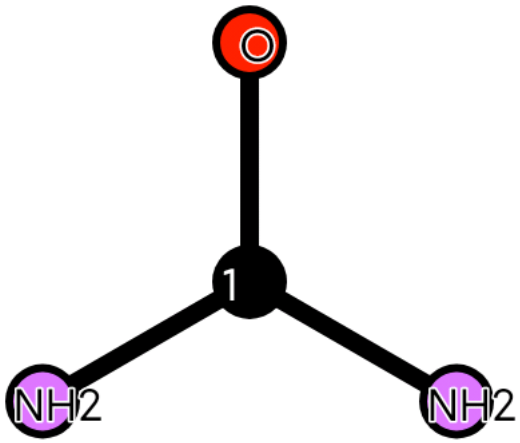
Print calculated values

Report generated by:root, 16.02.2020 - 17:56:00

The following determinant is calculated:

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

It is about this molecule:

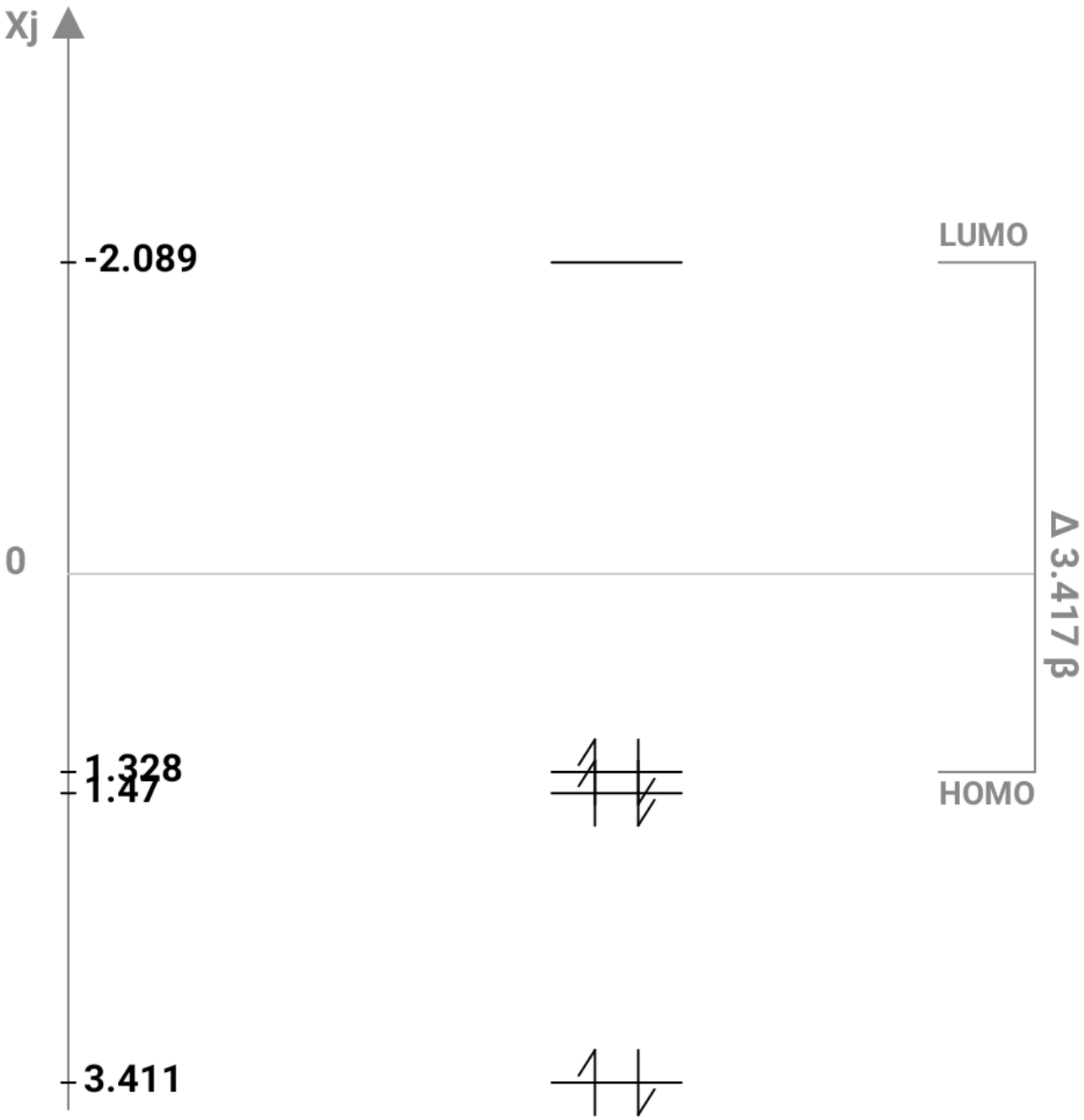


HMO-Energies

x1 = 3.411; x2 = 1.47; x3 = 1.328; x4 = -2.089;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 4α + 12.418β -

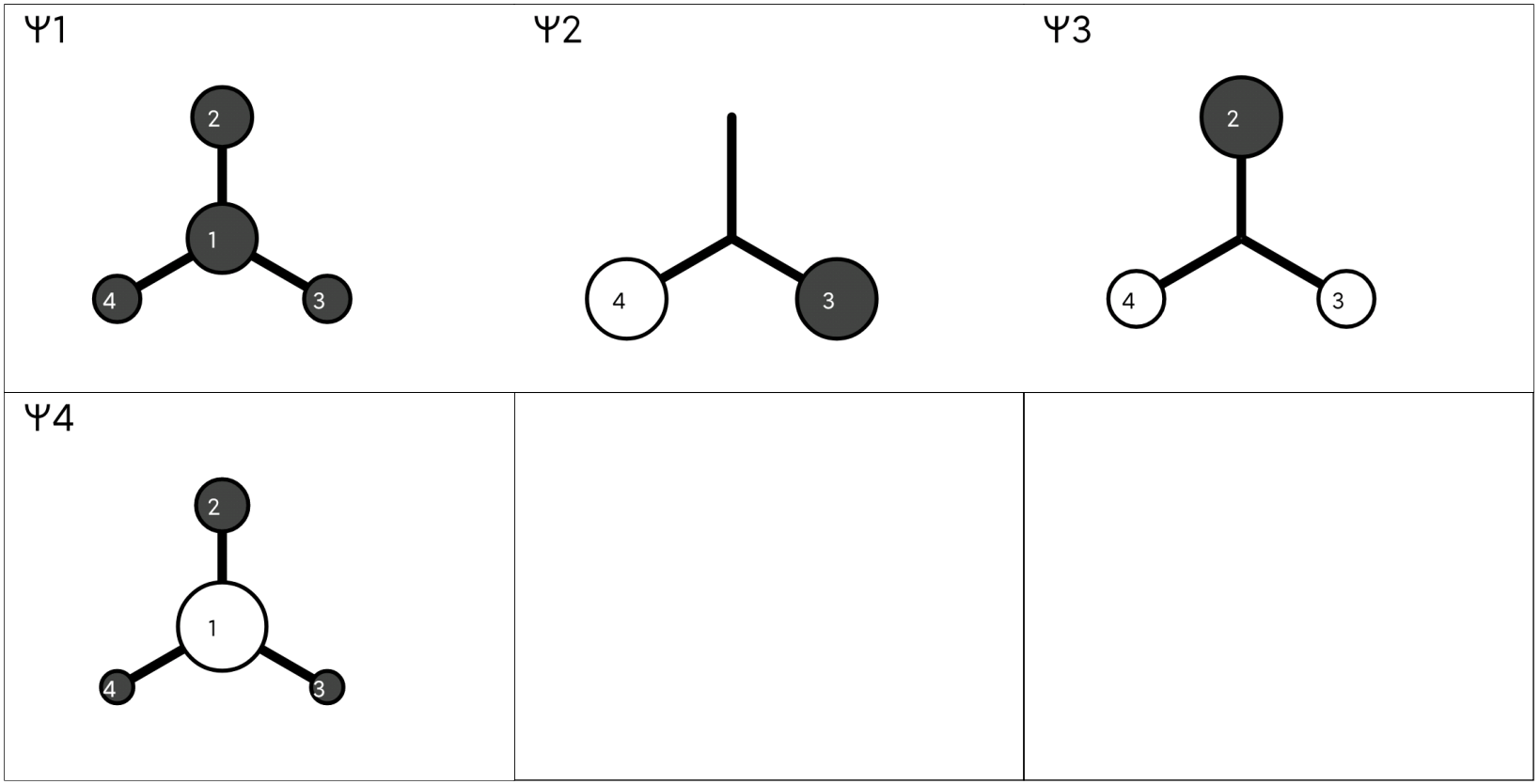
this corresponds to one πelectron: 2.07β

2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4
	x1= 3.411	**x2= 1.47**	**x3= 1.328**	**x4= -2.089**
1	-0.615	0.0	-0.054	0.787
2	-0.532	0.0	-0.708	-0.465
3	-0.412	-0.707	0.498	-0.287
4	-0.412	0.707	0.498	-0.287

2.2. Molecule orbital presentation:

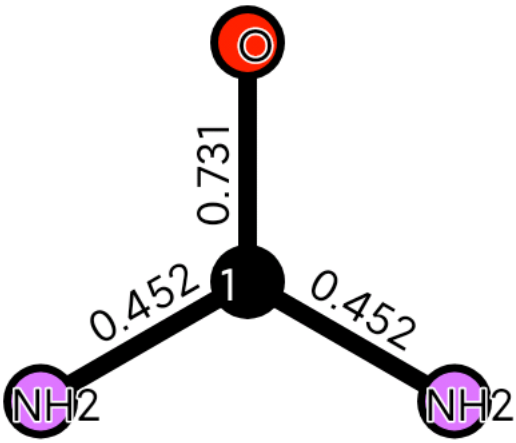


3. Bond Order

3.1. Calculated values:

	1	2	3	4
1	0.762			
2	0.731	1.568		
3	0.452	-0.267	1.835	
4	0.452	-0.267	-0.165	1.835

3.2. Presentation of bond order:

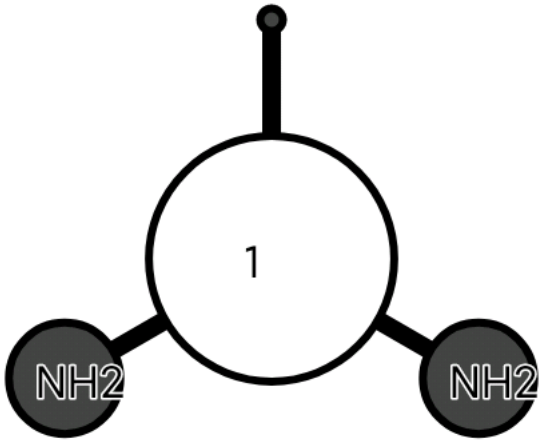


4. Net Charge

4.1. Calculated values:

	1	2	3	4
1	0.738			
2		-0.068		
3			-0.335	
4				-0.335

4.2. Presentation of molecule:

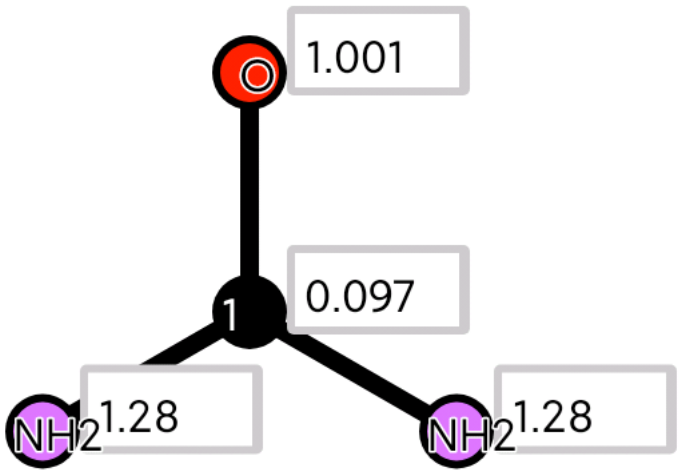


5. Free valences

5.1. Calculated values:

1	2	3	4
0.097	1.001	1.28	1.28

5.2. Presentation of molecule:

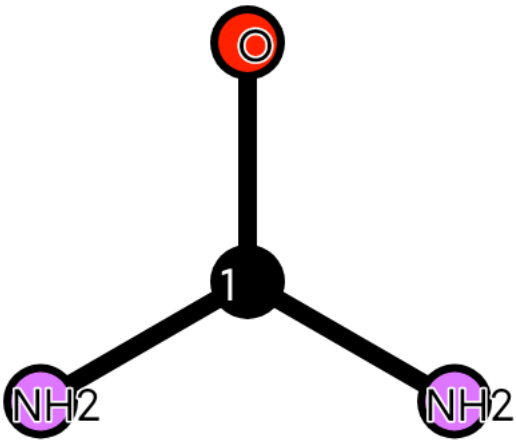


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4
1	0.172			
2	-0.103	0.171		
3	-0.034	-0.034	0.081	
4	-0.034	-0.034	-0.012	0.081

6.2. Presentation of molecule:

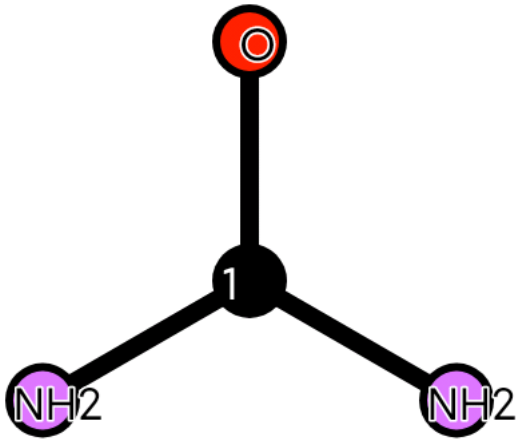


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4
1 2	0.037	-0.114	0.039	0.039
1 3	0.016	0.065	-0.104	0.023
1 4	0.016	0.065	0.023	-0.104

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3	1 4
1 2	0.172		
1 3	-0.12	0.279	
1 4	-0.12	-0.069	0.279

8.2. Presentation of molecule: