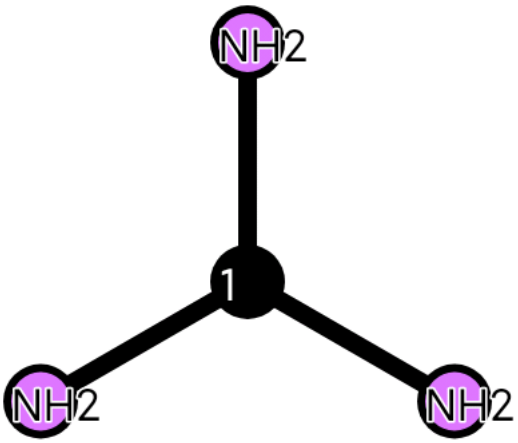
Print calculated values

Report generated by:root, 20.01.2020 - 12:19:39

The following determinant is calculated:

-x	1.3	1.3	1.3
1.3	-x+1.47	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:

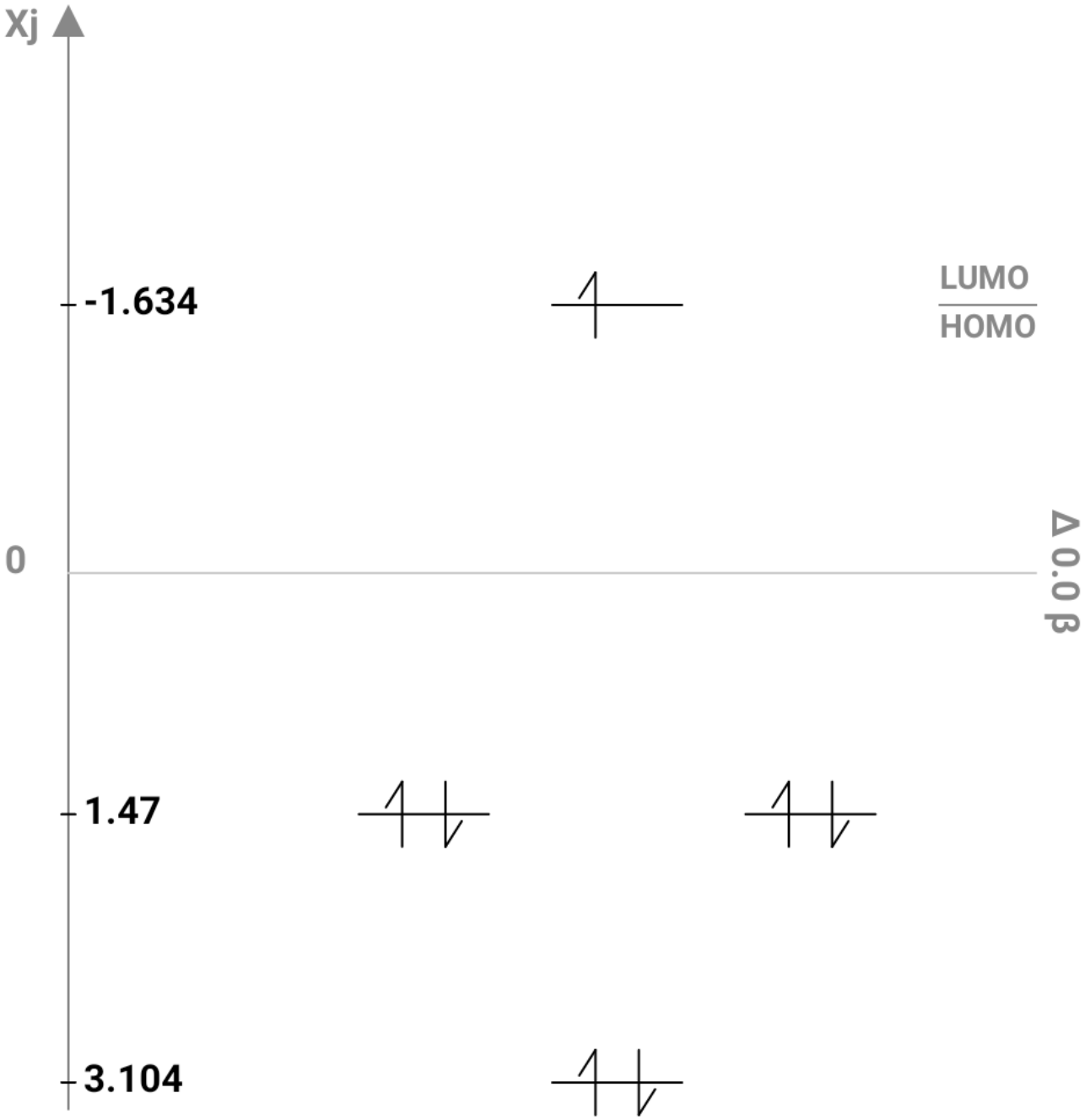


HMO-Energies

x1 = 3.104; x2 = 1.47; x3 = 1.47; x4 = -1.634;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 4α + 10.454β -

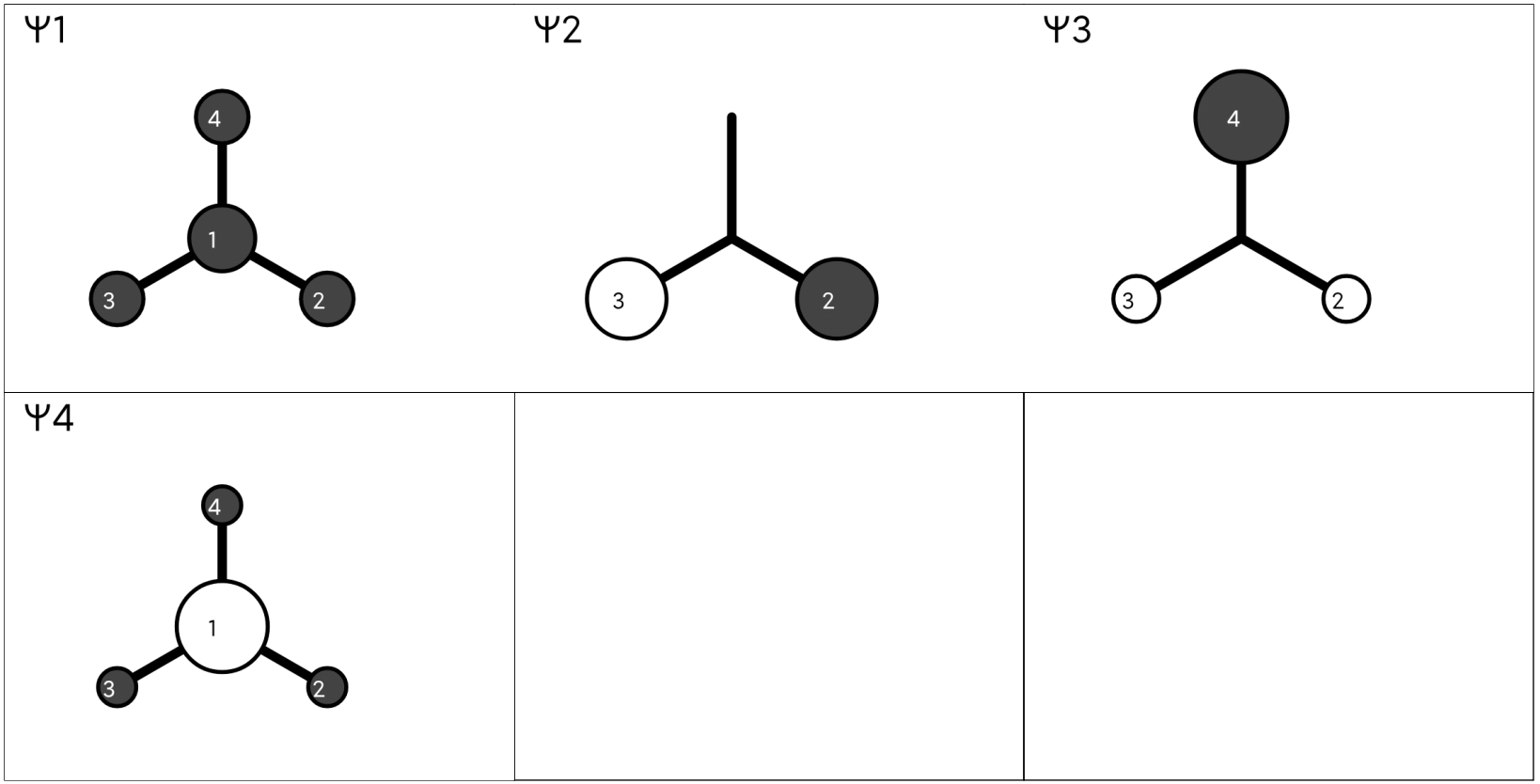
this corresponds to one πelectron: 1.493β

2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4
	x1= 3.104	**x2= 1.47**	**x3= 1.47**	**x4= -1.634**
1	-0.587	0.0	0.0	0.809
2	-0.467	-0.707	0.408	-0.339
3	-0.467	0.707	0.408	-0.339
4	-0.467	0.0	-0.816	-0.339

2.2. Molecule orbital presentation:

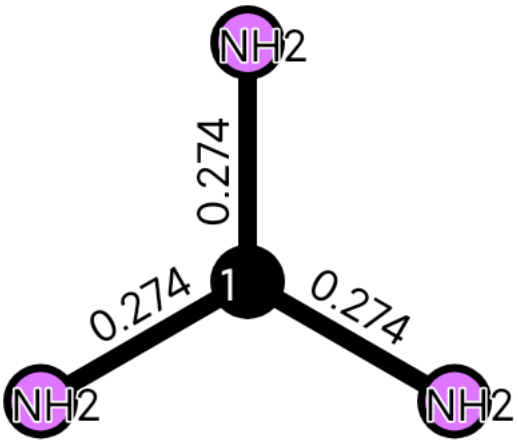


3. Bond Order

3.1. Calculated values:

	1	2	3	4
1	1.345			
2	0.274	1.885		
3	0.274	-0.115	1.885	
4	0.274	-0.115	-0.115	1.885

3.2. Presentation of bond order:

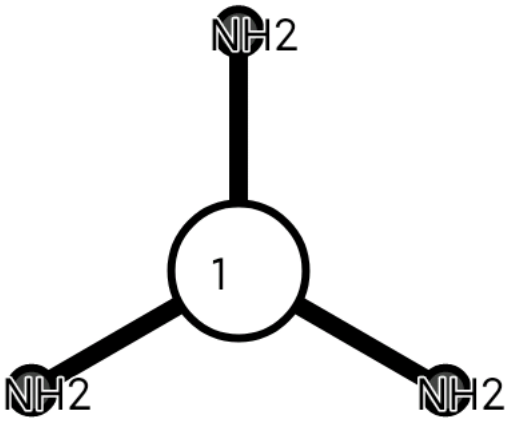


4. Net Charge

4.1. Calculated values:

	1	2	3	4
1	0.405			
2		-0.135		
3			-0.135	
4				-0.135

4.2. Presentation of molecule:

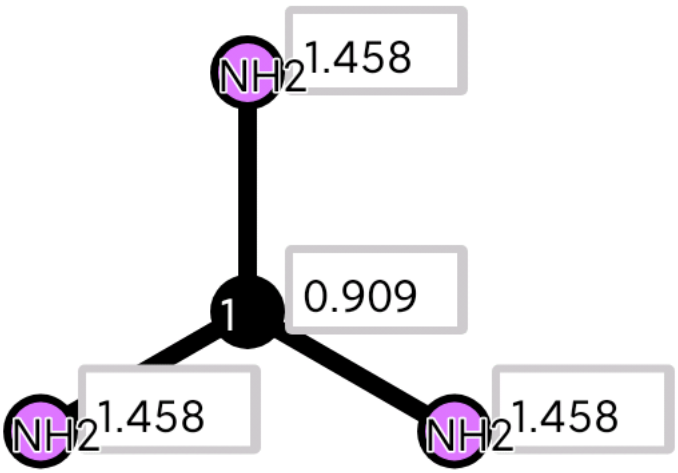


5. Free valences

5.1. Calculated values:

1	2	3	4
0.909	1.458	1.458	1.458

5.2. Presentation of molecule:

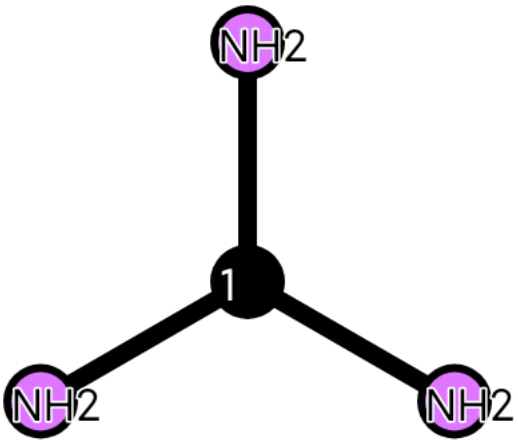


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4
1	0.095			
2	-0.032	0.06		
3	-0.032	-0.014	0.06	
4	-0.032	-0.014	-0.014	0.06

6.2. Presentation of molecule:

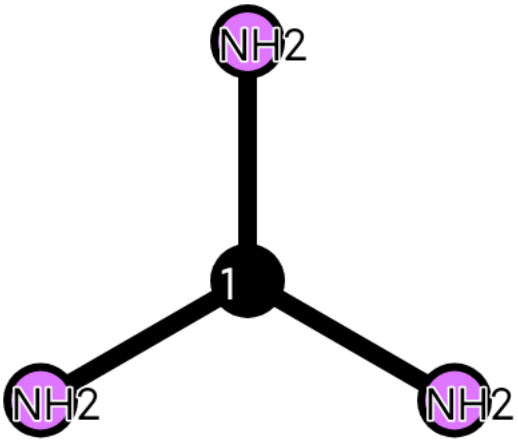


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4
1 2	0.018	-0.065	0.023	0.023
1 3	0.018	0.023	-0.065	0.023
1 4	0.018	0.023	0.023	-0.065

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3	1 4
1 2	0.147		
1 3	-0.064	0.147	
1 4	-0.064	-0.064	0.147

8.2. Presentation of molecule: