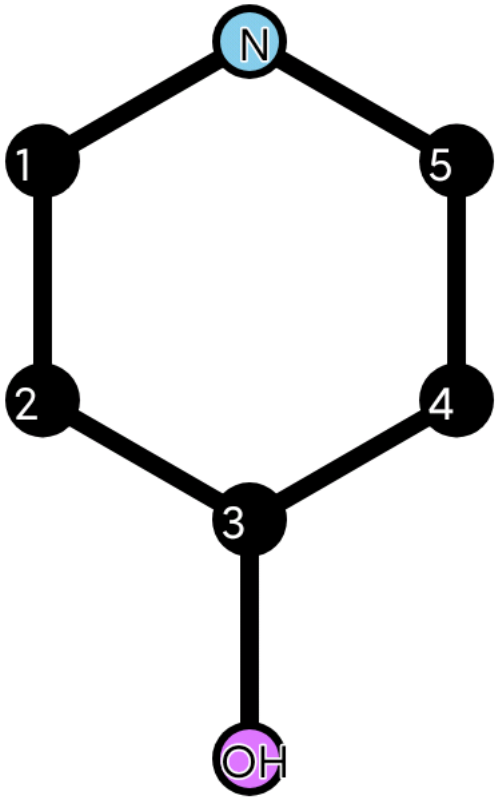
Print calculated values

Report generated by:root, 26.03.2020 - 17:39:32

The following determinant is calculated:

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

It is about this molecule:

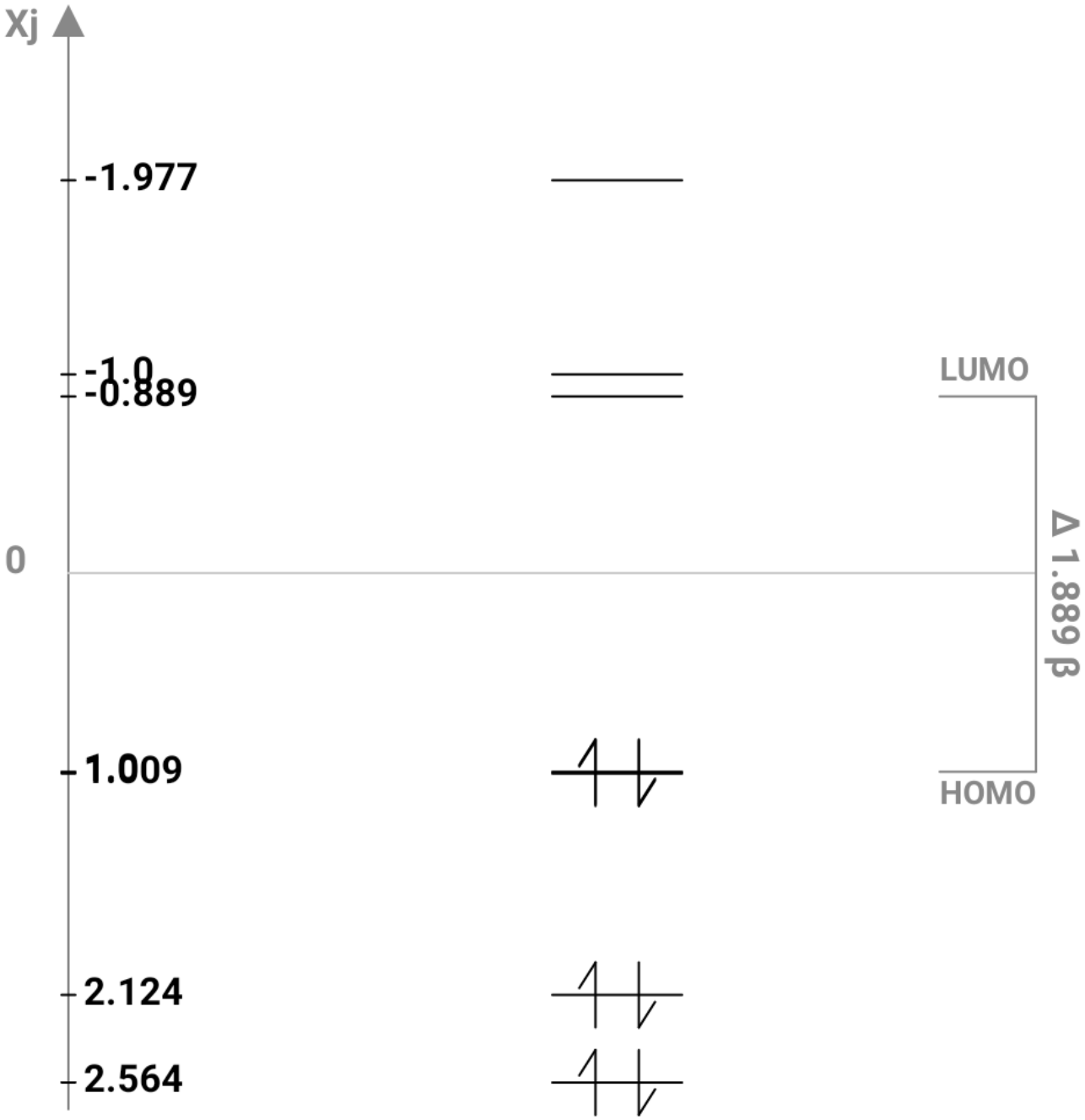


HMO-Energies

x1 = 2.564; x2 = 2.124; x3 = 1.009; x4 = 1.0; x5 = -0.889; x6 = -1.0; x7 = -1.977;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 7α + 13.394β -

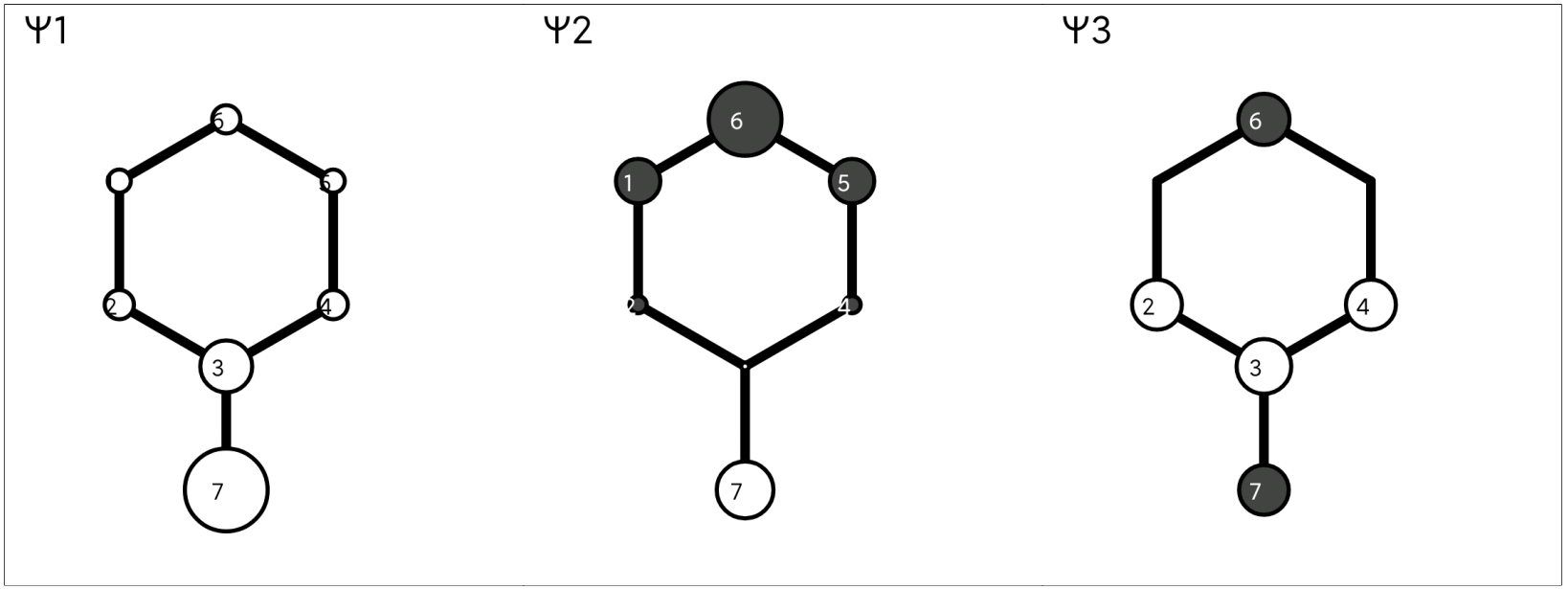
this corresponds to one πelectron: 1.674β

2. Hueckel-coefficient

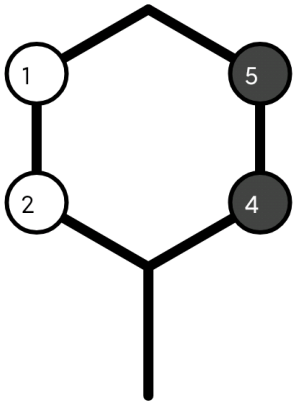
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7
	x1= 2.564	x2= 2.124	x3= 1.009	x4= 1.0	x5= -0.889	x6= -1.0	x7= -1.977
1	0.201	-0.388	-0.038	0.5	0.411	-0.5	-0.373
2	0.255	-0.15	0.436	0.5	0.171	0.5	0.439
3	0.453	0.068	0.478	0.0	-0.563	0.0	-0.495
4	0.255	-0.15	0.436	-0.5	0.171	-0.5	0.439
5	0.201	-0.388	-0.038	-0.5	0.411	0.5	-0.373
6	0.246	-0.635	-0.447	0.0	-0.506	0.0	0.282
7	0.723	0.496	-0.434	0.0	0.175	0.0	0.112

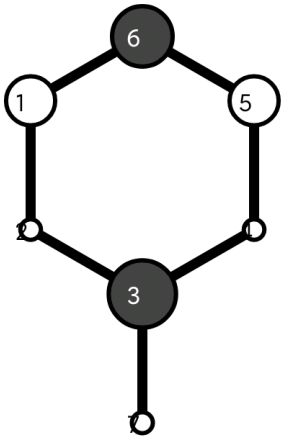
2.2. Molecule orbital presentation:



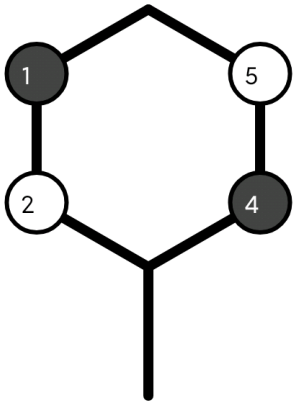
Ψ4



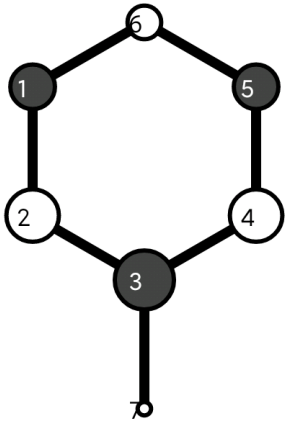
Ψ5



Ψ6



Ψ7

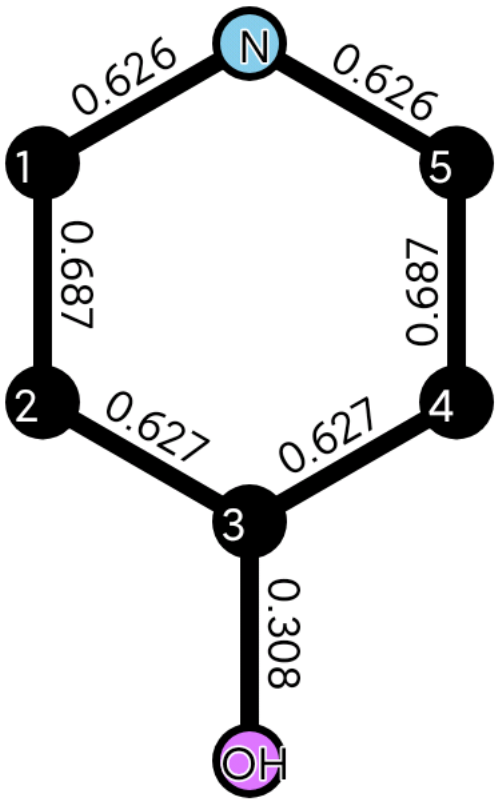


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7
1	0.885						
2	0.687	1.056					
3	0.093	0.627	0.876				
4	-0.313	0.056	0.627	1.056			
5	-0.115	-0.313	0.093	0.687	0.885		
6	0.626	-0.074	-0.291	-0.074	0.626	1.329	
7	-0.061	-0.158	0.308	-0.158	-0.061	0.115	1.913

3.2. Presentation of bond order:

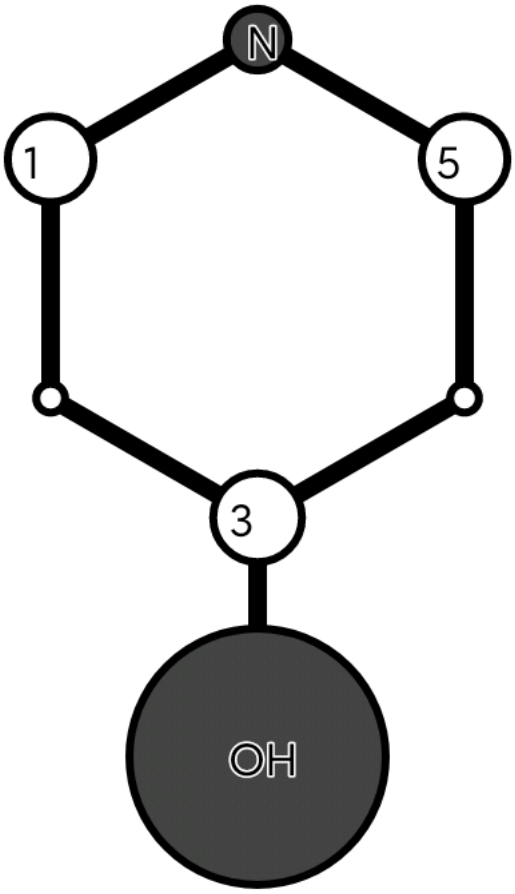


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7
1	0.258						
2		0.087					
3			0.267				
4				0.087			
5					0.258		
6						-0.186	
7							-0.771

4.2. Presentation of molecule:

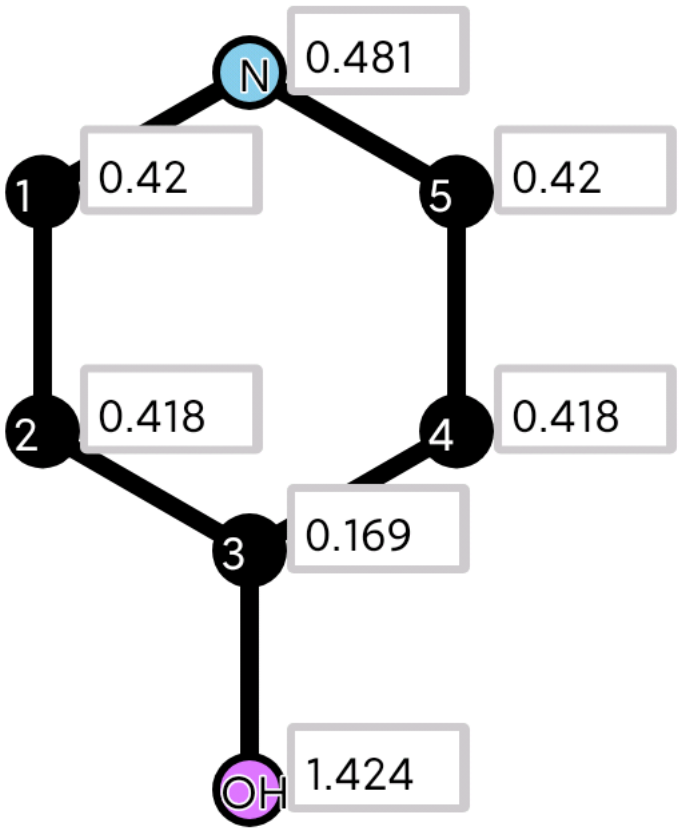


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7
0.42	0.418	0.169	0.418	0.42	0.481	1.424

5.2. Presentation of molecule:

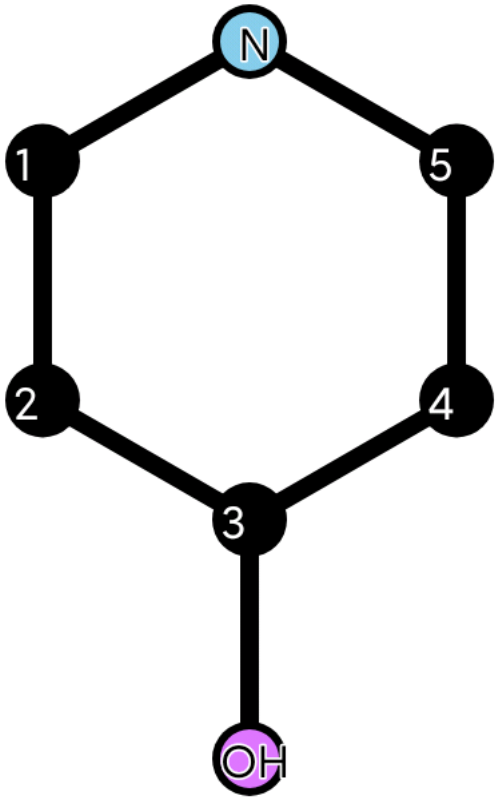


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7
1	0.389						
2	-0.174	0.405					
3	-0.002	-0.135	0.35				
4	-0.088	0.004	-0.135	0.405			
5	-0.003	-0.088	-0.002	-0.174	0.389		
6	-0.12	0.004	-0.076	0.004	-0.12	0.32	
7	-0.002	-0.017	-0.001	-0.017	-0.002	-0.014	0.053

6.2. Presentation of molecule:

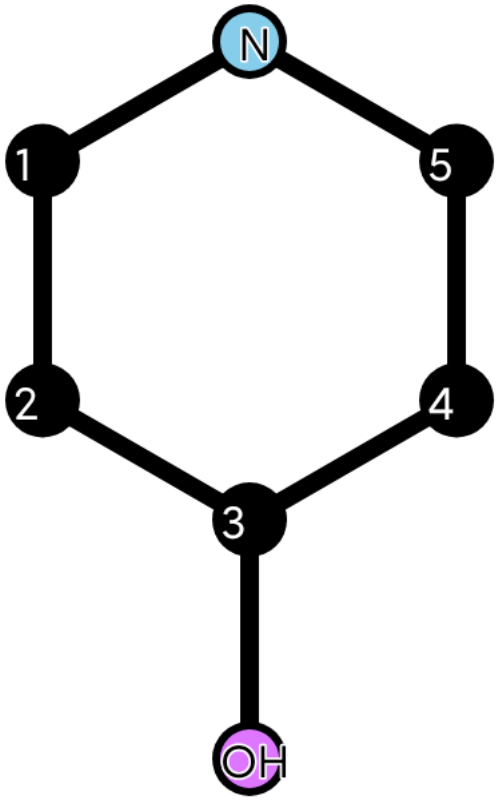


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7
1 2	0.049	-0.017	-0.035	0.016	-0.034	0.029	-0.009
1 6	-0.001	0.025	0.025	-0.02	0.043	-0.078	0.007
2 3	-0.04	-0.012	0.046	-0.021	0.028	-0.02	0.019
3 4	0.028	-0.021	0.046	-0.012	-0.04	-0.02	0.019
3 7	0.003	0.049	-0.046	0.049	0.003	0.034	-0.092
4 5	-0.034	0.016	-0.035	-0.017	0.049	0.029	-0.009
5 6	0.043	-0.02	0.025	0.025	-0.001	-0.078	0.007

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	0.237						
1 6	-0.2	0.26					
2 3	-0.203	0.126	0.256				
3 4	0.106	-0.068	-0.167	0.256			
3 7	0.038	-0.027	-0.084	-0.084	0.34		
4 5	-0.074	0.1	0.106	-0.203	0.038	0.237	
5 6	0.1	-0.148	-0.068	0.126	-0.027	-0.2	0.26

8.2. Presentation of molecule: