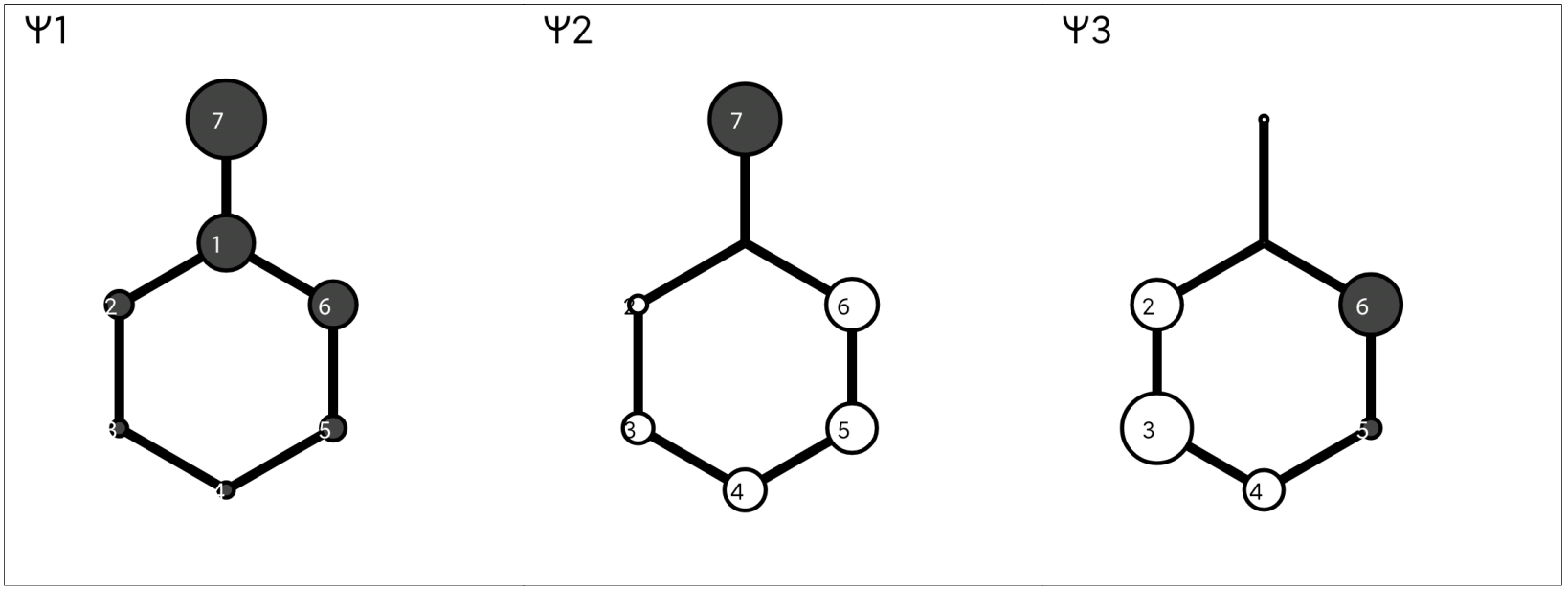
this corresponds to one πelectron: 1.676β

2. Hueckel-coefficient

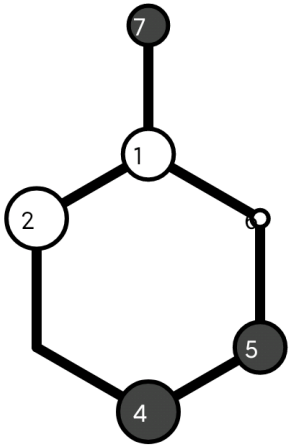
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7
	x1= 2.643	x2= 1.941	x3= 1.278	x4= 0.84	x5= -0.828	x6= -1.077	x7= -1.967
1	-0.484	0.041	-0.053	0.425	-0.271	0.561	0.438
2	-0.236	0.159	0.437	0.505	-0.359	-0.383	-0.445
3	-0.14	0.267	0.611	-0.001	0.569	-0.149	0.437
4	-0.134	0.36	0.343	-0.506	-0.112	0.543	-0.414
5	-0.215	0.431	-0.172	-0.424	-0.476	-0.436	0.377
6	-0.409	0.45	-0.531	0.141	0.477	-0.07	-0.309
7	-0.678	-0.619	0.066	-0.33	0.086	-0.164	-0.099

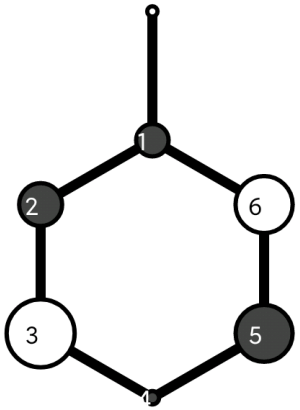
2.2. Molecule orbital presentation:



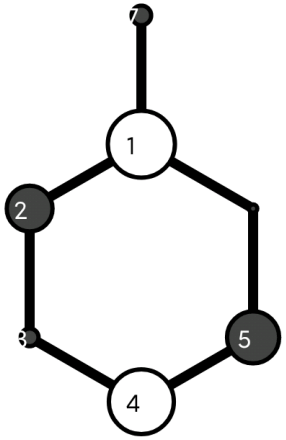
Ψ4



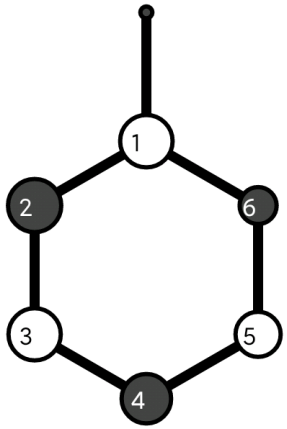
Ψ5



Ψ6



Ψ7

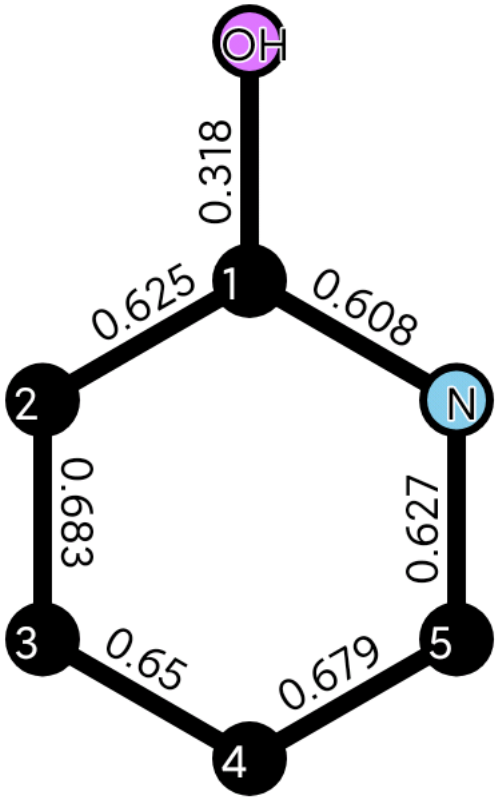


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7
1	0.839						
2	0.625	1.053					
3	0.092	0.683	0.928				
4	-0.307	-0.033	0.65	1.043			
5	-0.1	-0.34	0.082	0.679	0.883		
6	0.608	0.014	-0.294	-0.073	0.627	1.343	
7	0.318	-0.152	-0.06	0.115	0.014	-0.167	1.911

3.2. Presentation of bond order:

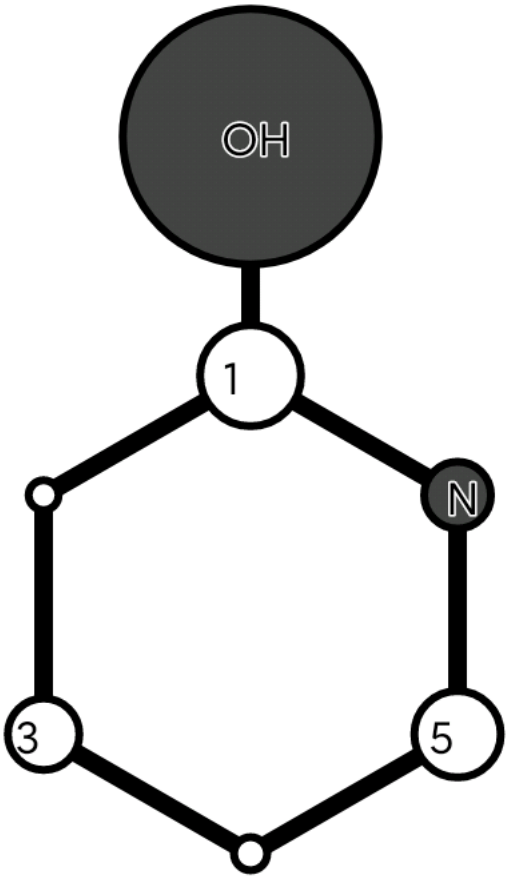


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7
1	0.304						
2		0.09					
3			0.215				
4				0.1			
5					0.26		
6						-0.201	
7							-0.769

4.2. Presentation of molecule:

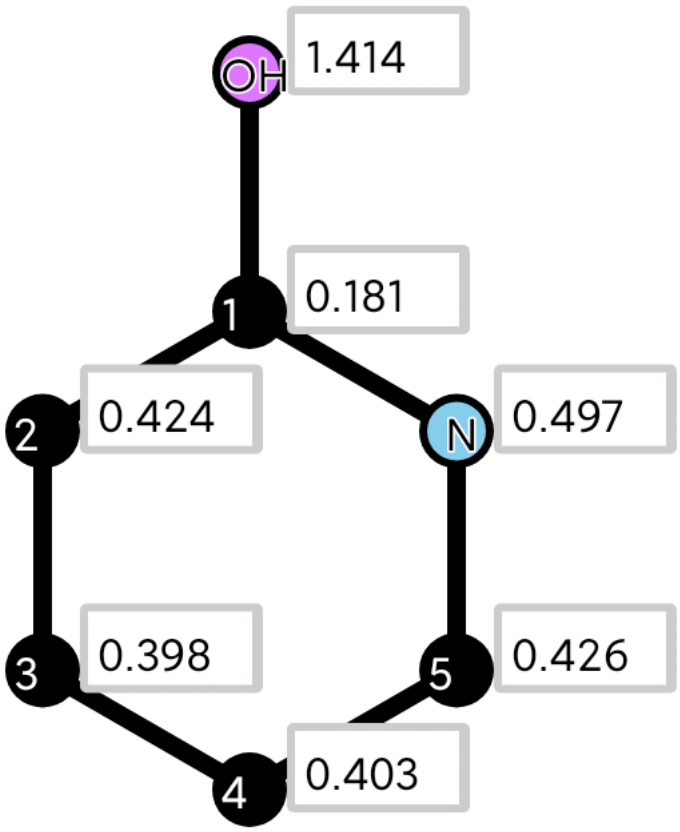


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7
0.181	0.424	0.398	0.403	0.426	0.497	1.414

5.2. Presentation of molecule:

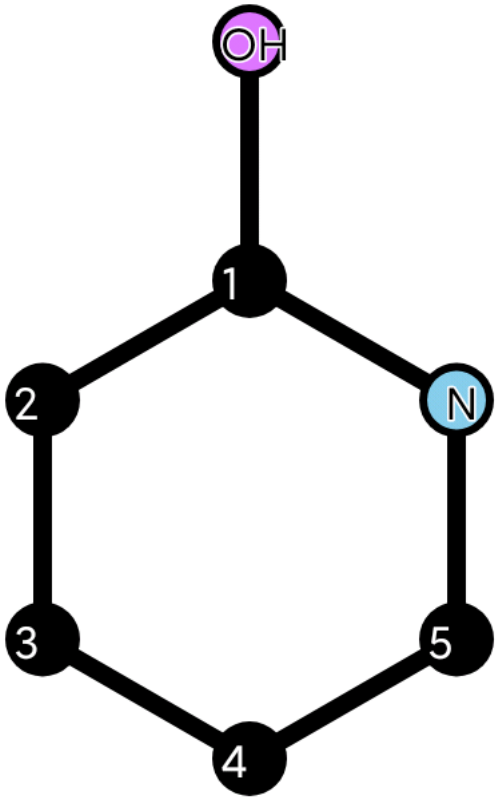


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7
1	0.342						
2	-0.131	0.411					
3	-0.002	-0.17	0.391				
4	-0.086	0.009	-0.144	0.399			
5	-0.002	-0.109	0.002	-0.168	0.395		
6	-0.116	0.004	-0.075	0.004	-0.117	0.318	
7	-0.004	-0.014	-0.002	-0.014	0.0	-0.018	0.053

6.2. Presentation of molecule:

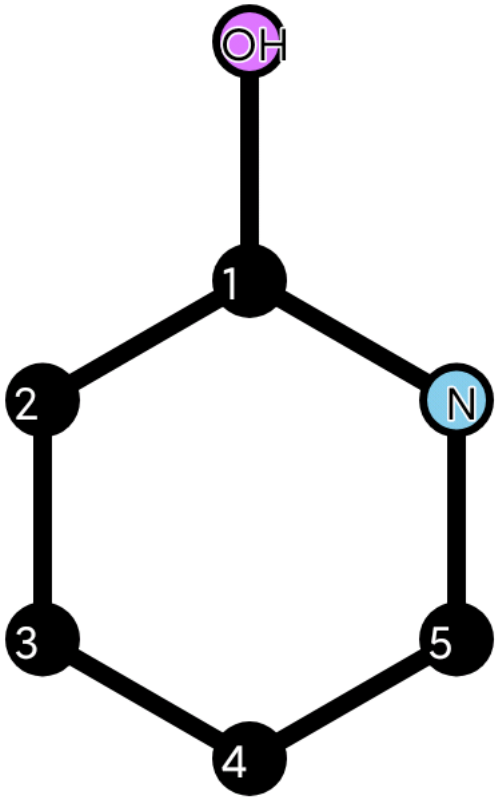


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7
1 2	0.065	0.002	-0.036	-0.013	-0.034	-0.006	0.021
1 6	0.021	-0.014	0.024	-0.018	0.04	-0.07	0.018
1 7	-0.039	0.045	0.003	0.036	0.0	0.048	-0.093
2 3	-0.038	-0.03	0.025	0.015	0.03	0.006	-0.009
3 4	0.029	0.018	0.025	-0.02	-0.038	-0.021	0.007
4 5	-0.029	-0.016	-0.03	-0.007	0.055	0.03	-0.003
5 6	0.036	0.011	0.021	0.023	-0.007	-0.087	0.003

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	0.261						
1 6	-0.161	0.25					
1 7	-0.096	-0.07	0.345				
2 3	-0.203	0.103	0.039	0.241			
3 4	0.13	-0.067	-0.03	-0.211	0.261		
4 5	-0.092	0.099	0.019	0.133	-0.211	0.241	
5 6	0.117	-0.145	-0.021	-0.087	0.126	-0.2	0.267

8.2. Presentation of molecule: