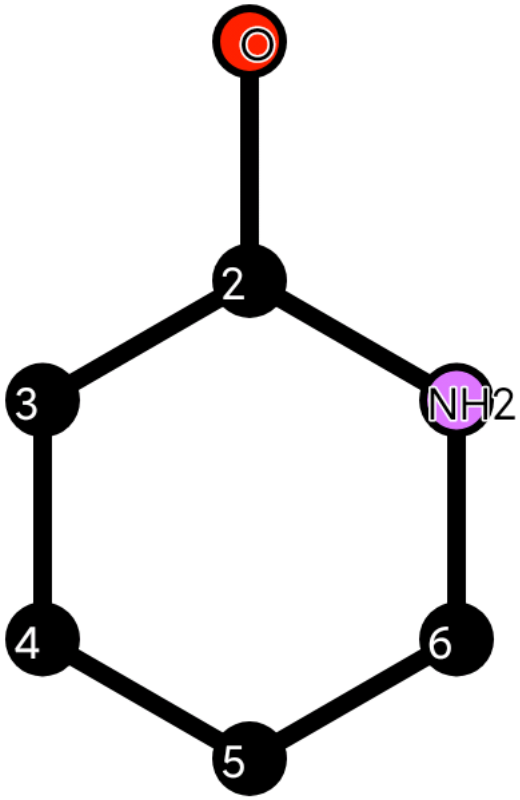
Print calculated values

Report generated by:root, 20.01.2020 - 12:39:01

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	0.0	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
0.0	0.0	0.0	1.0	-x	1.0	0.0
0.0	0.0	0.0	0.0	1.0	-x	1.3
0.0	1.3	0.0	0.0	0.0	1.3	-x+1.47

It is about this molecule:

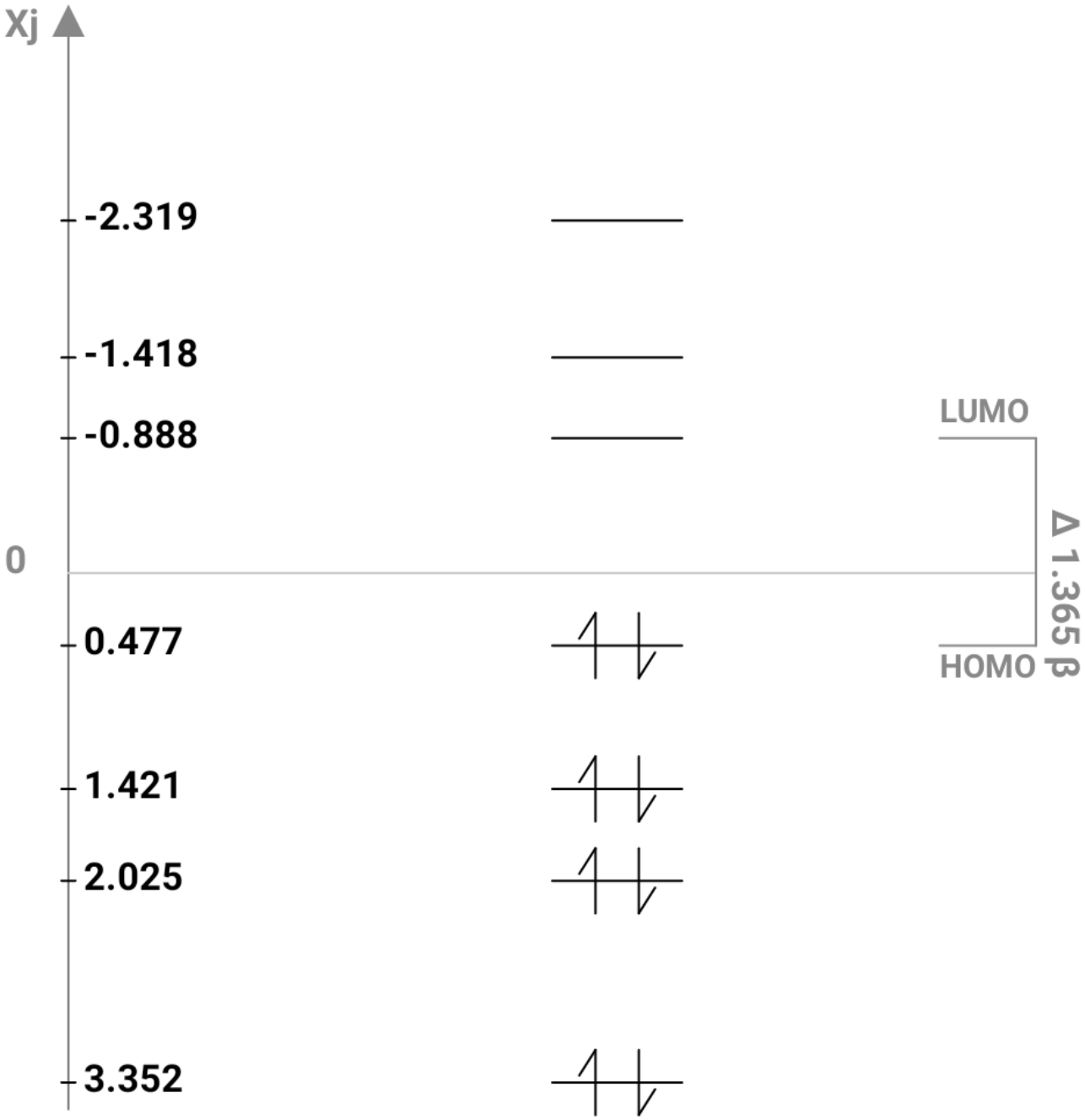


HMO-Energies

x1 = 3.352; x2 = 2.025; x3 = 1.421; x4 = 0.477; x5 = -0.888; x6 = -1.418; x7 = -2.319;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 7α + 14.55β -

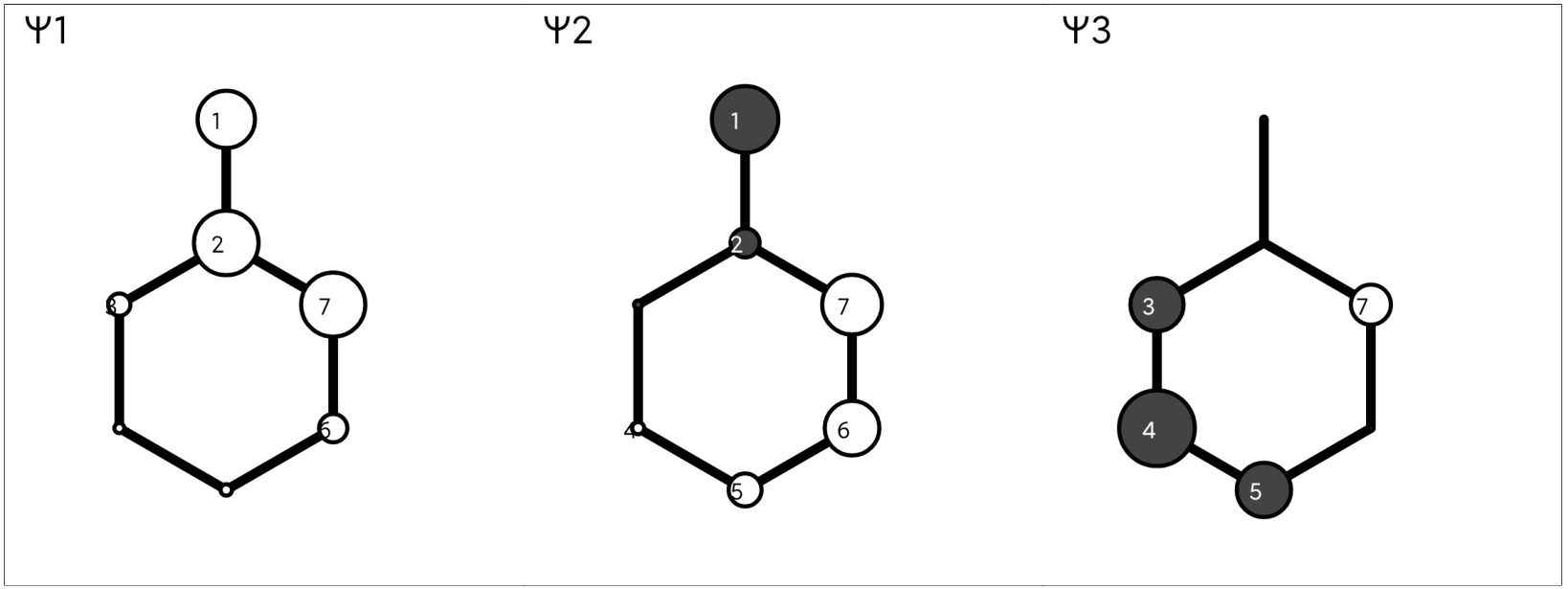
this corresponds to one πelectron: 1.819β

2. Hueckel-coefficient

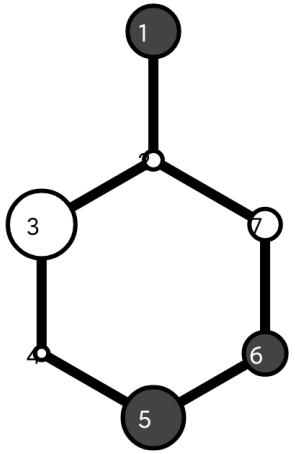
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7
	x1= 3.352	x2= 2.025	x3= 1.421	x4= 0.477	x5= -0.888	x6= -1.418	x7= -2.319
1	0.501	-0.58	0.005	-0.431	0.062	-0.313	0.354
2	0.564	-0.254	0.001	0.157	-0.066	0.421	-0.641
3	0.194	-0.073	-0.464	0.565	-0.516	0.004	0.394
4	0.088	0.106	-0.661	0.113	0.525	-0.427	-0.272
5	0.1	0.288	-0.475	-0.511	0.05	0.601	0.238
6	0.247	0.477	-0.014	-0.357	-0.569	-0.426	-0.28
7	0.56	0.522	0.35	0.262	0.351	0.002	0.316

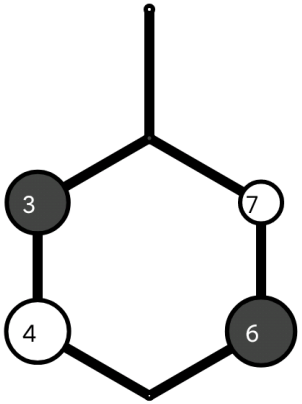
2.2. Molecule orbital presentation:



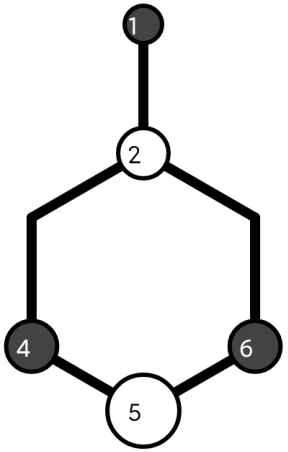
Ψ4



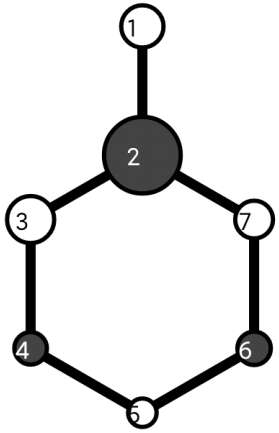
Ψ5



Ψ6



Ψ7

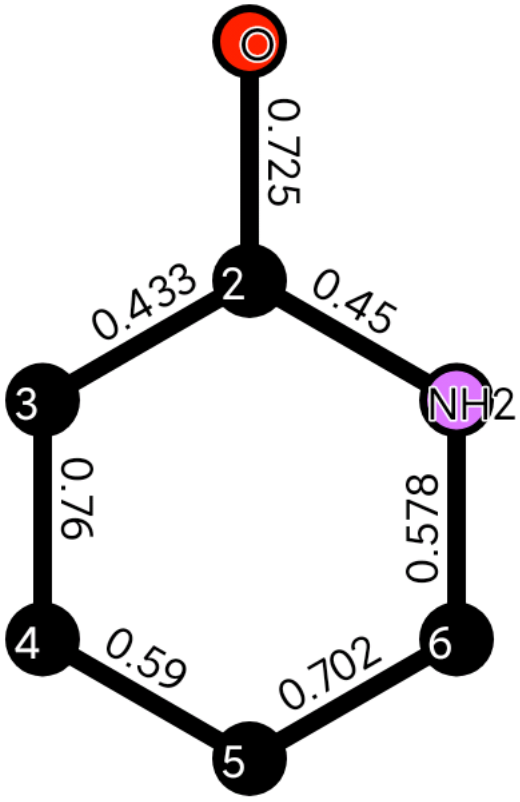


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7
1	1.547						
2	0.725	0.814					
3	-0.212	0.433	1.157				
4	-0.139	0.08	0.76	0.936			
5	0.202	-0.194	-0.14	0.59	1.159		
6	0.002	-0.076	-0.364	0.082	0.702	0.832	
7	-0.265	0.45	0.113	-0.194	-0.188	0.578	1.555

3.2. Presentation of bond order:

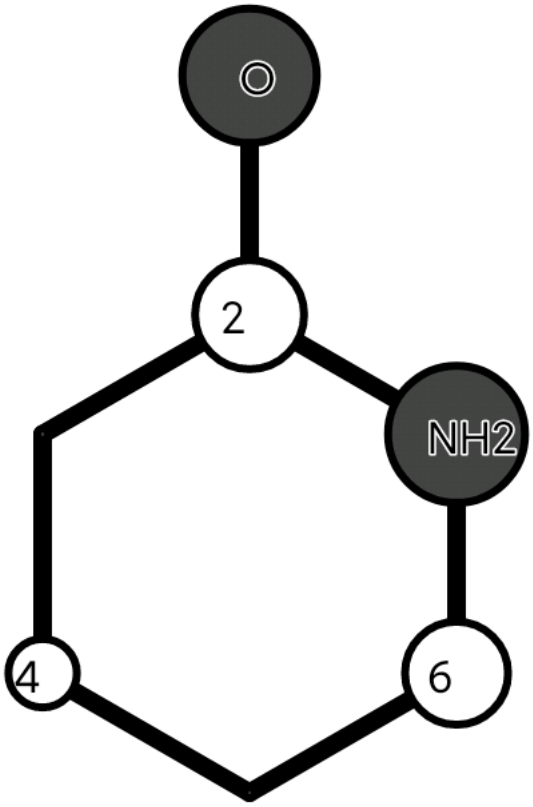


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7
1	-0.404						
2		0.328					
3			-0.014				
4				0.206			
5					-0.016		
6						0.31	
7							-0.412

4.2. Presentation of molecule:

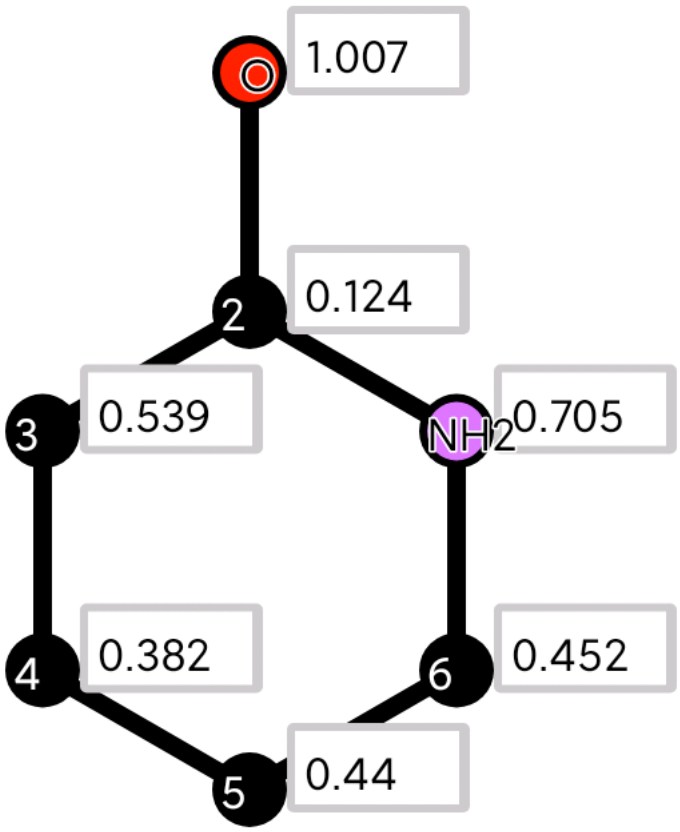


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7
1.007	0.124	0.539	0.382	0.44	0.452	0.705

5.2. Presentation of molecule:

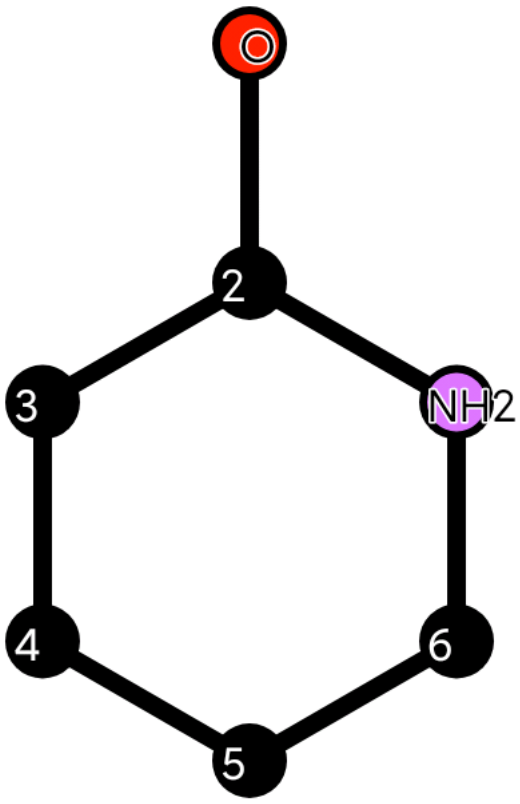


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7
1	0.196						
2	-0.09	0.203					
3	-0.015	-0.042	0.472				
4	-0.016	-0.004	-0.243	0.382			
5	-0.04	-0.03	-0.006	-0.1	0.395		
6	0.002	0.001	-0.14	0.006	-0.196	0.381	
7	-0.037	-0.038	-0.027	-0.025	-0.022	-0.055	0.203

6.2. Presentation of molecule:

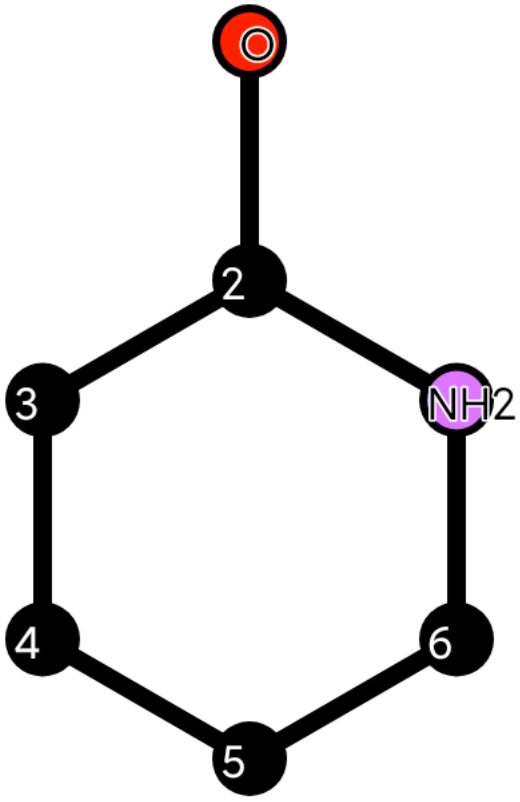


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7
1 2	-0.125	0.01	0.03	0.01	0.037	-0.003	0.041
2 3	0.066	0.041	0.002	-0.037	-0.027	-0.023	-0.022
2 7	0.068	0.013	-0.028	0.011	-0.03	0.026	-0.061
3 4	-0.027	-0.018	-0.093	0.03	0.048	0.036	0.025
4 5	0.028	0.014	0.086	0.012	-0.057	-0.046	-0.037
5 6	-0.005	-0.01	-0.066	-0.021	-0.05	0.091	0.06
6 7	0.002	0.013	0.061	0.008	0.073	-0.037	-0.119

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	2 3	2 7	3 4	4 5	5 6	6 7
1 2	0.195						
2 3	-0.142	0.285					
2 7	-0.118	-0.036	0.233				
3 4	0.05	-0.147	0.026	0.21			
4 5	-0.043	0.106	-0.011	-0.237	0.325		
5 6	0.015	-0.064	0.041	0.138	-0.214	0.246	
6 7	-0.013	0.072	-0.066	-0.076	0.108	-0.208	0.297

8.2. Presentation of molecule: