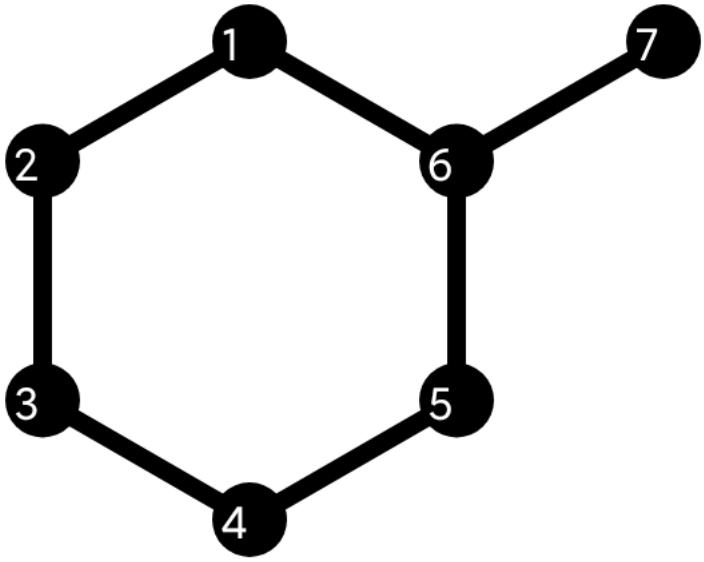
Print calculated values

Report generated by:root, 13.02.2020 - 11:35:16

The following determinant is calculated:

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

It is about this molecule:

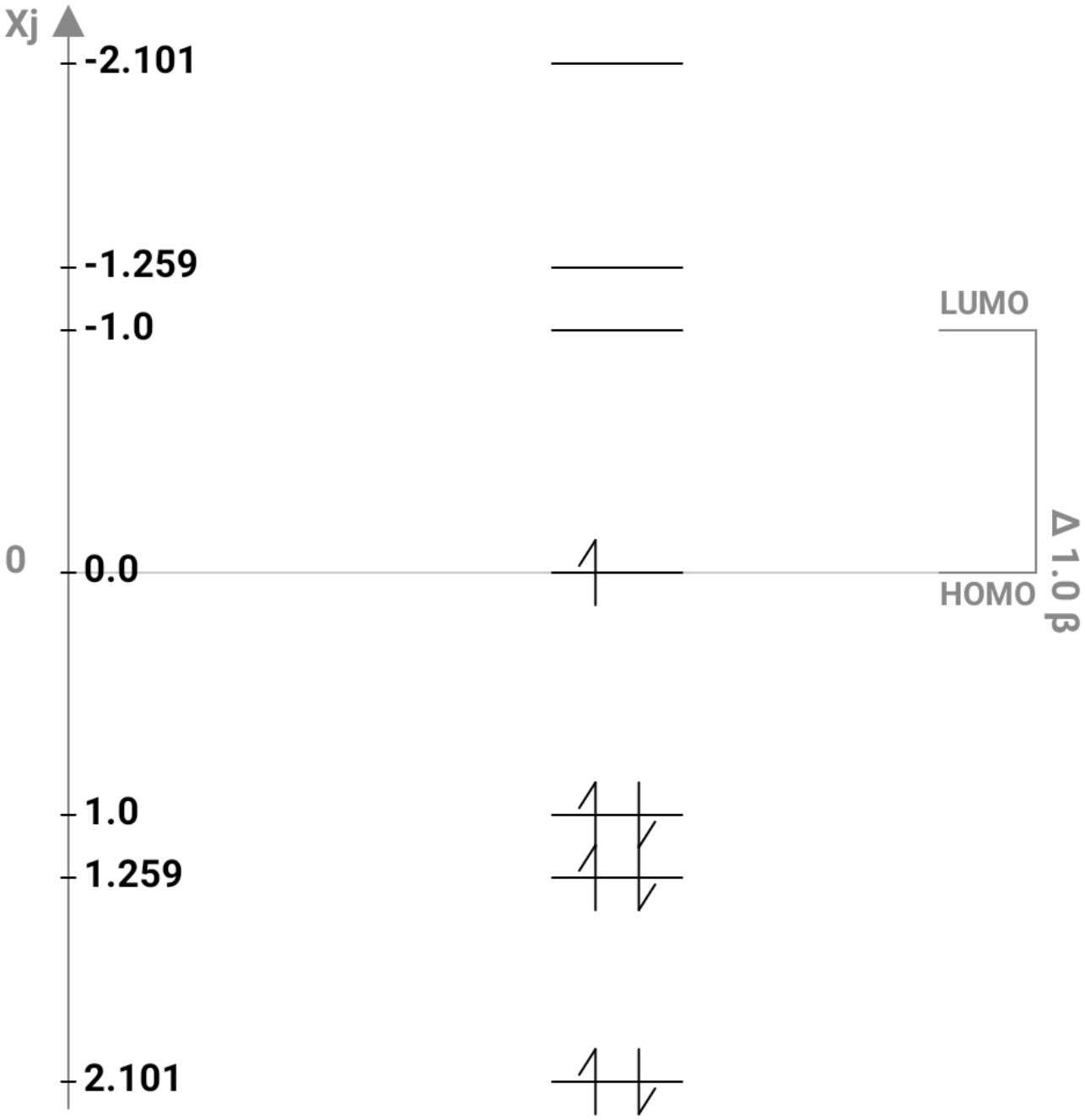


HMO-Energies

x1 = 2.101; x2 = 1.259; x3 = 1.0; x4 = 0.0; x5 = -1.0; x6 = -1.259; x7 = -2.101;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 7α + 8.72β -

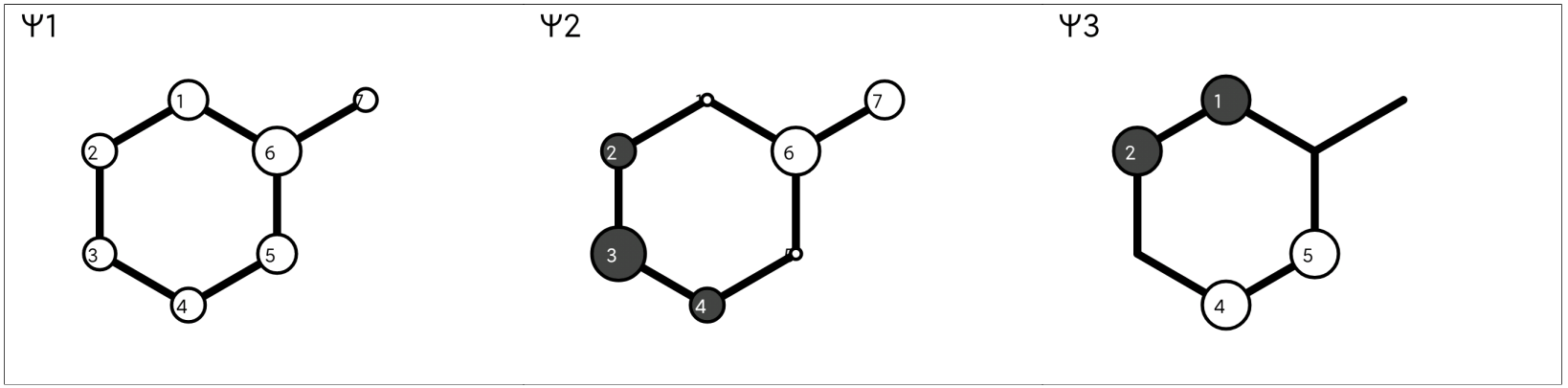
this corresponds to one πelectron: 1.246β

2. Hueckel-coefficient

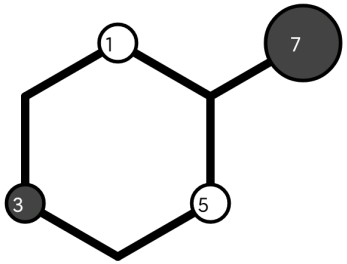
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7
	x1= 2.101	x2= 1.259	x3= 1.0	x4= 0.0	x5= -1.0	x6= -1.259	x7= -2.101
1	0.406	0.116	-0.5	0.378	-0.5	0.116	0.406
2	0.354	-0.354	-0.5	0.0	0.5	0.354	-0.354
3	0.337	-0.562	0.0	-0.378	0.0	-0.562	0.337
4	0.354	-0.354	0.5	0.0	-0.5	0.354	-0.354
5	0.406	0.116	0.5	0.378	0.5	0.116	0.406
6	0.5	0.5	0.0	0.0	0.0	-0.5	-0.5
7	0.238	0.397	0.0	-0.756	0.0	0.397	0.238

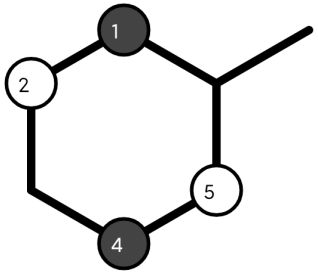
2.2. Molecule orbital presentation:



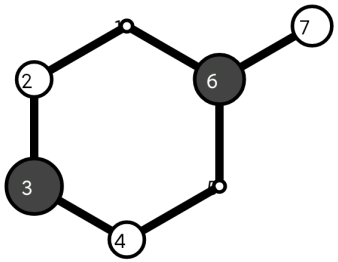
Ψ4



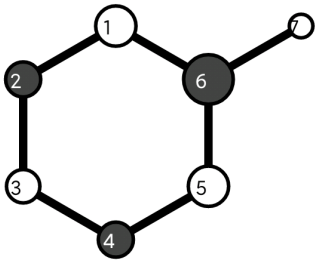
Ψ5



Ψ6



Ψ7

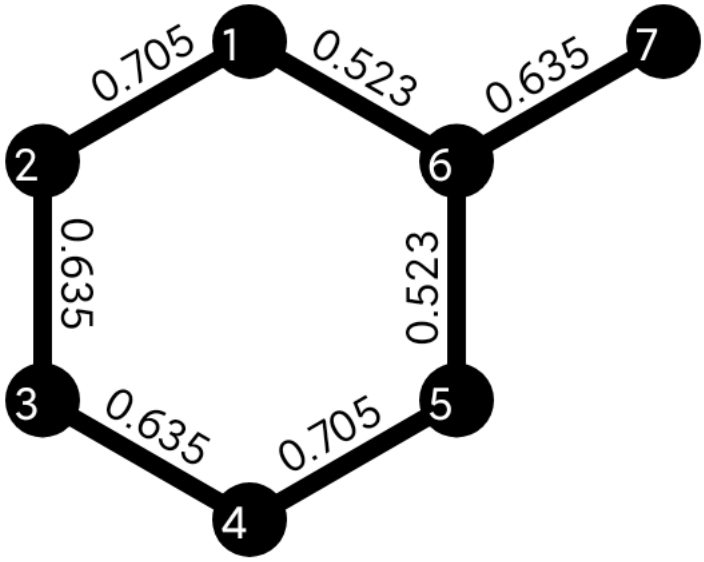


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7
1	1.0						
2	0.705	1.0					
3	0.0	0.635	1.0				
4	-0.295	0.0	0.635	1.0			
5	0.0	-0.295	0.0	0.705	1.0		
6	0.523	0.0	-0.225	0.0	0.523	1.0	
7	0.0	-0.112	0.0	-0.112	0.0	0.635	1.0

3.2. Presentation of bond order:

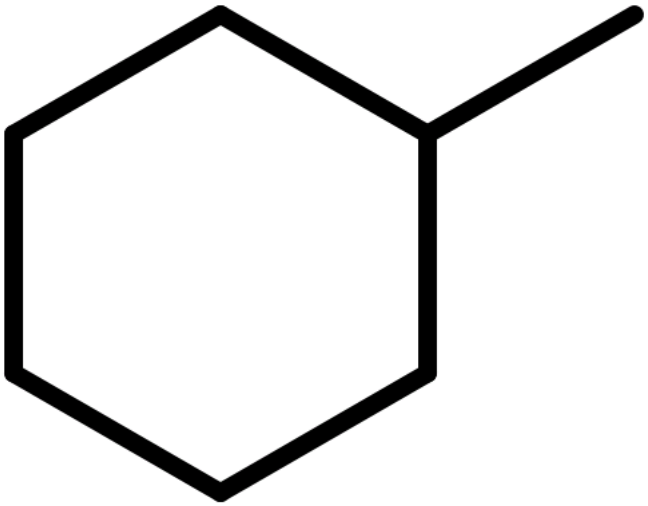


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7
1	0.0						
2		0.0					
3			0.0				
4				0.0			
5					0.0		
6						0.0	
7							0.0

4.2. Presentation of molecule:

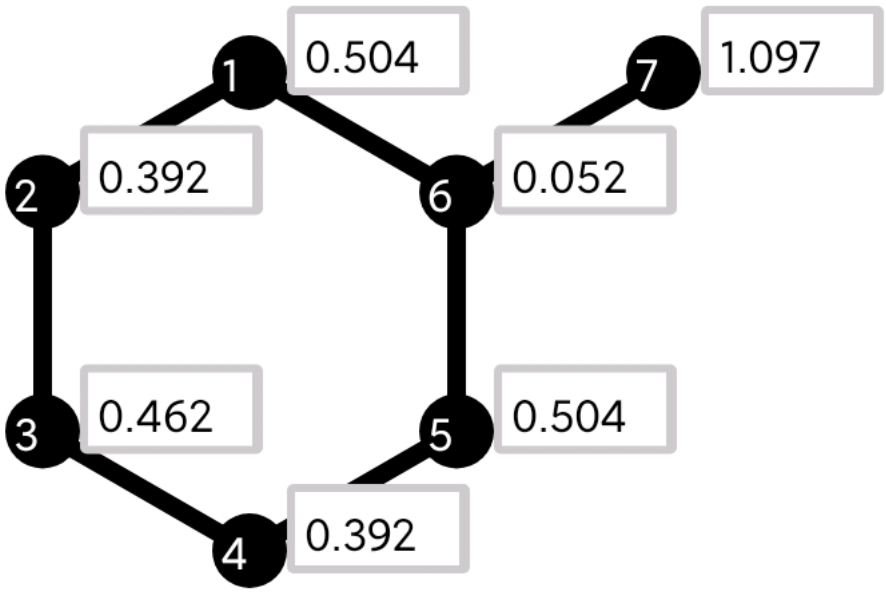


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7
0.504	0.392	0.462	0.392	0.504	0.052	1.097

5.2. Presentation of molecule:

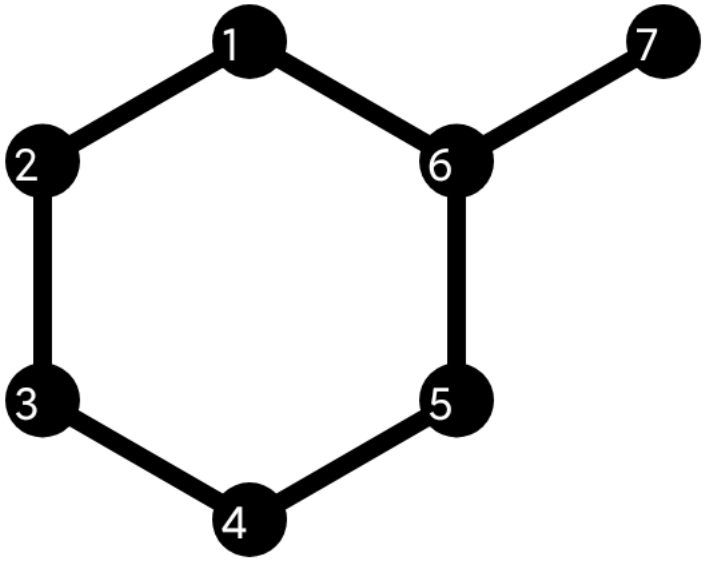


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7
1	0.469						
2	-0.189	0.393					
3	-0.004	-0.132	0.429				
4	-0.077	0.011	-0.132	0.393			
5	-0.054	-0.077	-0.004	-0.189	0.469		
6	-0.073	0.005	-0.04	0.005	-0.073	0.308	
7	-0.072	-0.01	-0.116	-0.01	-0.072	-0.132	0.412

6.2. Presentation of molecule:

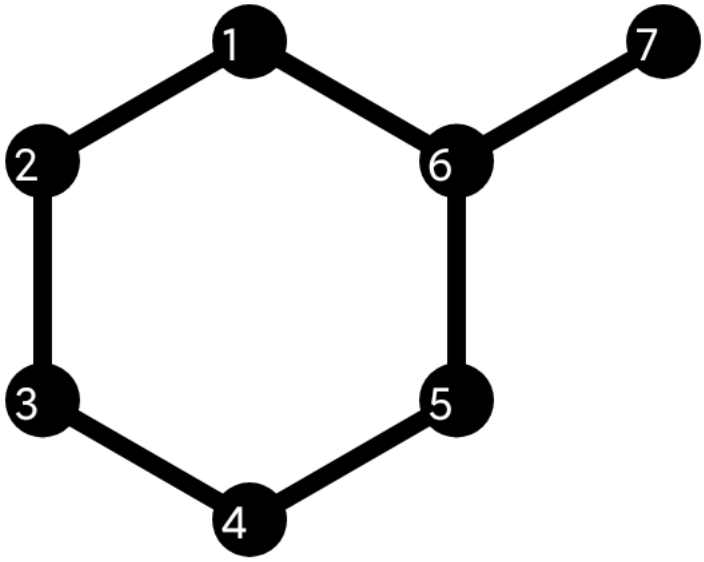


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7
1 2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1 6	0.0	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	0.0
3 4	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4 5	0.0	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	0.0
6 7	0.0	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 6	2 3	3 4	4 5	5 6	6 7
1 2	0.256						
1 6	-0.16	0.307					
2 3	-0.245	0.1	0.3				
3 4	0.12	-0.04	-0.195	0.3			
4 5	-0.084	0.065	0.12	-0.245	0.256		
5 6	0.065	-0.076	-0.04	0.1	-0.16	0.307	
6 7	0.05	-0.195	-0.04	-0.04	0.05	-0.195	0.37

8.2. Presentation of molecule: