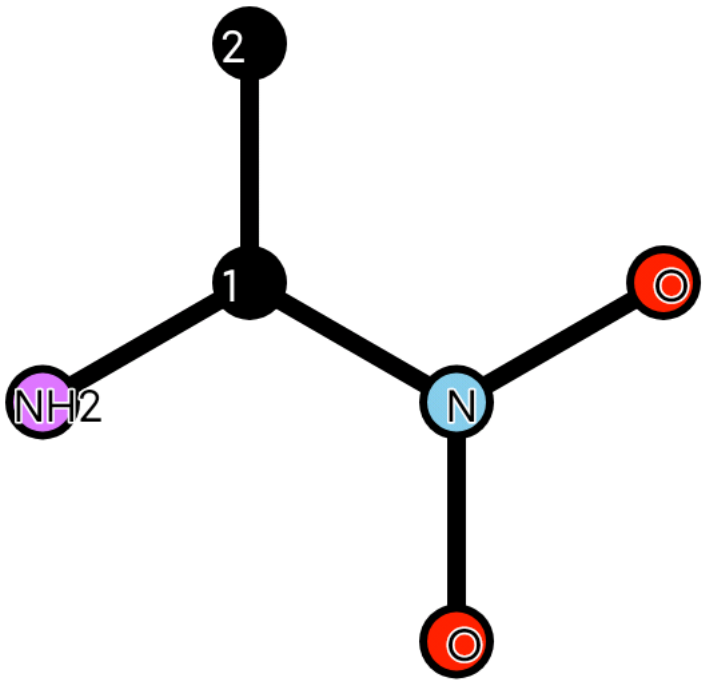
Print calculated values

Report generated by:root, 22.02.2020 - 23:21:19

The following determinant is calculated:

-x	1.0	1.3	1.3	0.0	0.0
1.0	-x	0.0	0.0	0.0	0.0
1.3	0.0	-x+1.47	0.0	0.0	0.0
1.3	0.0	0.0	-x+1.47	1.95	1.95
0.0	0.0	0.0	1.95	-x+1.18	0.0
0.0	0.0	0.0	1.95	0.0	-x+1.18

It is about this molecule:

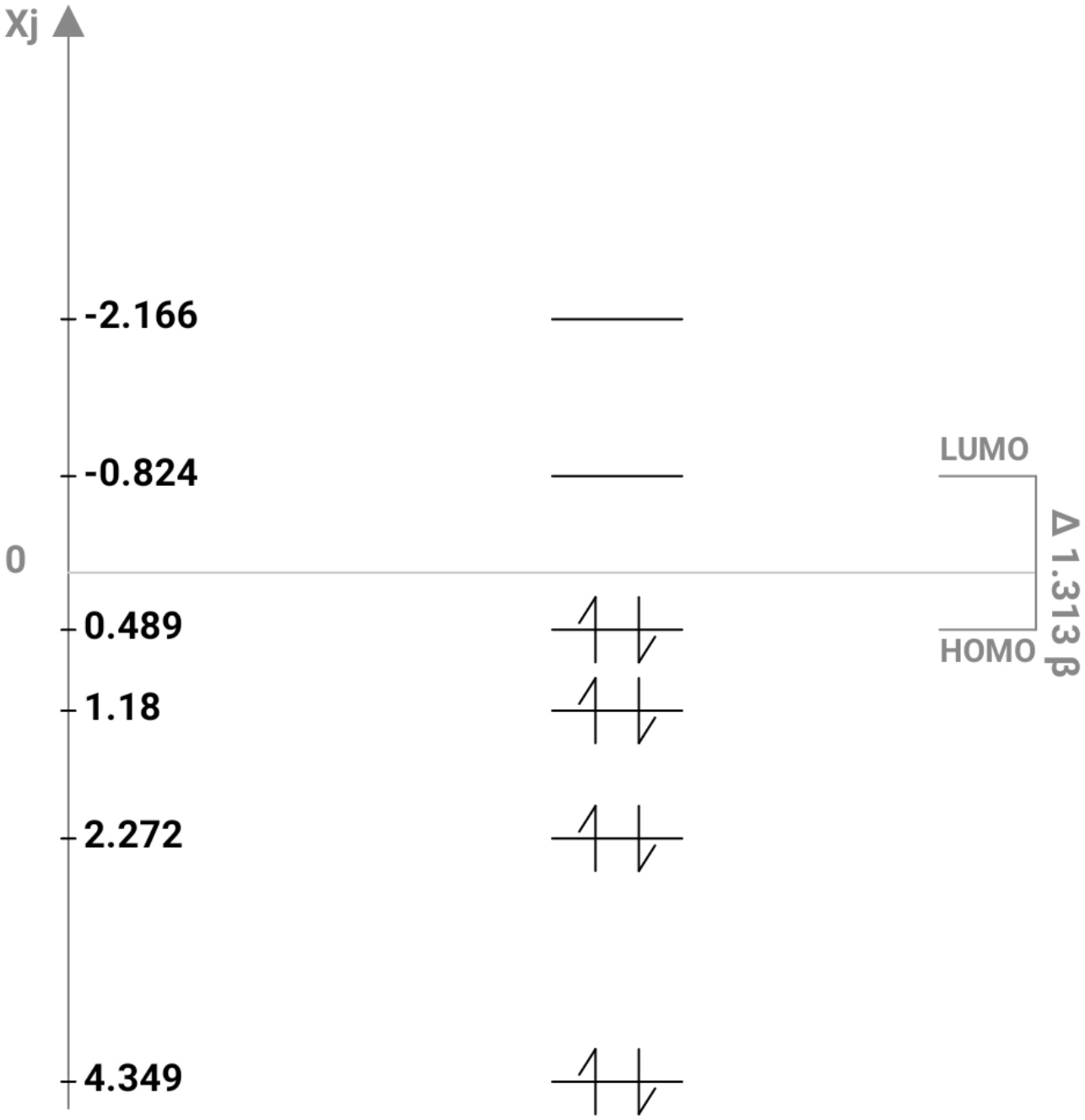


HMO-Energies

x1 = 4.349; x2 = 2.272; x3 = 1.18; x4 = 0.489; x5 = -0.824; x6 = -2.166;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 6α + 16.58β -

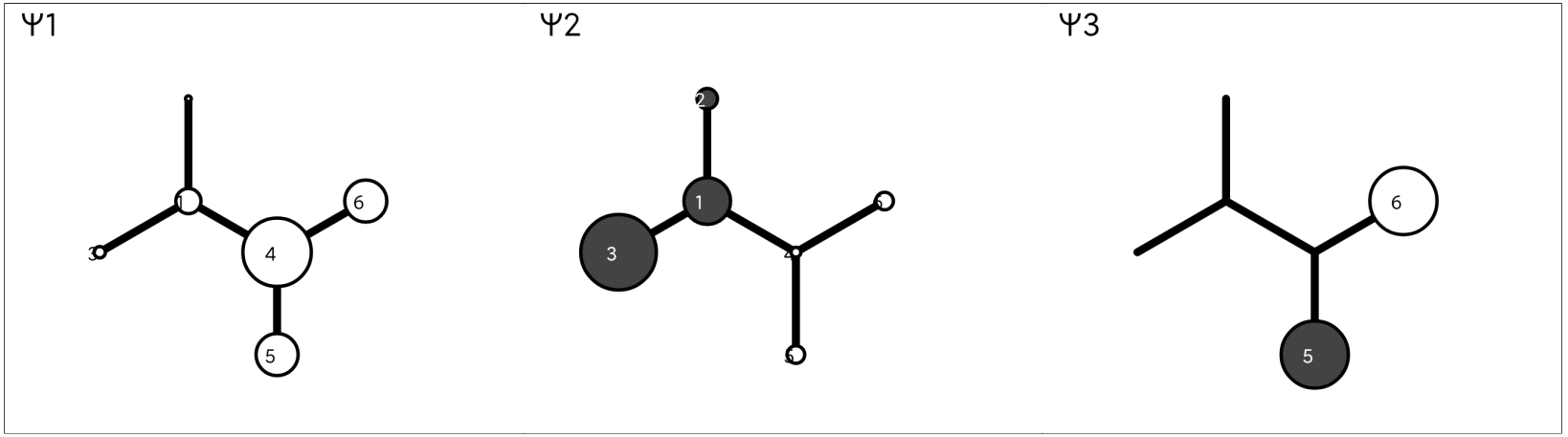
this corresponds to one πelectron: 2.073β

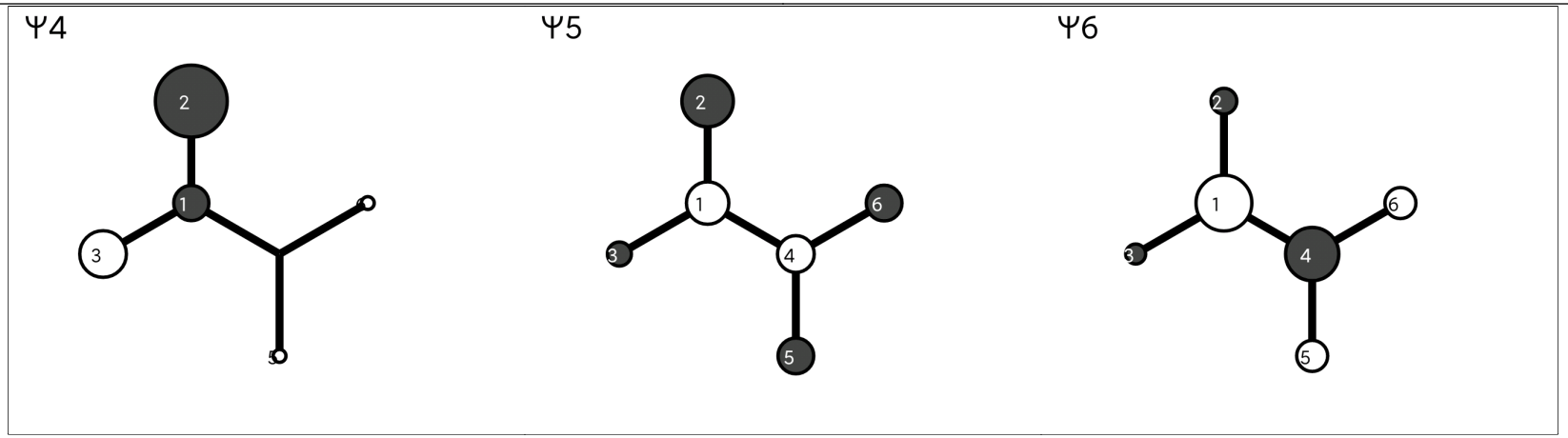
2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6
	x1= 4.349	x2= 2.272	x3= 1.18	x4= 0.489	x5= -0.824	x6= -2.166
1	0.265	-0.491	0.0	-0.372	0.449	0.59
2	0.061	-0.216	0.0	-0.761	-0.545	-0.273
3	0.12	-0.796	0.0	0.493	-0.254	-0.211
4	0.72	0.104	0.0	-0.048	0.389	-0.563
5	0.443	0.185	-0.707	0.136	-0.378	0.328
6	0.443	0.185	0.707	0.136	-0.378	0.328

2.2. Molecule orbital presentation:



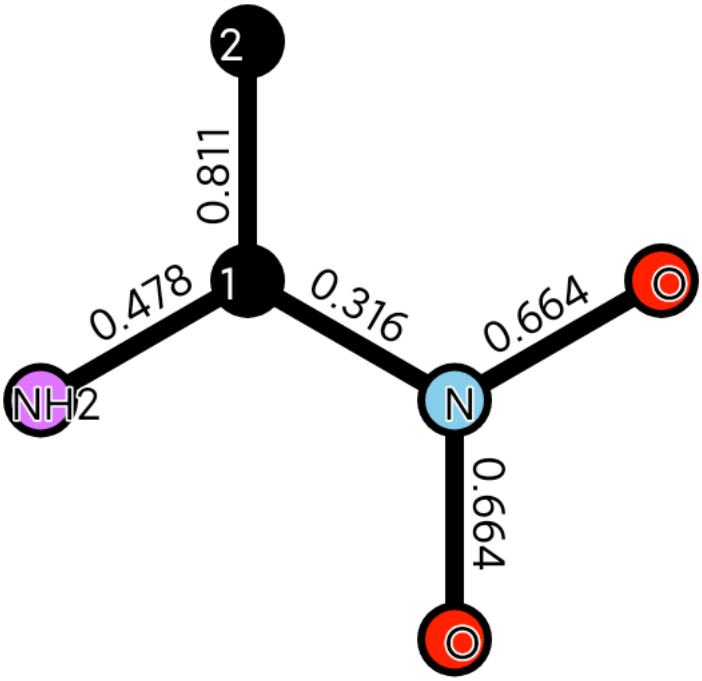

Ψ4
2
1
3
Ψ5
2
1
6
3
4
5
Ψ6
2
1
6
3
4
5

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6
1	0.9					
2	0.811	1.258				
3	0.478	-0.392	1.782			
4	0.316	0.116	-0.04	1.064		
5	-0.048	-0.233	-0.054	0.664	1.498	
6	-0.048	-0.233	-0.054	0.664	-0.502	1.498

3.2. Presentation of bond order:

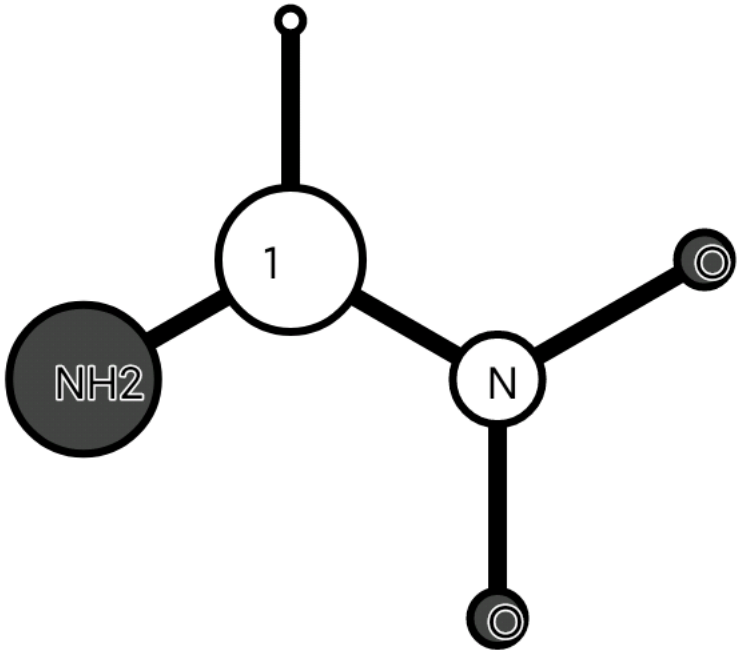


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6
1	0.434					
2		0.075				
3			-0.448			
4				0.27		
5					-0.165	
6						-0.165

4.2. Presentation of molecule:

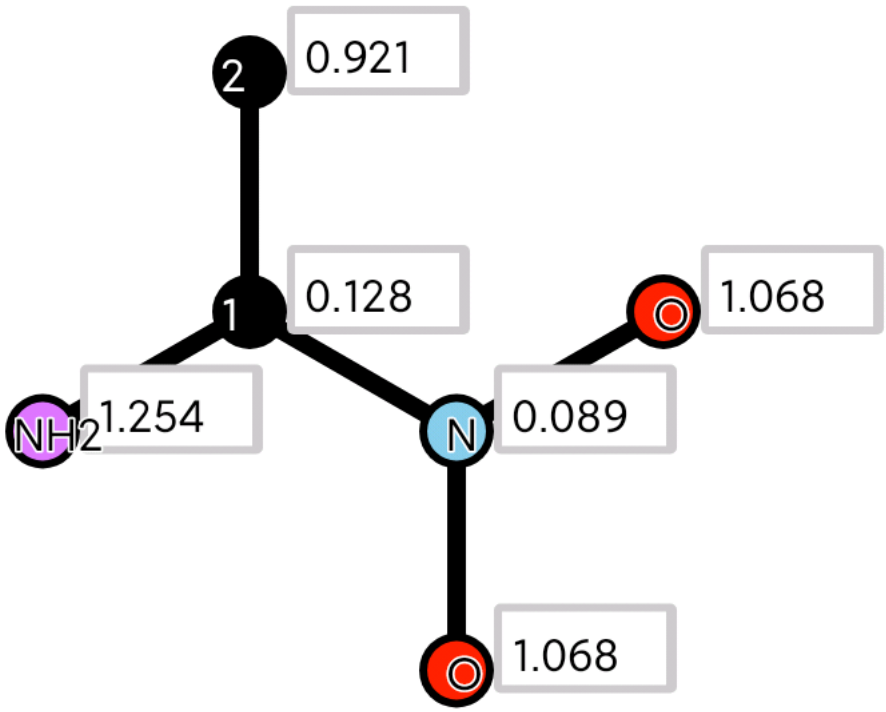


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6
0.128	0.921	1.254	0.089	1.068	1.068

5.2. Presentation of molecule:

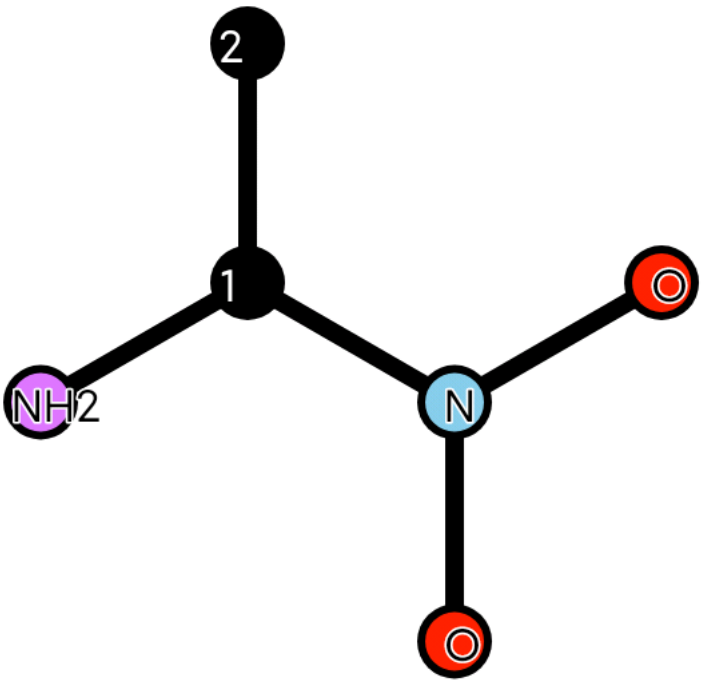


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6
1	0.322					
2	-0.333	0.61				
3	-0.008	-0.15	0.144			
4	-0.009	-0.015	0.004	0.169		
5	0.014	-0.056	0.005	-0.075	0.263	
6	0.014	-0.056	0.005	-0.075	-0.152	0.263

6.2. Presentation of molecule:

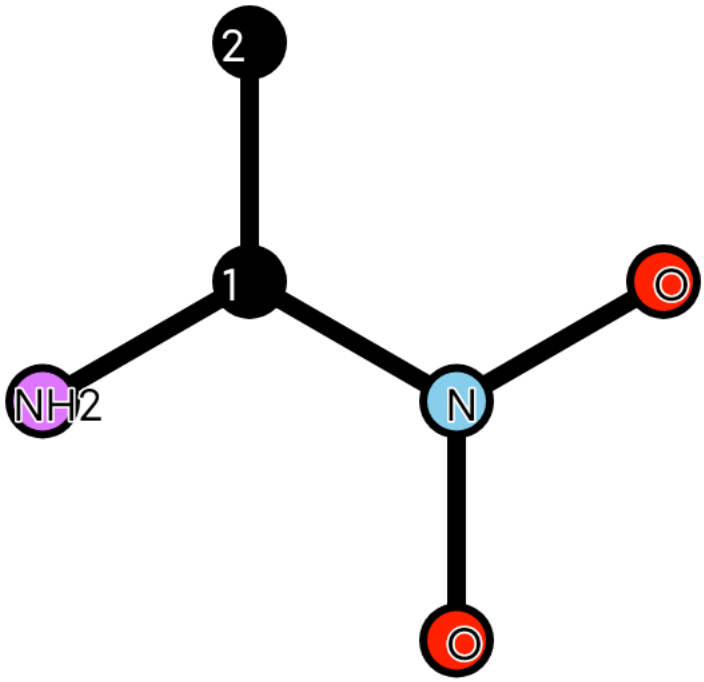


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6
1 2	0.061	-0.127	0.078	-0.007	-0.002	-0.002
1 3	-0.061	0.23	-0.147	-0.001	-0.01	-0.01
1 4	0.022	-0.086	0.017	0.008	0.02	0.02
4 5	-0.004	0.032	-0.006	-0.01	-0.135	0.122
4 6	-0.004	0.032	-0.006	-0.01	0.122	-0.135

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3	1 4	4 5	4 6
1 2	0.145				
1 3	-0.19	0.351			
1 4	-0.05	-0.065	0.225		
4 5	0.017	0.016	-0.062	0.191	
4 6	0.017	0.016	-0.062	-0.149	0.191

8.2. Presentation of molecule: