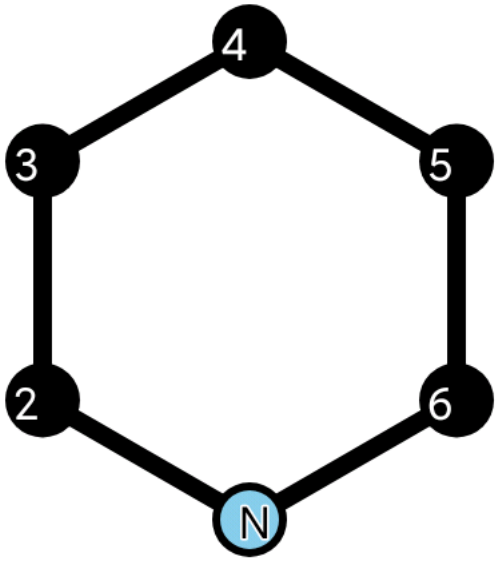
Print calculated values

Report generated by:root, 16.02.2020 - 17:58:57

The following determinant is calculated:

-x+0.83	1.06	0.0	0.0	0.0	1.06
1.06	-x	1.0	0.0	0.0	0.0
0.0	1.0	-x	1.0	0.0	0.0
0.0	0.0	1.0	-x	1.0	0.0
0.0	0.0	0.0	1.0	-x	1.0
1.06	0.0	0.0	0.0	1.0	-x

It is about this molecule:

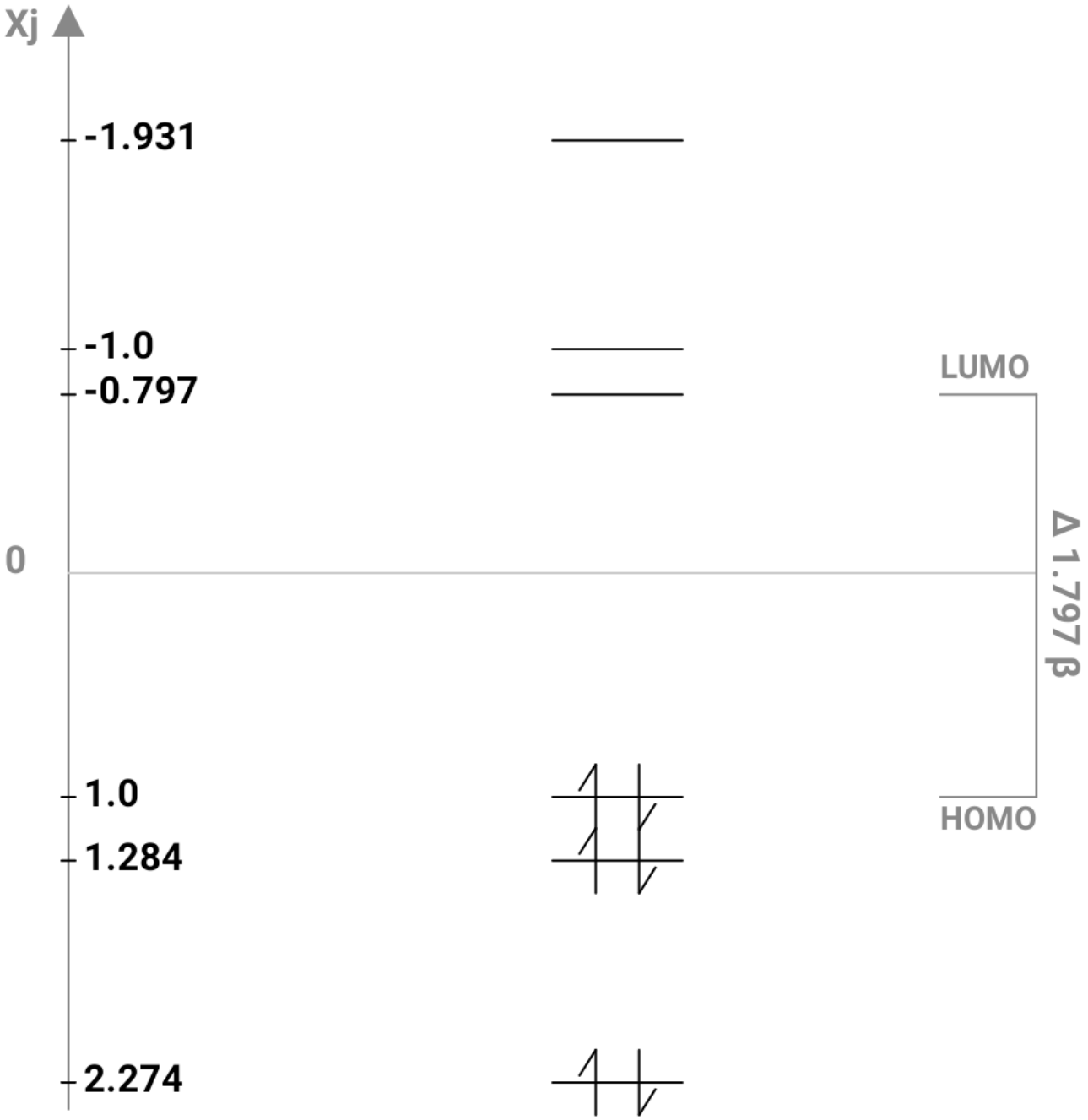


HMO-Energies

x1 = 2.274; x2 = 1.284; x3 = 1.0; x4 = -0.797; x5 = -1.0; x6 = -1.931;

1. Energy-eigenvalues

1.1. Calculated values:



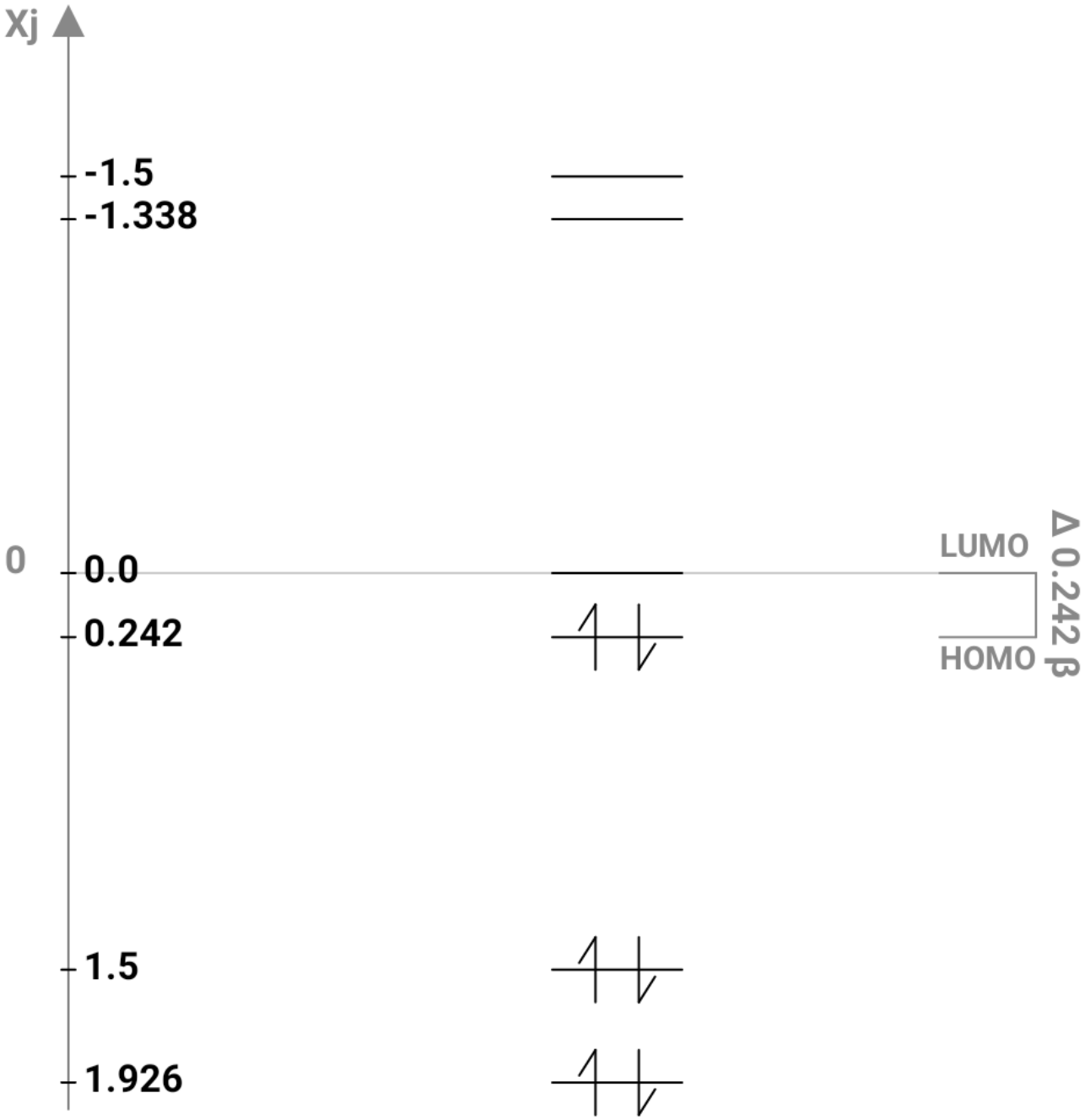
total Power Eπ: 6α + 9.116β -

this corresponds to one πelectron: 1.519β

1. Moebius-Energy-eigenvalues

1.1. Calculated values:

$$\beta = \beta * \cos(\pi / n)$$



total Power Eπ: 6α + 7.336β -

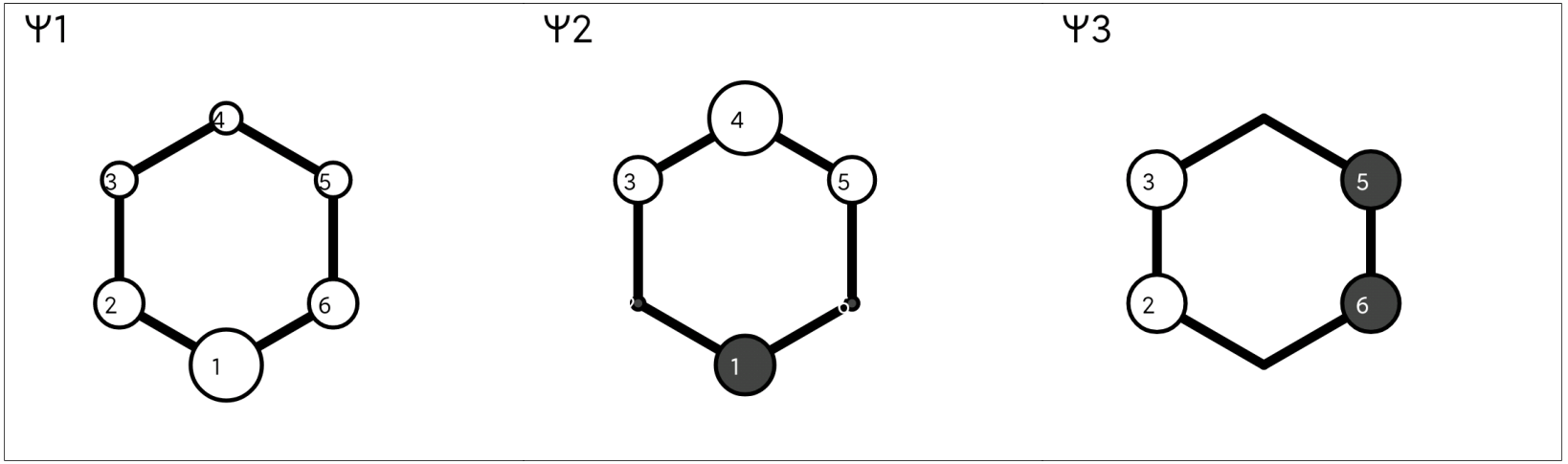
this corresponds to one πelectron: 1.223β

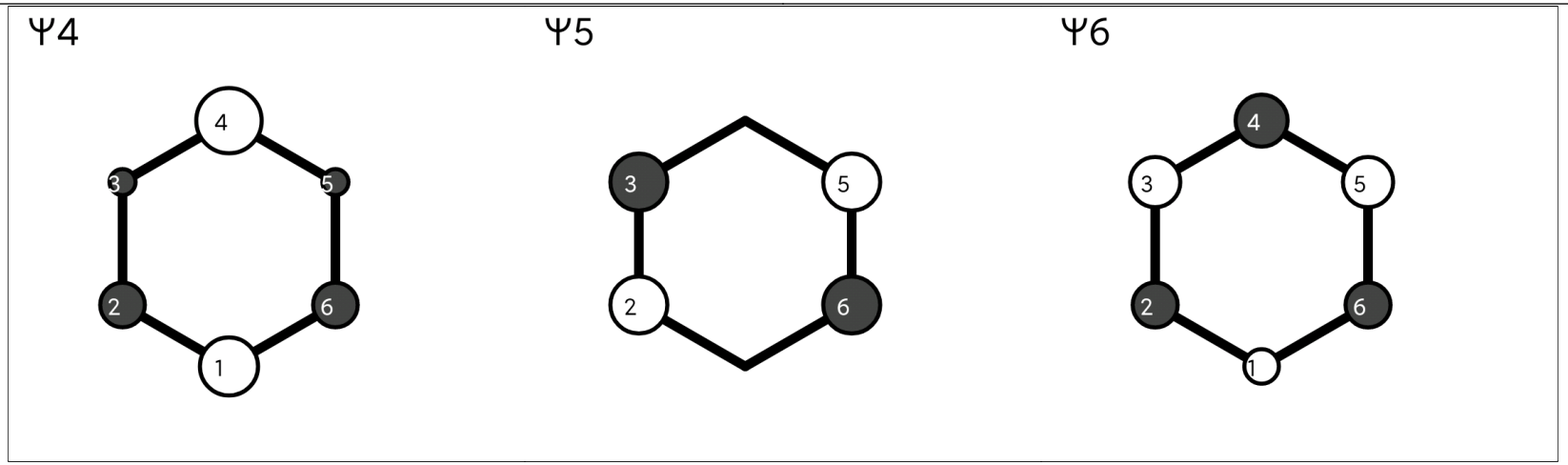
2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6
	x1= 2.274	x2= 1.284	x3= 1.0	x4= -0.797	x5= -1.0	x6= -1.931
1	0.621	-0.512	0.0	0.51	0.0	0.303
2	0.423	-0.11	0.5	-0.391	0.5	-0.395
3	0.304	0.402	0.5	-0.229	-0.5	0.441
4	0.267	0.626	0.0	0.574	0.0	-0.456
5	0.304	0.402	-0.5	-0.229	0.5	0.441
6	0.423	-0.11	-0.5	-0.391	-0.5	-0.395

2.2. Molecule orbital presentation:



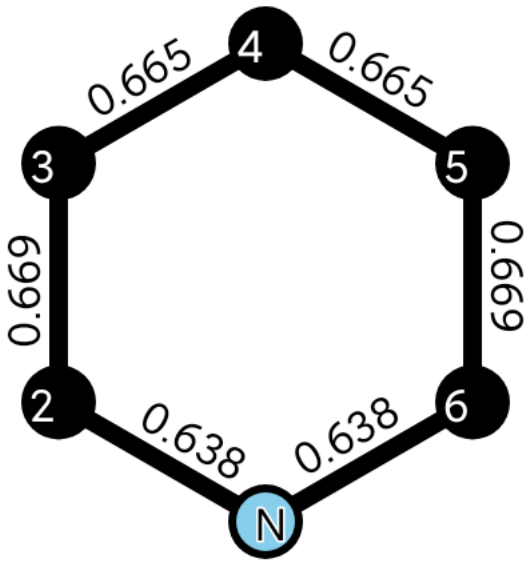

Ψ4
4
3
5
2
6
1
Ψ5
3
5
2
6
Ψ6
4
3
5
2
6
1

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6
1	1.296					
2	0.638	0.882				
3	-0.034	0.669	1.007			
4	-0.308	0.089	0.665	0.925		
5	-0.034	-0.331	0.007	0.665	1.007	
6	0.638	-0.118	-0.331	0.089	0.669	0.882

3.2. Presentation of bond order:

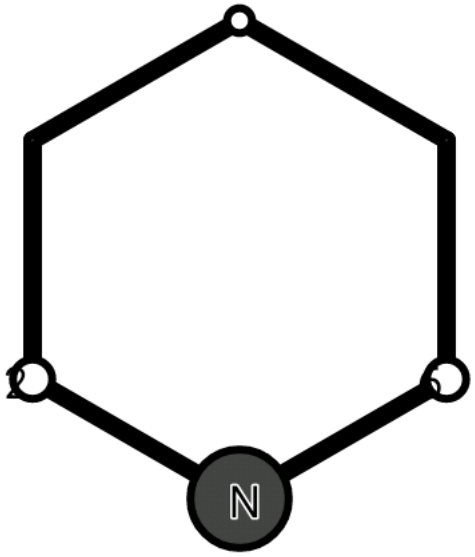


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6
1	-0.296					
2		0.118				
3			-0.007			
4				0.075		
5					-0.007	
6						0.118

4.2. Presentation of molecule:

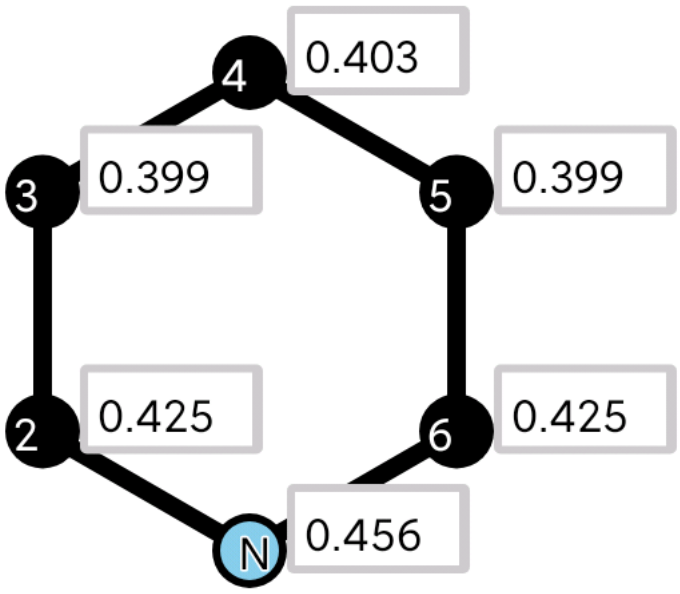


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6
0.456	0.425	0.399	0.403	0.399	0.425

5.2. Presentation of molecule:

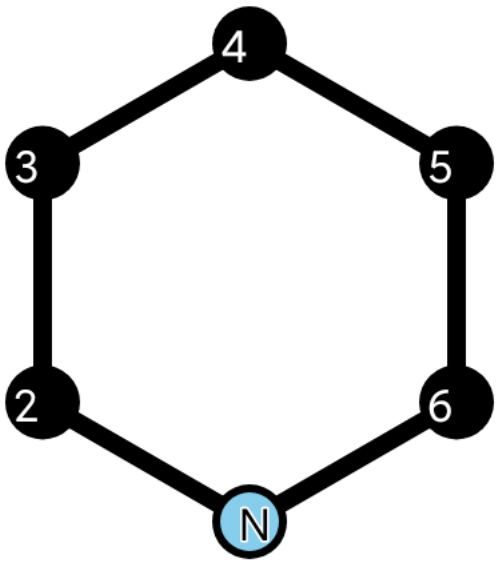


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6
1	0.325					
2	-0.128	0.391				
3	0.007	-0.159	0.398			
4	-0.084	0.001	-0.156	0.394		
5	0.007	-0.1	0.009	-0.156	0.398	
6	-0.128	-0.005	-0.1	0.001	-0.159	0.391

6.2. Presentation of molecule:

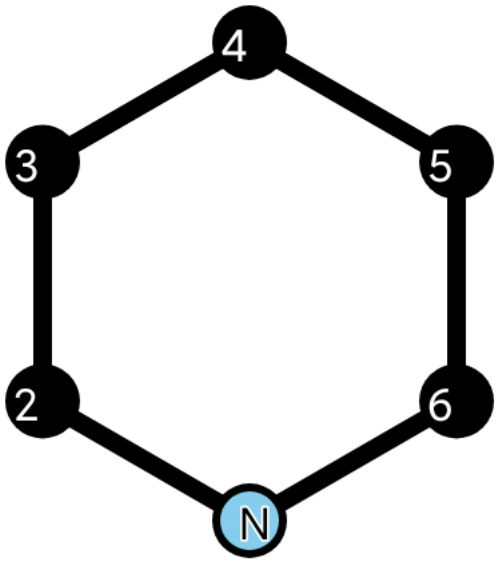


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6
1 2	-0.069	-0.001	0.006	0.024	-0.007	0.046
1 3	-0.035	-0.148	-0.043	0.11	0.009	0.108
1 4	0.036	-0.025	0.009	-0.006	0.009	-0.025
1 6	-0.069	0.046	-0.007	0.024	0.006	-0.001
2 3	0.015	0.051	0.006	-0.034	-0.001	-0.037
3 4	-0.009	-0.038	-0.007	0.026	-0.001	0.03
4 5	-0.009	0.03	-0.001	0.026	-0.007	-0.038
5 6	0.015	-0.037	-0.001	-0.034	0.006	0.051

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3	1 4	1 6	2 3	3 4	4 5	5 6
1 2	0.249							
1 3	-0.015	0.374						
1 4	0.05	-0.051	0.29					
1 6	-0.16	0.041	0.05	0.249				
2 3	-0.194	-0.035	-0.133	0.114	0.243			
3 4	0.124	0.031	0.065	-0.082	-0.207	0.245		
4 5	-0.082	0.005	0.065	0.124	0.128	-0.202	0.245	
5 6	0.114	-0.001	-0.133	-0.194	-0.091	0.128	-0.207	0.243

8.2. Presentation of molecule: