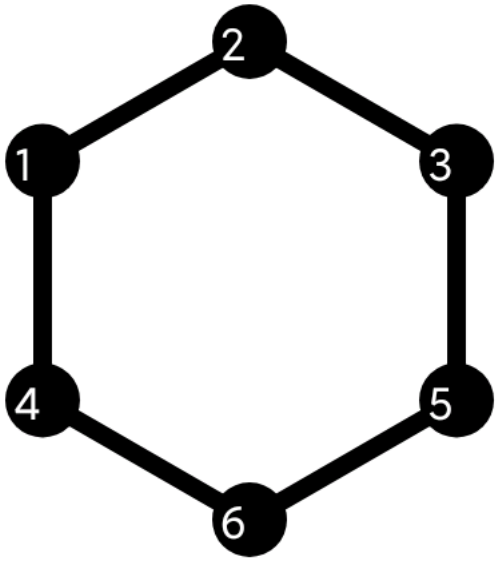
Print calculated values

Report generated by:root, 20.01.2020 - 21:02:57

The following determinant is calculated:

-x	1.0	0.0	1.0	0.0	0.0
1.0	-x	1.0	0.0	0.0	0.0
0.0	1.0	-x	0.0	1.0	0.0
1.0	0.0	0.0	-x	0.0	1.0
0.0	0.0	1.0	0.0	-x	1.0
0.0	0.0	0.0	1.0	1.0	-x

It is about this molecule:

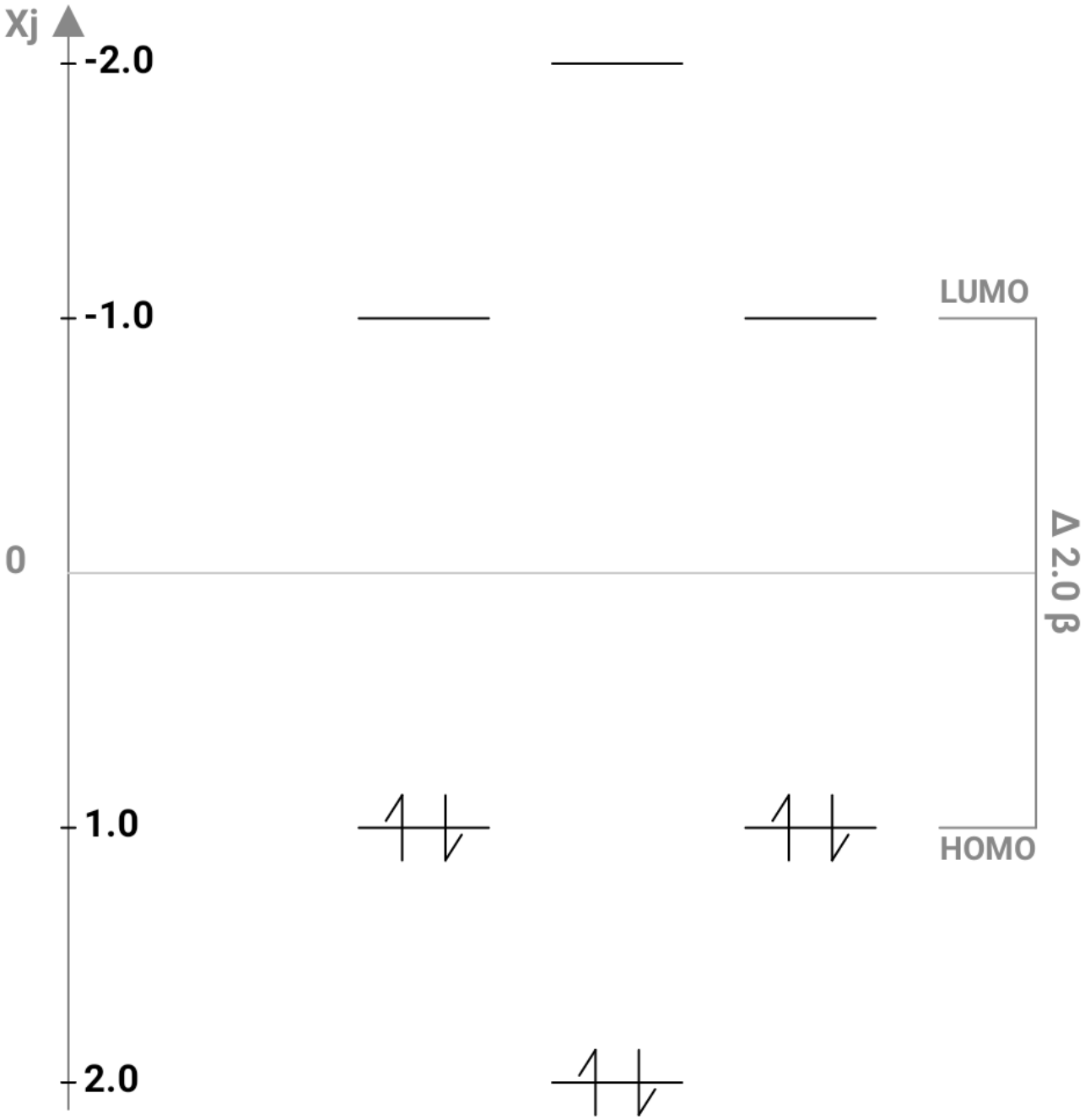


HMO-Energies

x1 = 2.0; x2 = 1.0; x3 = 1.0; x4 = -1.0; x5 = -1.0; x6 = -2.0;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 6α + 8.0β -

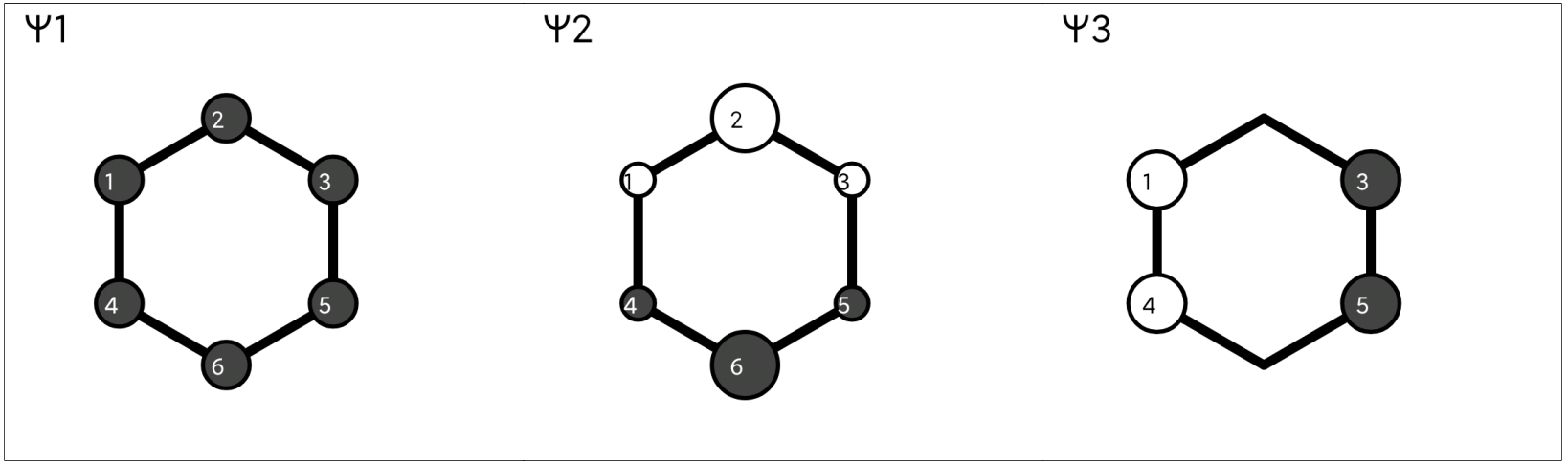
this corresponds to one πelectron: 1.333β

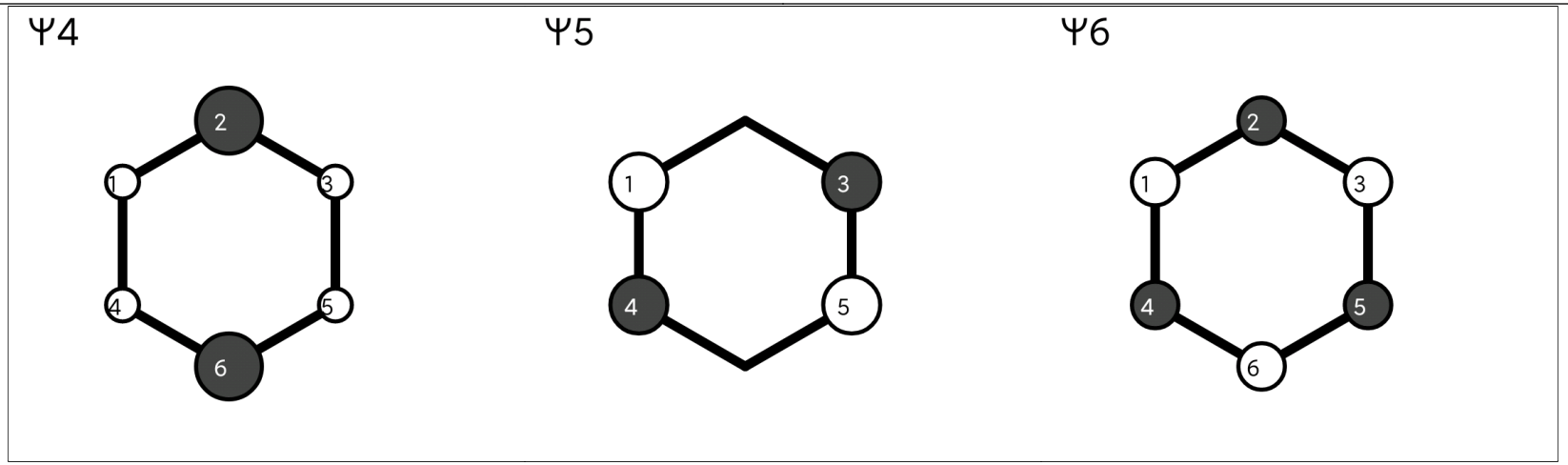
2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6
	x1= 2.0	x2= 1.0	x3= 1.0	x4= -1.0	x5= -1.0	x6= -2.0
1	-0.408	0.289	0.5	0.289	0.5	0.408
2	-0.408	0.577	0.0	-0.577	0.0	-0.408
3	-0.408	0.289	-0.5	0.289	-0.5	0.408
4	-0.408	-0.289	0.5	0.289	-0.5	-0.408
5	-0.408	-0.289	-0.5	0.289	0.5	-0.408
6	-0.408	-0.577	0.0	-0.577	0.0	0.408

2.2. Molecule orbital presentation:



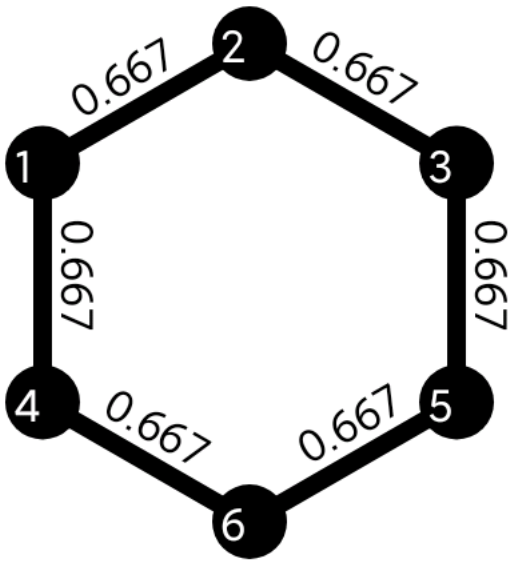

Ψ4
2
1
3
4
5
6
Ψ5
1
3
4
5
Ψ6
2
1
3
4
5
6

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6
1	1.0					
2	0.667	1.0				
3	0.0	0.667	1.0			
4	0.667	0.0	-0.333	1.0		
5	-0.333	0.0	0.667	0.0	1.0	
6	0.0	-0.333	0.0	0.667	0.667	1.0

3.2. Presentation of bond order:

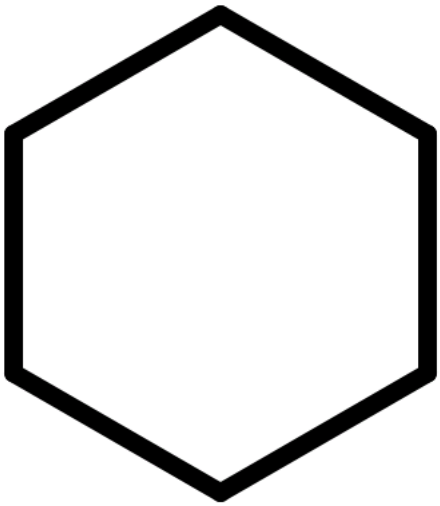


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6
1	0.0					
2		0.0				
3			0.0			
4				0.0		
5					0.0	
6						0.0

4.2. Presentation of molecule:

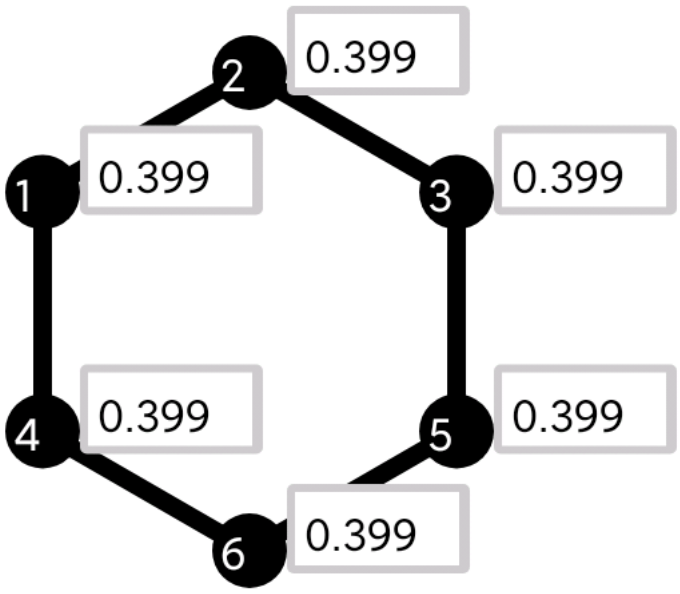


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6
0.399	0.399	0.399	0.399	0.399	0.399

5.2. Presentation of molecule:

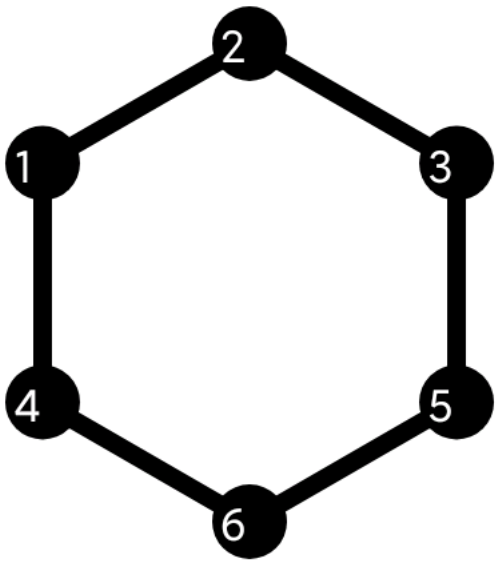


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6
1	0.398					
2	-0.157	0.398				
3	0.009	-0.157	0.398			
4	-0.157	0.009	-0.102	0.398		
5	-0.102	0.009	-0.157	0.009	0.398	
6	0.009	-0.102	0.009	-0.157	-0.157	0.398

6.2. Presentation of molecule:

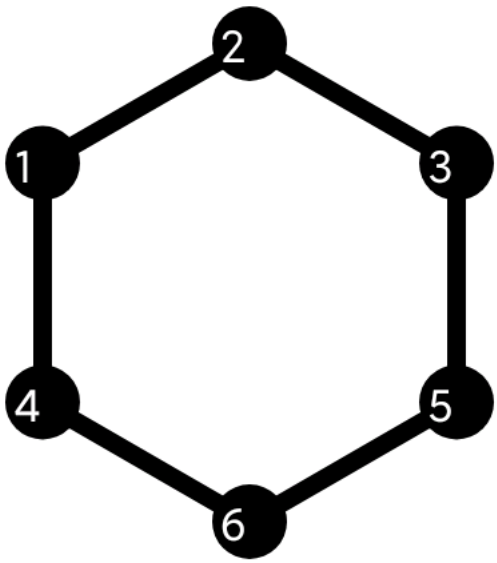


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6
1 2	0.0	0.0	0.0	0.0	0.0	0.0
1 4	0.0	0.0	0.0	0.0	0.0	0.0
2 3	0.0	0.0	0.0	0.0	0.0	0.0
3 5	0.0	0.0	0.0	0.0	0.0	0.0
4 6	0.0	0.0	0.0	0.0	0.0	0.0
5 6	0.0	0.0	0.0	0.0	0.0	0.0

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 4	2 3	3 5	4 6	5 6
1 2	0.241					
1 4	-0.204	0.241				
2 3	-0.204	0.13	0.241			
3 5	0.13	-0.093	-0.204	0.241		
4 6	0.13	-0.204	-0.093	0.13	0.241	
5 6	-0.093	0.13	0.13	-0.204	-0.204	0.241

8.2. Presentation of molecule: