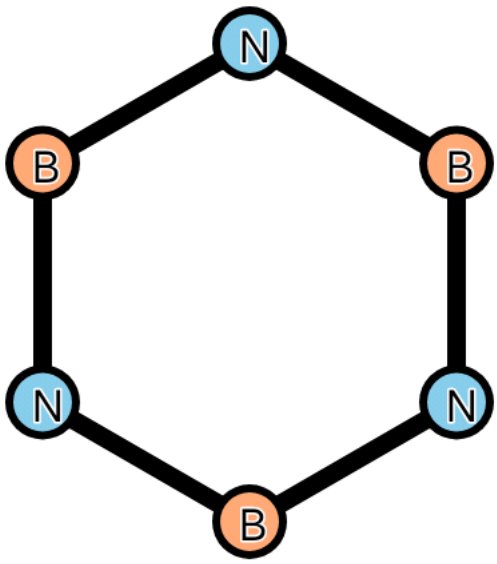
Print calculated values

Report generated by:root, 20.01.2020 - 20:35:54

The following determinant is calculated:

-x+0.83	0.8	0.8	0.0	0.0	0.0
0.8	-x+-1.0	0.0	0.0	0.8	0.0
0.8	0.0	-x+-1.0	0.8	0.0	0.0
0.0	0.0	0.8	-x+0.83	0.0	0.8
0.0	0.8	0.0	0.0	-x+0.83	0.8
0.0	0.0	0.0	0.8	0.8	-x+-1.0

It is about this molecule:

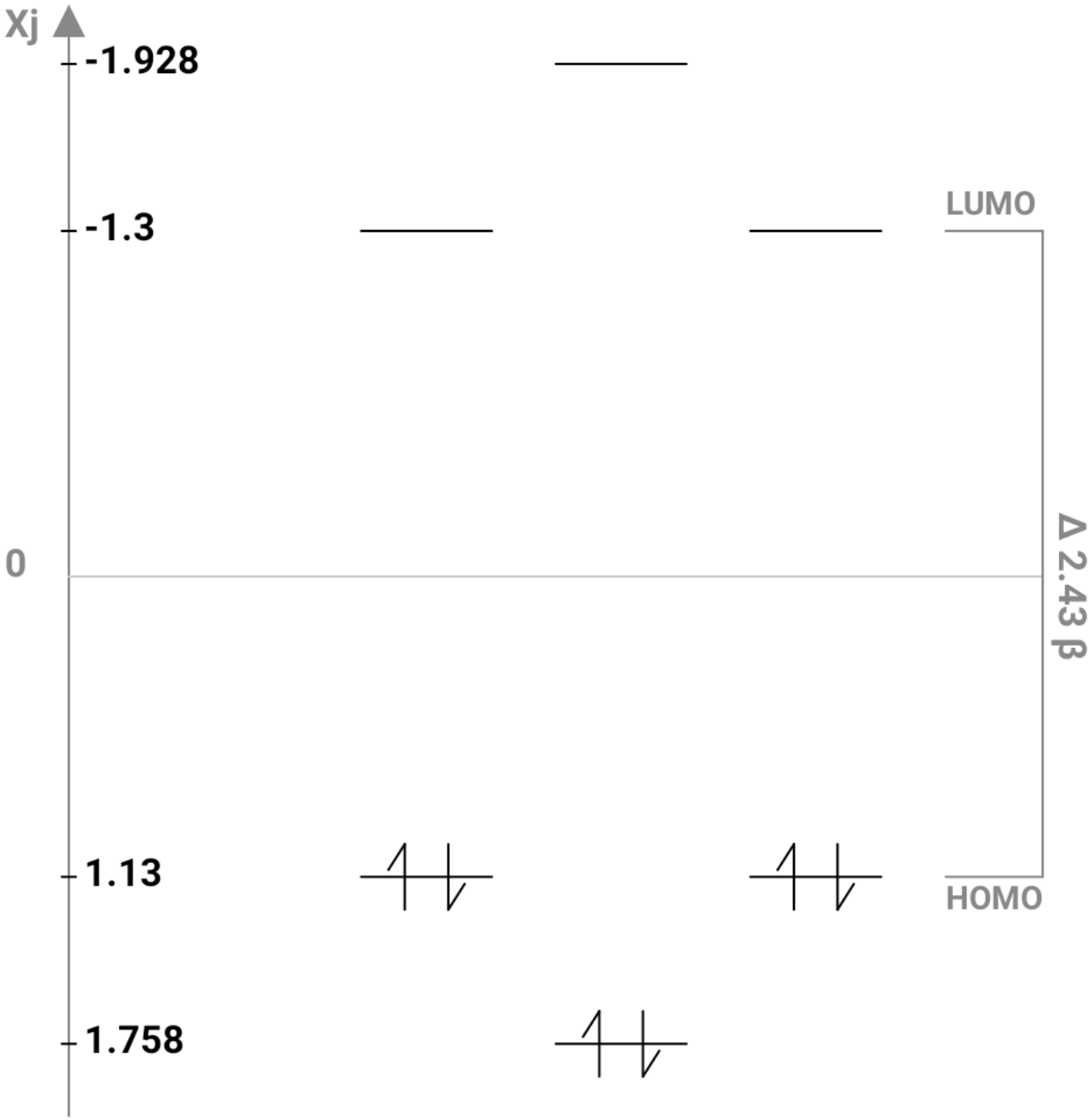


HMO-Energies

x1 = 1.758; x2 = 1.13; x3 = 1.13; x4 = -1.3; x5 = -1.3; x6 = -1.928;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 6α + 8.036β -

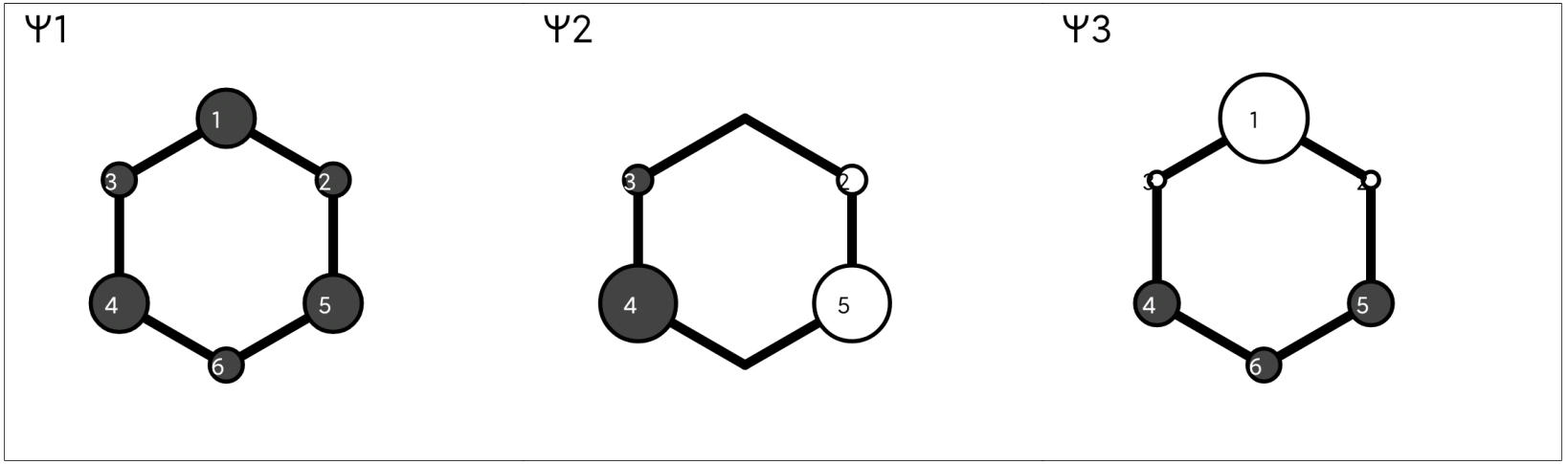
this corresponds to one πelectron: 1.339β

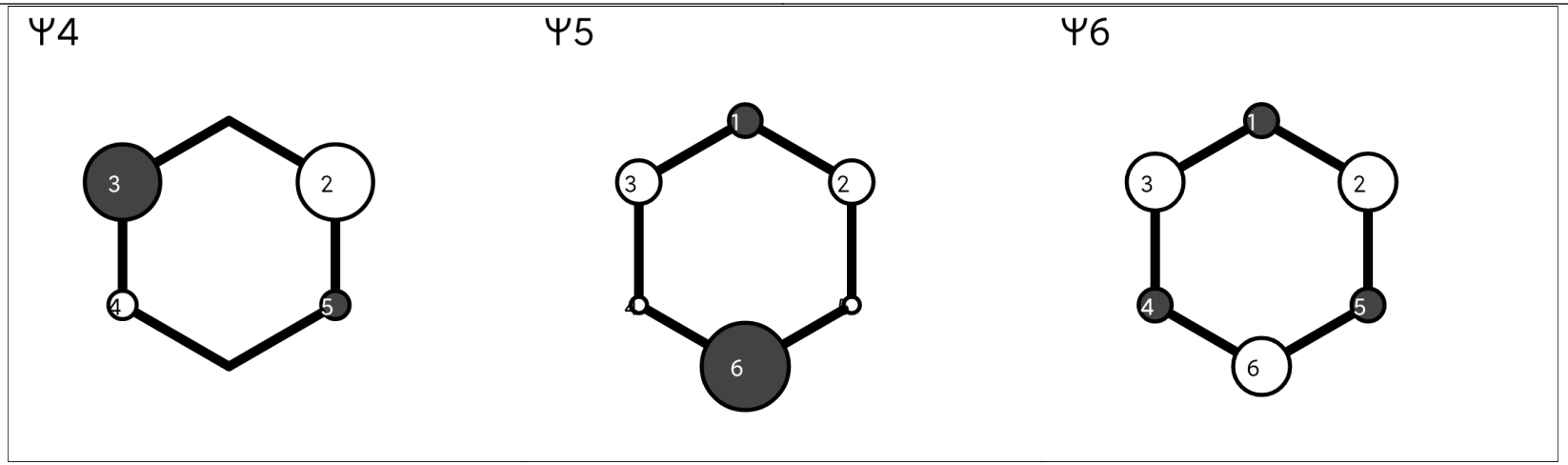
2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6
	x1= 1.758	x2= 1.13	x3= 1.13	x4= -1.3	x5= -1.3	x6= -1.928
1	-0.499	0.0	0.764	0.0	-0.287	-0.29
2	-0.29	0.249	0.144	0.662	0.382	0.499
3	-0.29	-0.249	0.144	-0.662	0.382	0.499
4	-0.499	-0.662	-0.382	0.249	0.144	-0.29
5	-0.499	0.662	-0.382	-0.249	0.144	-0.29
6	-0.29	0.0	-0.287	0.0	-0.764	0.499

2.2. Molecule orbital presentation:



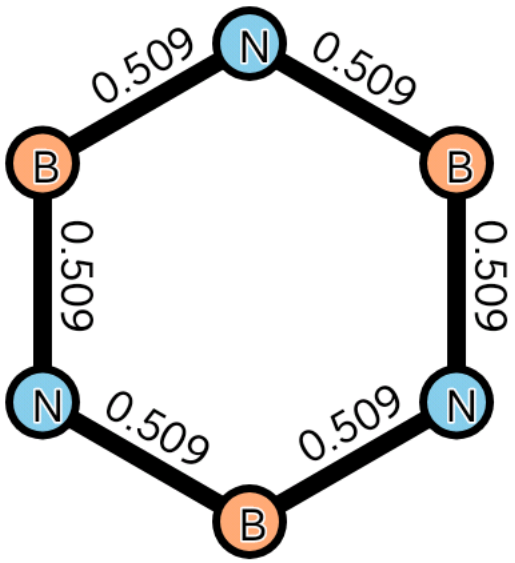

Ψ4
3
2
4
5
Ψ5
1
3
2
6
Ψ6
1
3
2
4
5
6

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6
1	1.667					
2	0.509	0.333				
3	0.509	0.085	0.333			
4	-0.085	-0.149	0.509	1.667		
5	-0.085	0.509	-0.149	-0.085	1.667	
6	-0.149	0.085	0.085	0.509	0.509	0.333

3.2. Presentation of bond order:

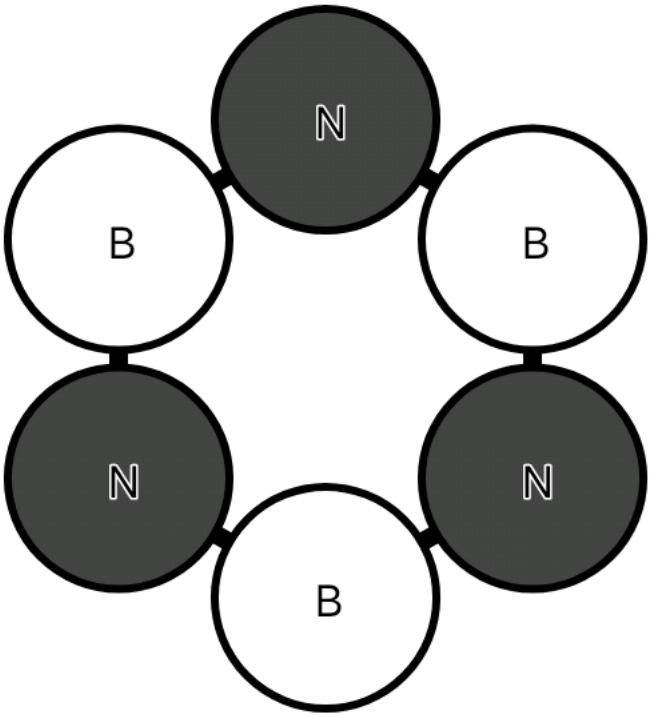


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6
1	-0.667					
2		0.667				
3			0.667			
4				-0.667		
5					-0.667	
6						0.667

4.2. Presentation of molecule:

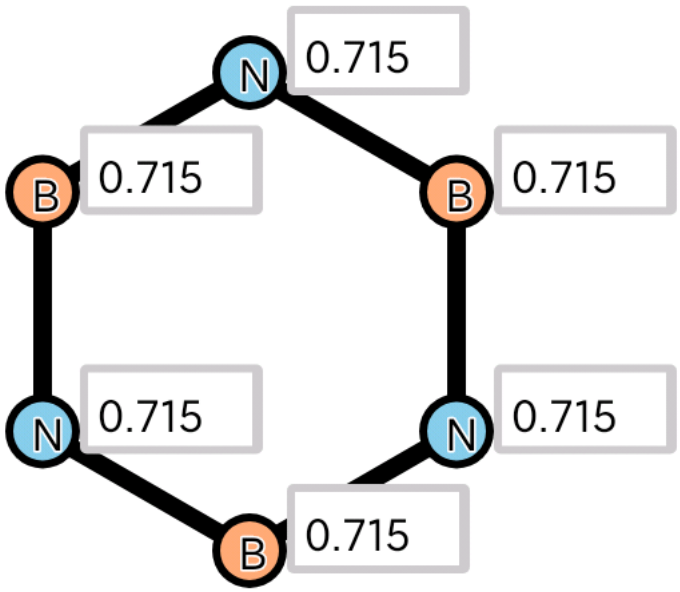


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6
0.715	0.715	0.715	0.715	0.715	0.715

5.2. Presentation of molecule:

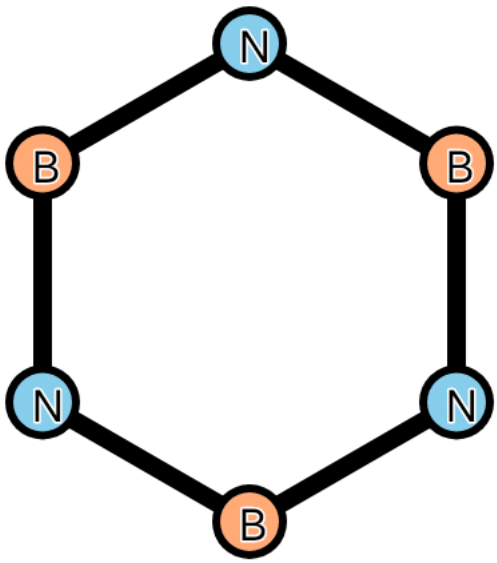


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6
1	0.193					
2	-0.084	0.193				
3	-0.084	-0.003	0.193			
4	-0.003	-0.019	-0.084	0.193		
5	-0.003	-0.084	-0.019	-0.003	0.193	
6	-0.019	-0.003	-0.003	-0.084	-0.084	0.193

6.2. Presentation of molecule:

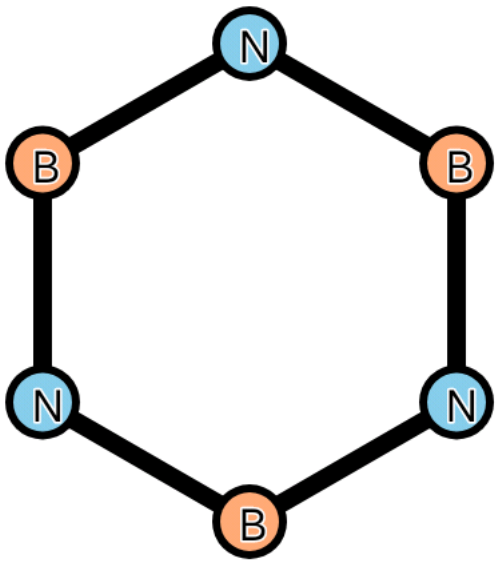


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6
1 2	-0.118	0.118	-0.022	-0.011	0.022	0.011
1 3	-0.118	-0.022	0.118	0.022	-0.011	0.011
2 5	0.022	0.118	0.011	-0.011	-0.118	-0.022
3 4	0.022	0.011	0.118	-0.118	-0.011	-0.022
4 6	-0.011	0.011	-0.022	-0.118	0.022	0.118
5 6	-0.011	-0.022	0.011	0.022	-0.118	0.118

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3	2 5	3 4	4 6	5 6
1 2	0.44					
1 3	-0.14	0.44				
2 5	-0.14	0.047	0.44			
3 4	0.047	-0.14	-0.01	0.44		
4 6	-0.01	0.047	0.047	-0.14	0.44	
5 6	0.047	-0.01	-0.14	0.047	-0.14	0.44

8.2. Presentation of molecule: