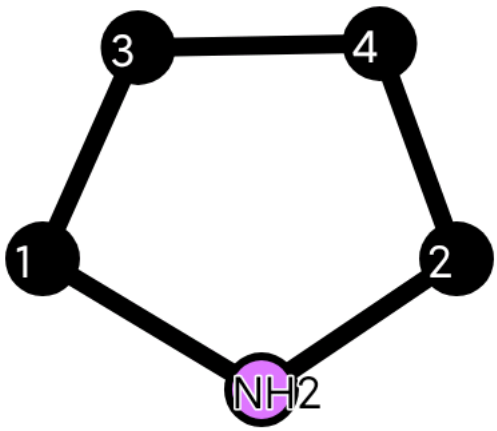
Print calculated values

Report generated by:root, 16.02.2020 - 18:00:28

The following determinant is calculated:

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

It is about this molecule:

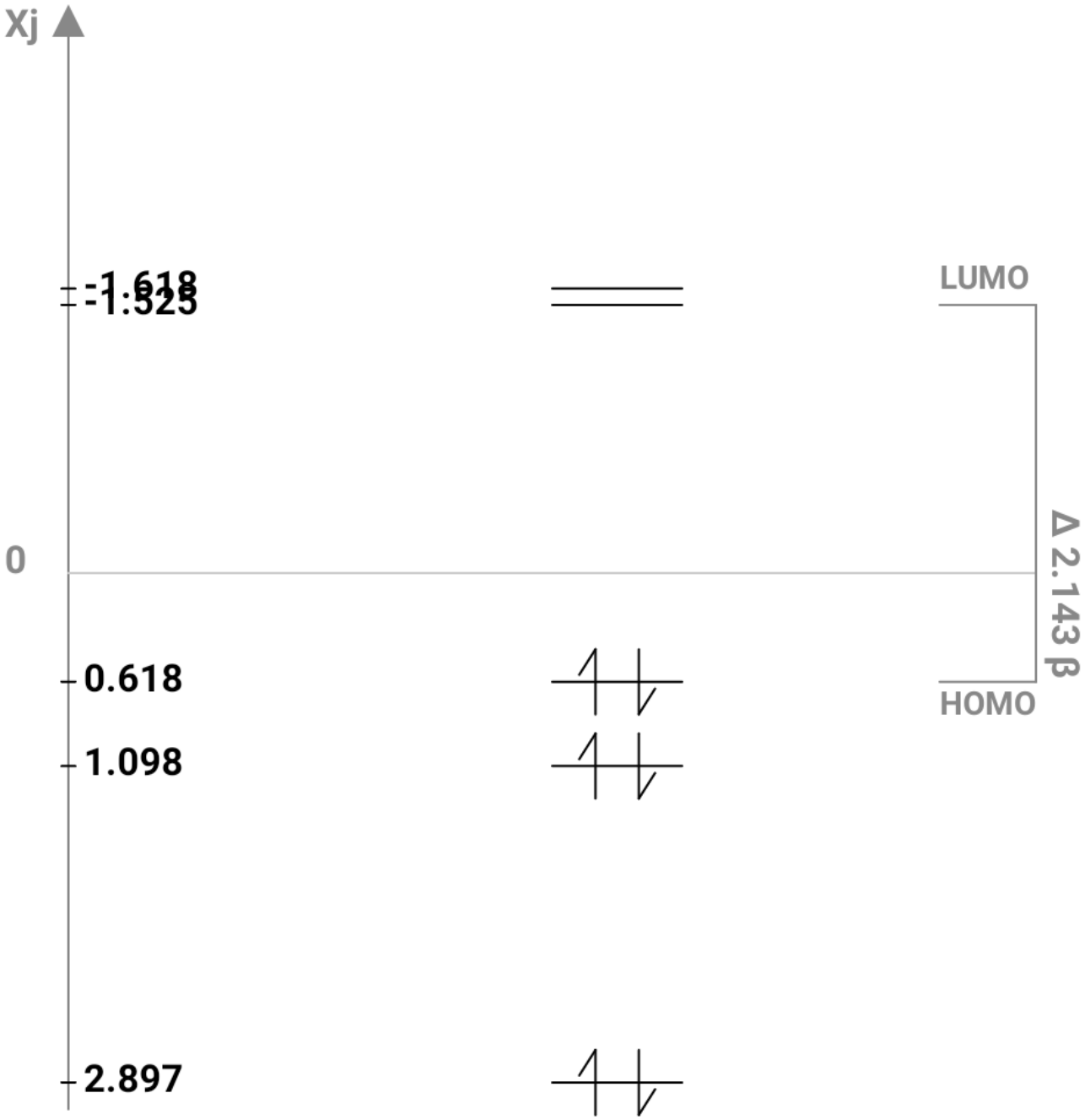


HMO-Energies

x1 = 2.897; x2 = 1.098; x3 = 0.618; x4 = -1.525; x5 = -1.618;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 5α + 9.226β -

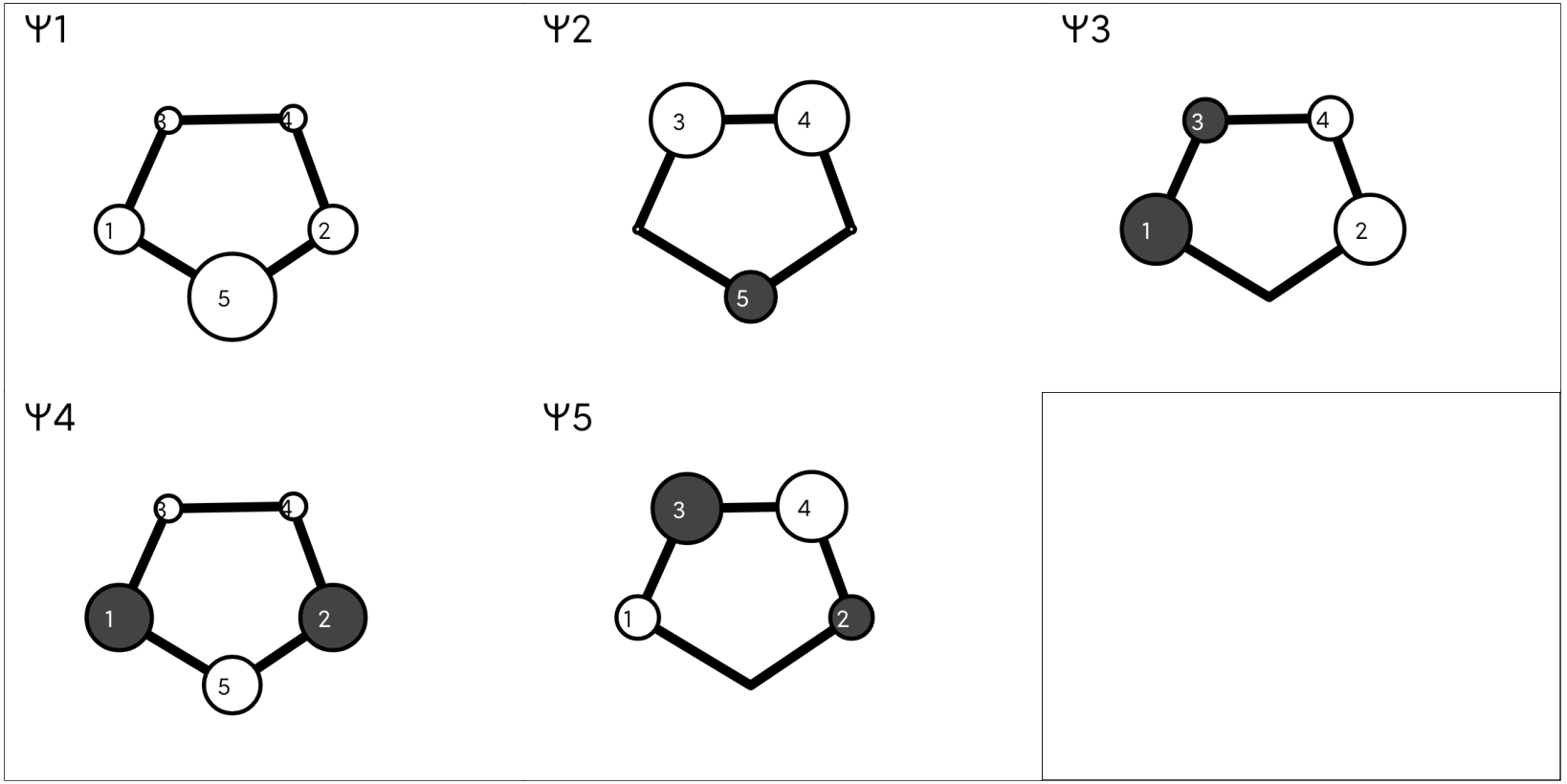
this corresponds to one πelectron: 1.538β

2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5
	x1= 2.897	**x2= 1.098**	**x3= 0.618**	**x4= -1.525**	**x5= -1.618**
1	0.412	0.062	-0.602	-0.571	0.372
2	0.412	0.062	0.602	-0.571	-0.372
3	0.217	0.634	-0.372	0.226	-0.602
4	0.217	0.634	0.372	0.226	0.602
5	0.752	-0.435	0.0	0.496	0.0

2.2. Molecule orbital presentation:

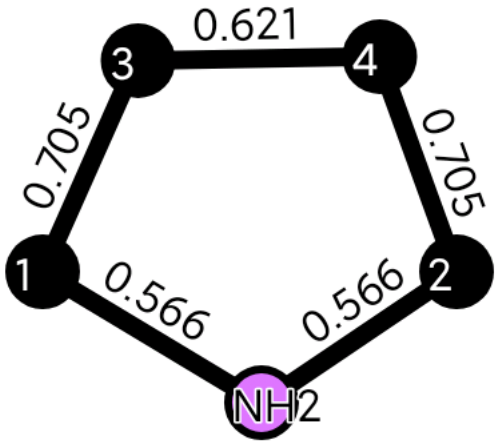


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5
1	1.072				
2	-0.376	1.072			
3	0.705	-0.189	1.174		
4	-0.189	0.705	0.621	1.174	
5	0.566	0.566	-0.224	-0.224	1.509

3.2. Presentation of bond order:

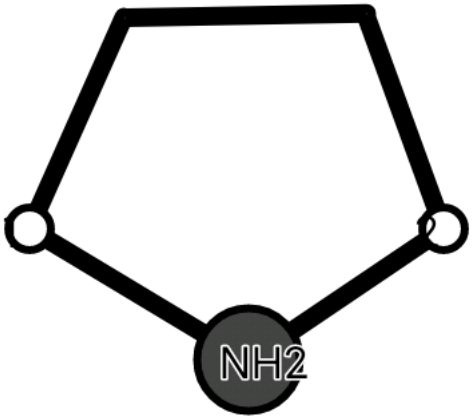


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5
1	0.128				
2		0.128			
3			0.026		
4				0.026	
5					-0.309

4.2. Presentation of molecule:

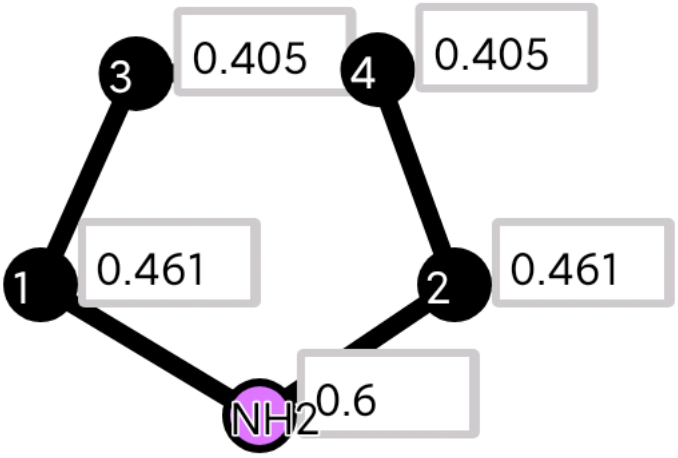


5. Free valences

5.1. Calculated values:

1	2	3	4	5
0.461	0.461	0.405	0.405	0.6

5.2. Presentation of molecule:

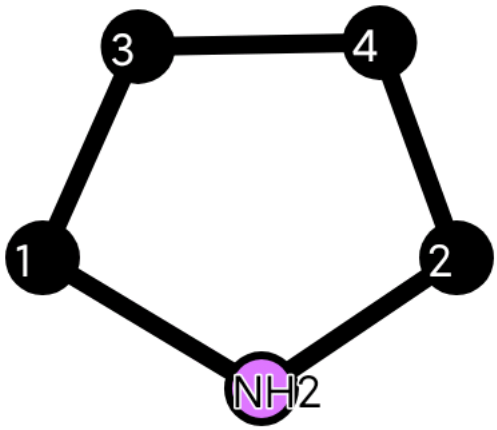


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5
1	0.383				
2	-0.1	0.383			
3	-0.192	-0.023	0.365		
4	-0.023	-0.192	-0.119	0.365	
5	-0.068	-0.068	-0.031	-0.031	0.196

6.2. Presentation of molecule:

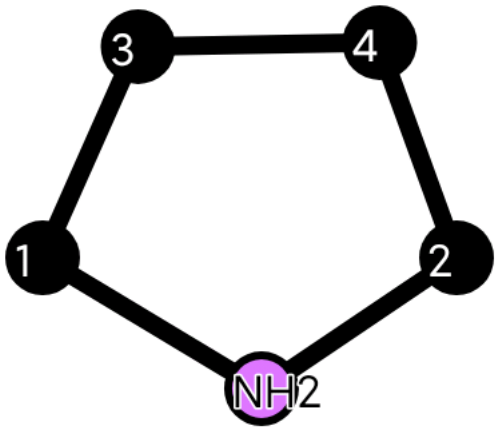


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5
1 3	-0.016	-0.048	-0.046	0.058	0.052
1 5	-0.063	0.096	0.078	-0.027	-0.084
2 4	-0.048	-0.016	0.058	-0.046	0.052
2 5	0.096	-0.063	-0.027	0.078	-0.084
3 4	0.071	0.071	-0.056	-0.056	-0.031

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 3	1 5	2 4	2 5	3 4
1 3	0.184				
1 5	-0.136	0.219			
2 4	0.091	-0.005	0.184		
2 5	-0.005	-0.055	-0.136	0.219	
3 4	-0.167	0.051	-0.167	0.051	0.246

8.2. Presentation of molecule: