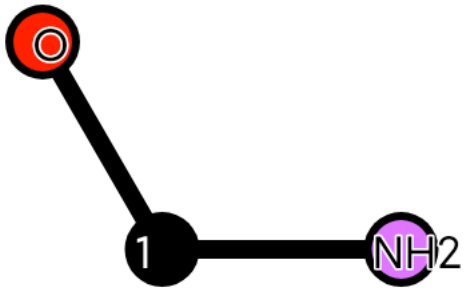
Print calculated values

Report generated by:root, 17.02.2020 - 10:02:27

The following determinant is calculated:

-x	1.93	1.3
1.93	-x+1.18	0.0
1.3	0.0	-x+1.47

It is about this molecule:

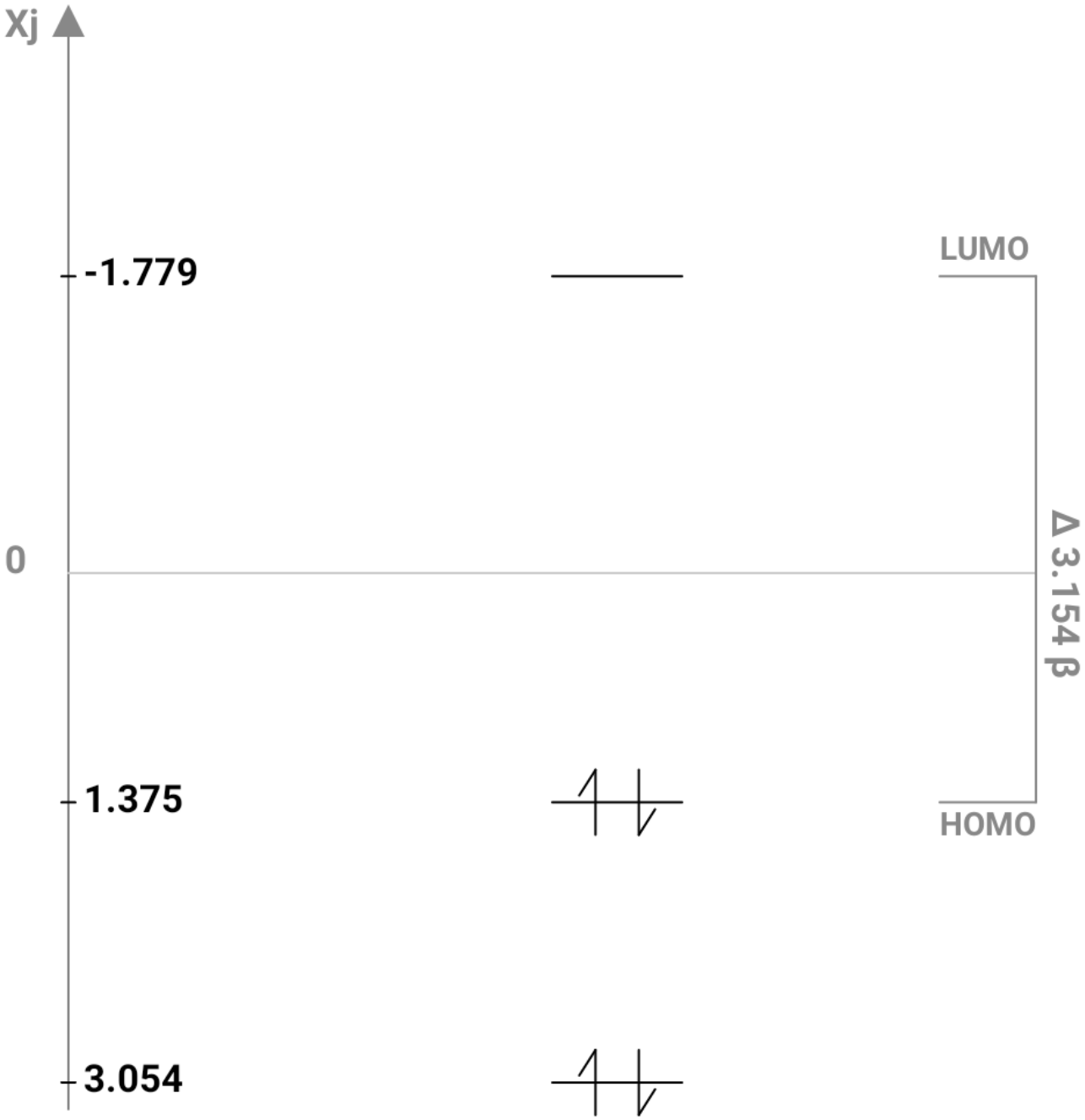


HMO-Energies

x1 = 3.054; x2 = 1.375; x3 = -1.779;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 3α + 8.858β -

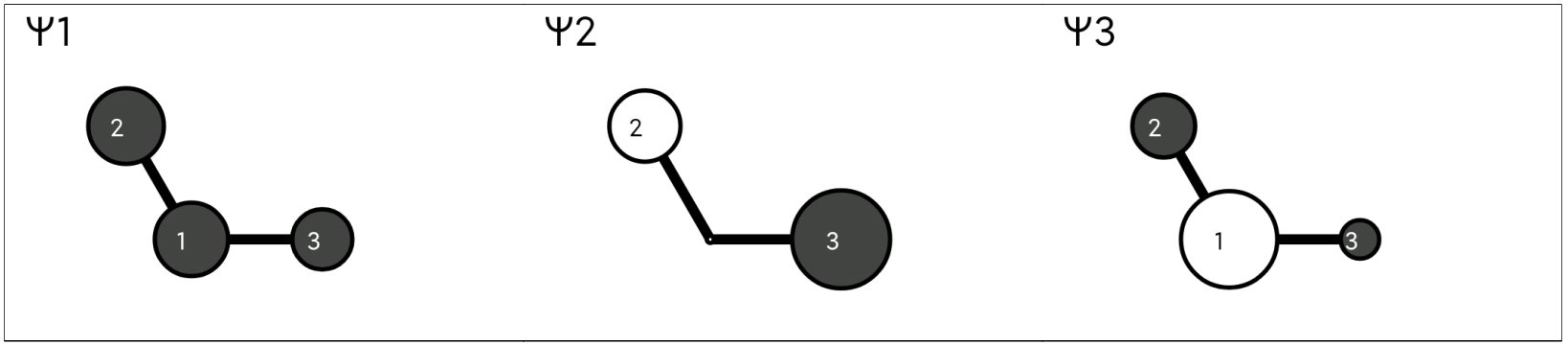
this corresponds to one πelectron: 2.215β

2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3
	x1= 3.054	x2= 1.375	x3= -1.779
1	-0.605	0.059	0.794
2	-0.623	0.586	-0.518
3	-0.496	-0.808	-0.318

2.2. Molecule orbital presentation:

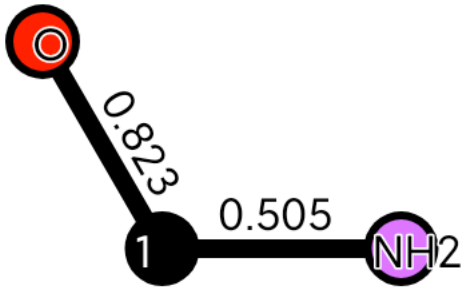


3. Bond Order

3.1. Calculated values:

	1	2	3
1	0.739		
2	0.823	1.463	
3	0.505	-0.329	1.798

3.2. Presentation of bond order:

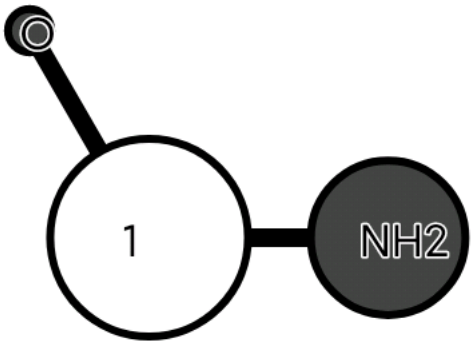


4. Net Charge

4.1. Calculated values:

	1	2	3
1	0.595		
2		-0.13	
3			-0.465

4.2. Presentation of molecule:

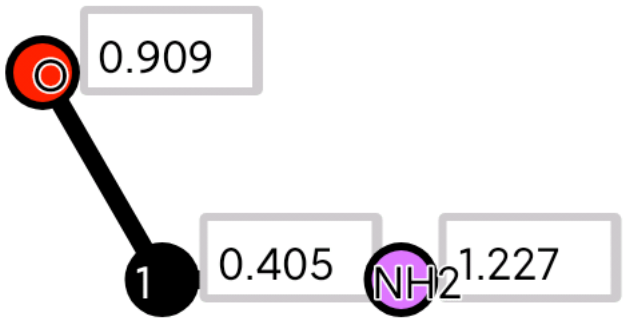


5. Free valences

5.1. Calculated values:

1	2	3
0.405	0.909	1.227

5.2. Presentation of molecule:

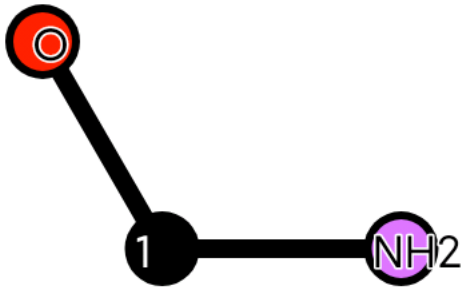


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3
1	0.194		
2	-0.146	0.203	
3	-0.047	-0.057	0.104

6.2. Presentation of molecule:

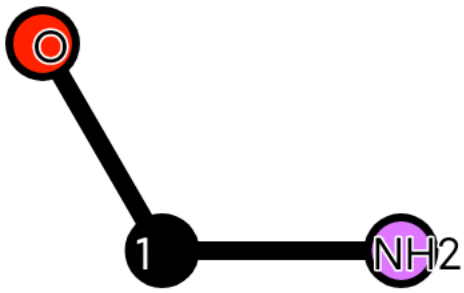


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3
1 2	0.049	-0.108	0.059
1 3	0.02	0.1	-0.121

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3
1 2	0.134	
1 3	-0.167	0.293

8.2. Presentation of molecule: