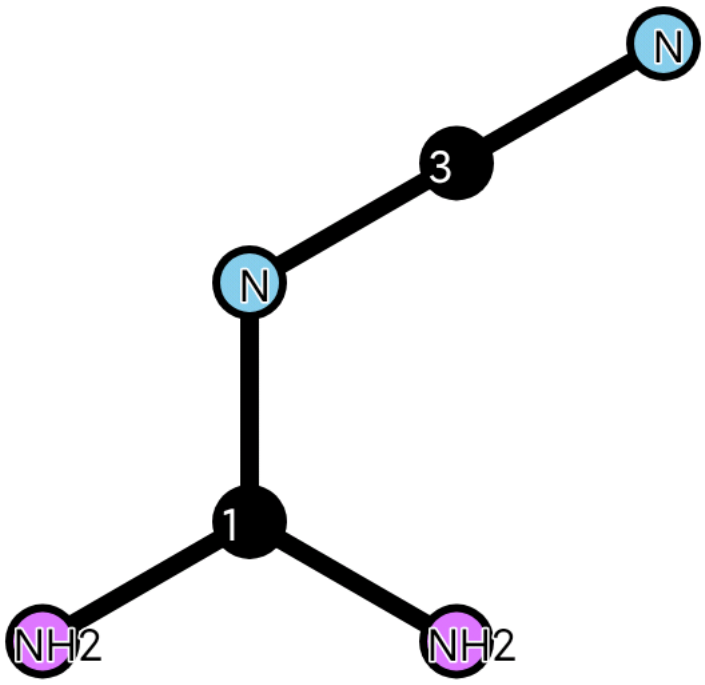
Print calculated values

Report generated by:root, 24.03.2020 - 20:51:40

The following determinant is calculated:

-x	1.06	0.0	0.0	1.3	1.3
1.06	-x+0.83	1.06	0.0	0.0	0.0
0.0	1.06	-x	1.66	0.0	0.0
0.0	0.0	1.66	-x+1.47	0.0	0.0
1.3	0.0	0.0	0.0	-x+1.47	0.0
1.3	0.0	0.0	0.0	0.0	-x+1.47

It is about this molecule:

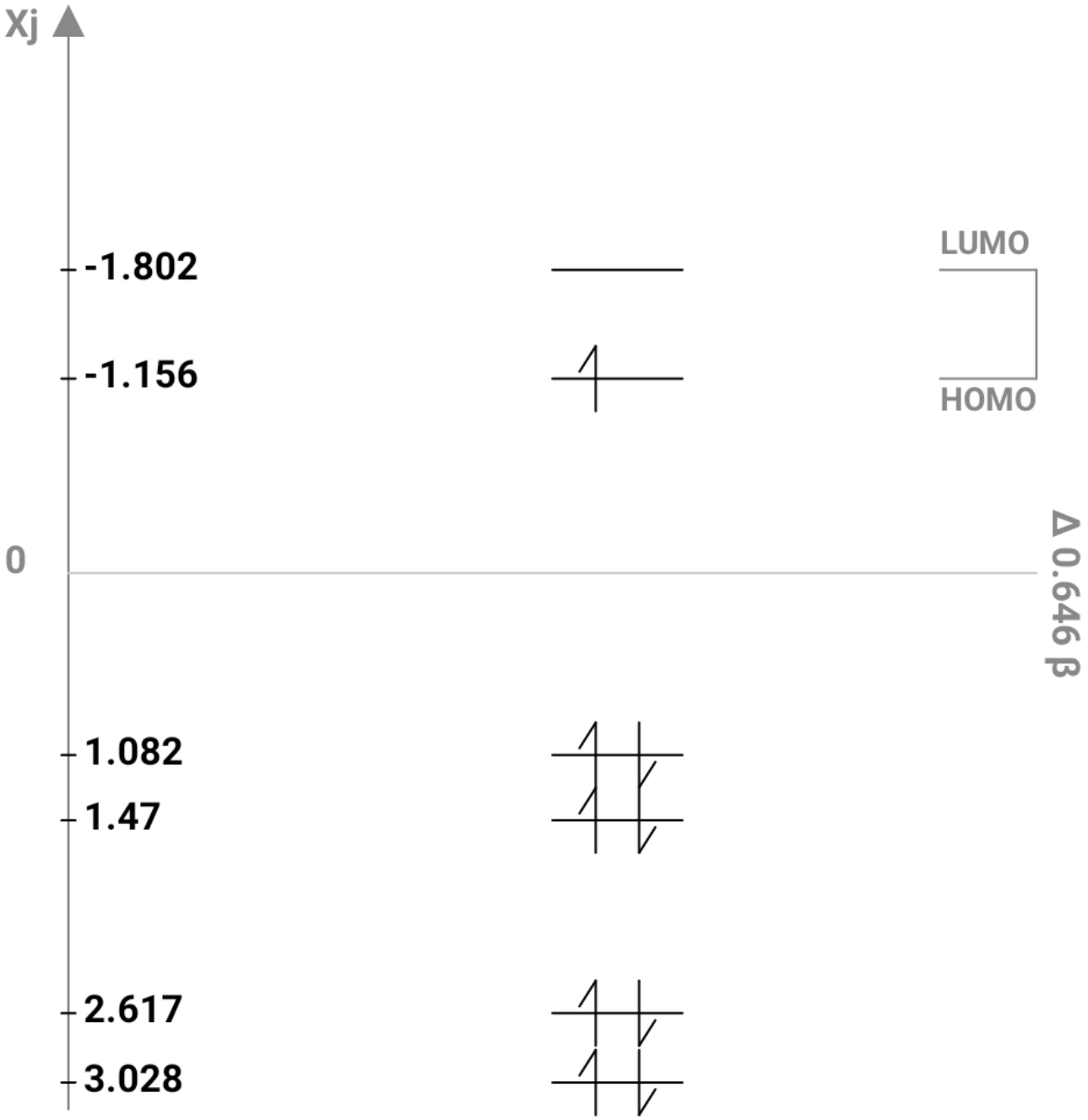


HMO-Energies

x1 = 3.028; x2 = 2.617; x3 = 1.47; x4 = 1.082; x5 = -1.156; x6 = -1.802;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 6α + 15.238β -

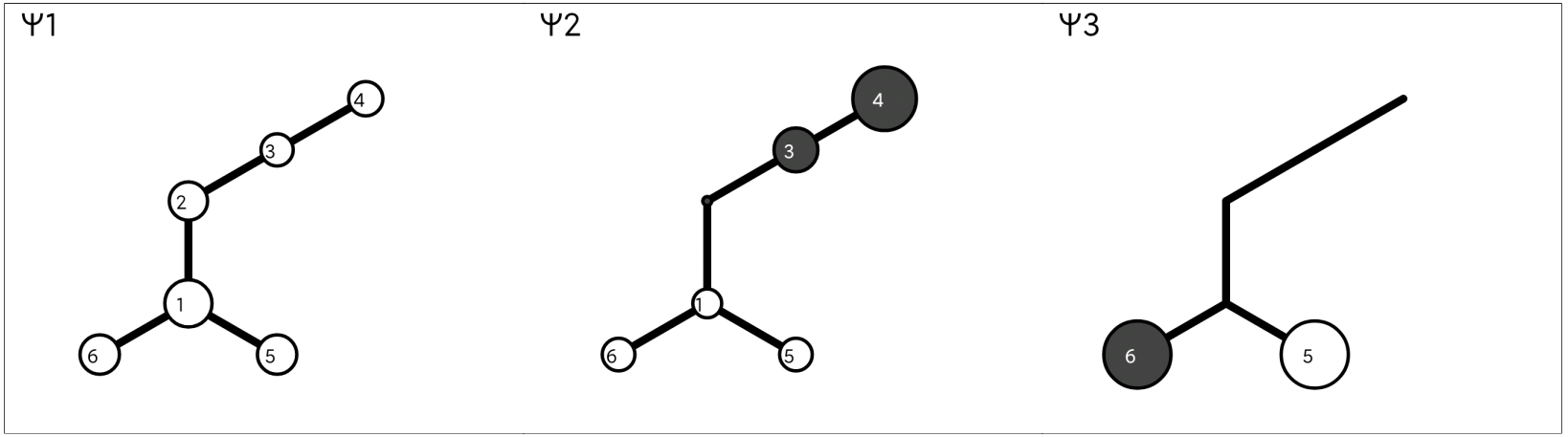
this corresponds to one πelectron: 1.693β

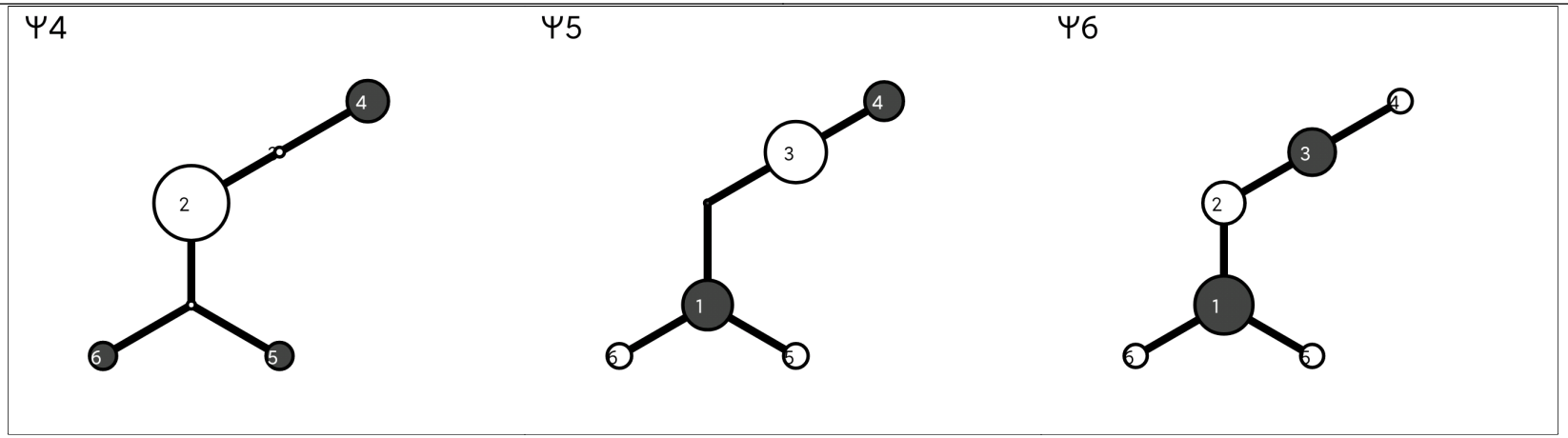
2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6
	x1= 3.028	x2= 2.617	x3= 1.47	x4= 1.082	x5= -1.156	x6= -1.802
1	0.497	0.304	0.0	0.086	-0.525	-0.614
2	0.403	-0.094	0.0	0.791	-0.065	0.446
3	0.339	-0.463	0.0	0.102	0.647	-0.492
4	0.361	-0.669	0.0	-0.438	-0.409	0.25
5	0.415	0.344	0.707	-0.287	0.26	0.244
6	0.415	0.344	-0.707	-0.287	0.26	0.244

2.2. Molecule orbital presentation:



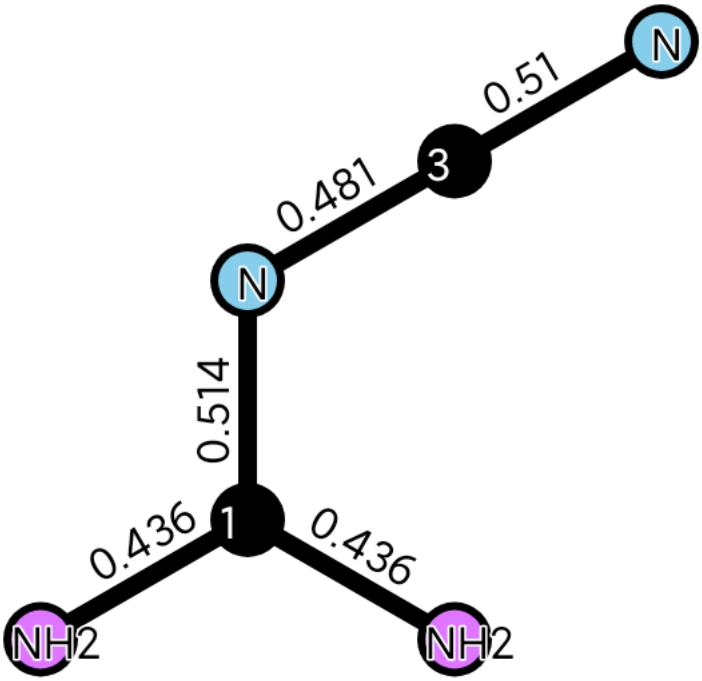

Ψ4
4
3
2
6
5
Ψ5
4
3
1
6
5
Ψ6
4
3
2
1
6
5

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6
1	0.97					
2	0.514	1.598				
3	-0.265	0.481	1.097			
4	0.092	-0.249	0.51	1.708		
5	0.436	-0.201	0.072	-0.016	1.813	
6	0.436	-0.201	0.072	-0.016	-0.187	1.813

3.2. Presentation of bond order:

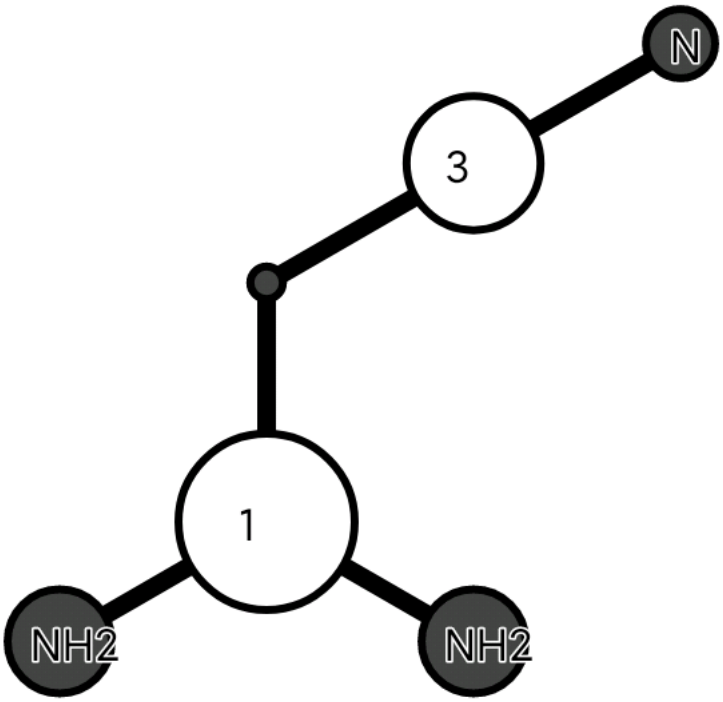


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6
1	0.53					
2		-0.098				
3			0.403			
4				-0.208		
5					-0.313	
6						-0.313

4.2. Presentation of molecule:

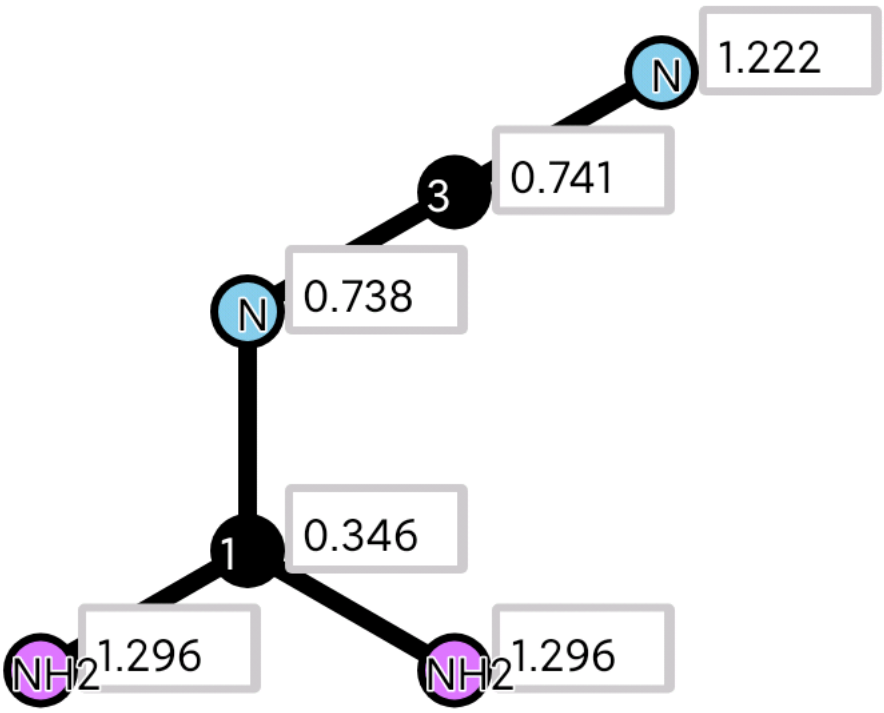


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6
0.346	0.738	0.741	1.222	1.296	1.296

5.2. Presentation of molecule:

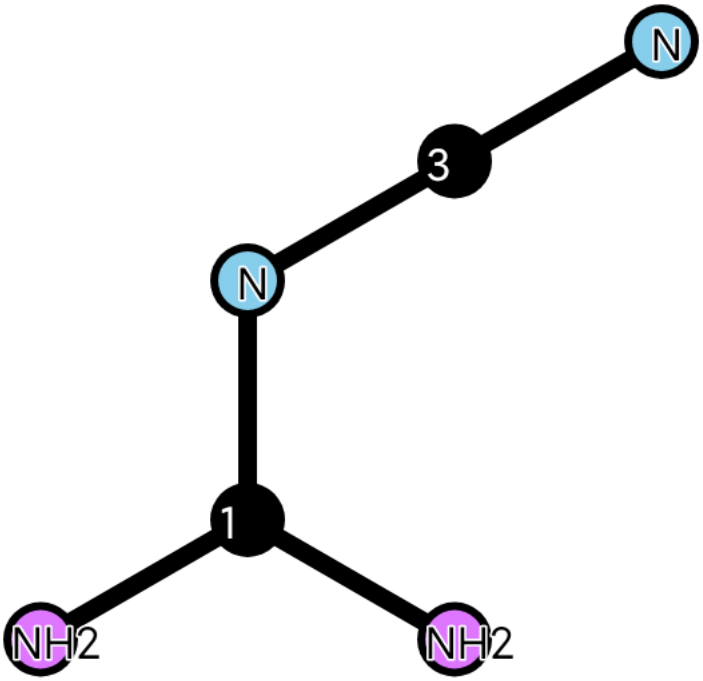


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6
1	0.483					
2	-0.088	0.206				
3	-0.315	-0.036	0.462			
4	-0.1	-0.03	0.013	0.16		
5	0.011	-0.026	-0.062	-0.021	0.111	
6	0.011	-0.026	-0.062	-0.021	-0.013	0.111

6.2. Presentation of molecule:

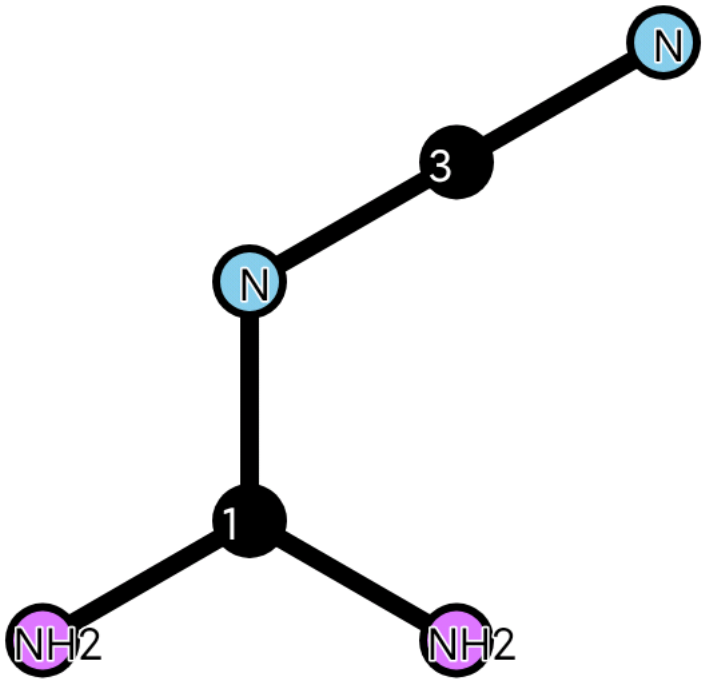


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6
1 2	-0.071	-0.095	0.105	0.026	0.017	0.017
1 5	-0.116	0.05	0.139	0.045	-0.131	0.013
1 6	-0.116	0.05	0.139	0.045	0.013	-0.131
2 3	0.168	-0.112	-0.129	0.016	0.029	0.029
3 4	0.177	0.038	-0.144	-0.142	0.036	0.036

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 5	1 6	2 3	3 4
1 2	0.308				
1 5	-0.013	0.357			
1 6	-0.013	0.021	0.357		
2 3	-0.112	-0.142	-0.142	0.381	
3 4	-0.11	-0.157	-0.157	0.043	0.334

8.2. Presentation of molecule: