

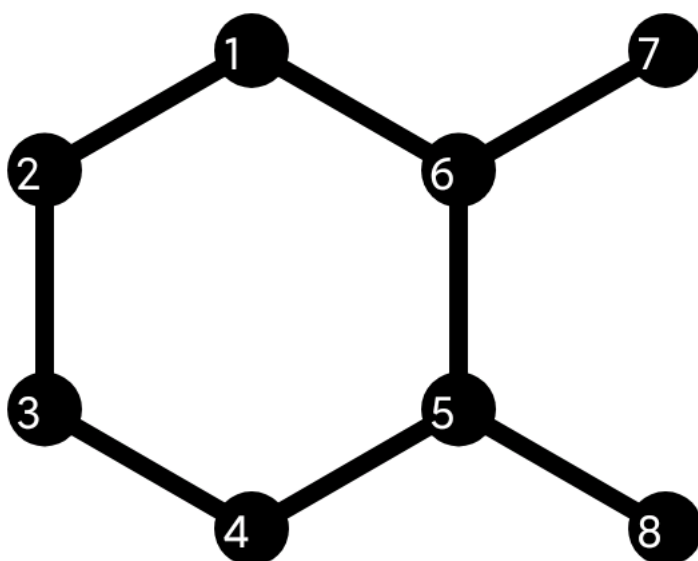
Print calculated values

Report generated by:root, 13.02.2020 - 09:31:35

The following determinant is calculated:

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

It is about this molecule:

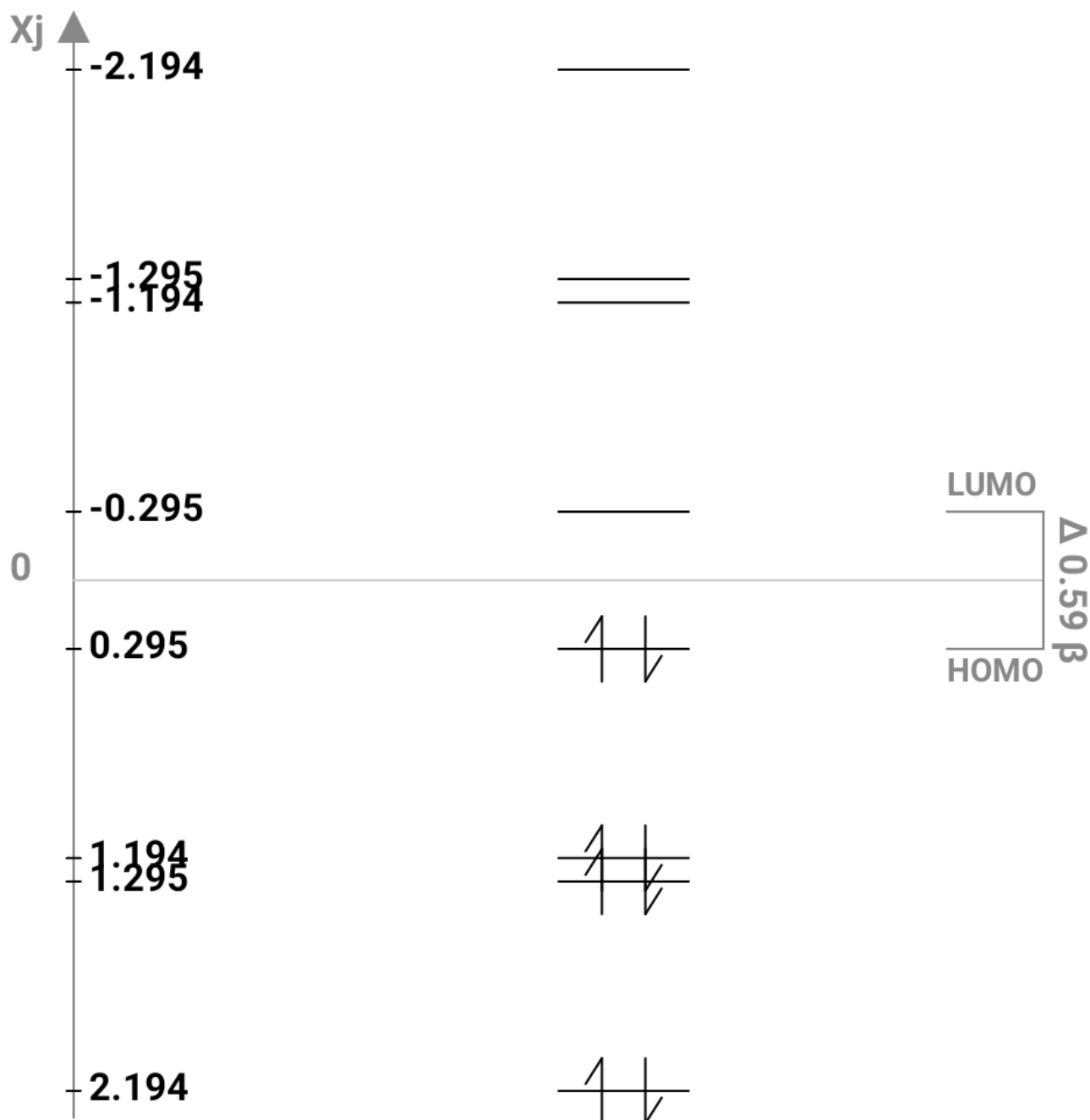


HMO-Energies

$x_1 = 2.194$; $x_2 = 1.295$; $x_3 = 1.194$; $x_4 = 0.295$; $x_5 = -0.295$; $x_6 = -1.194$; $x_7 = -1.295$; $x_8 = -2.194$;

1. Energy-eigenvalues

1.1. Calculated values:



total Power E_π : $8\alpha + 9.956\beta$ -

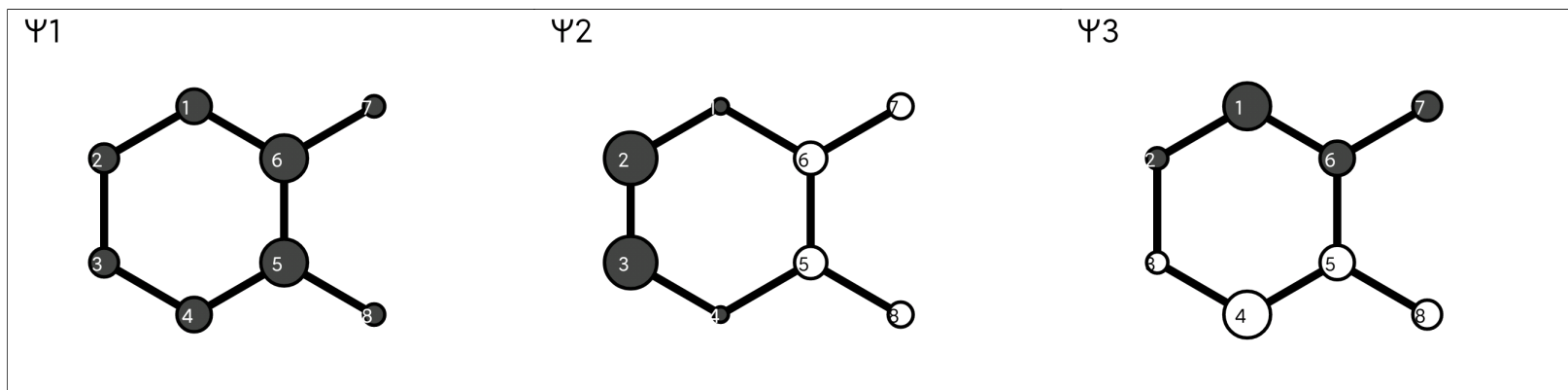
this corresponds to one π electron: 1.245β

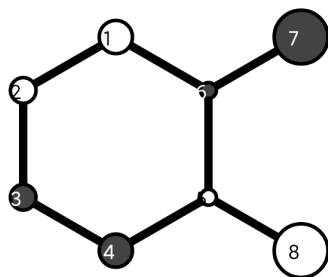
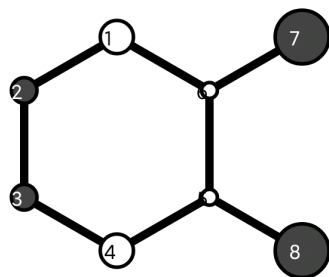
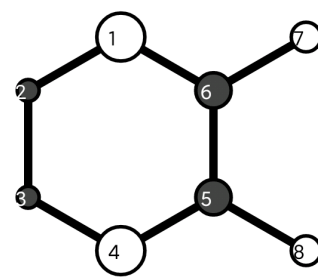
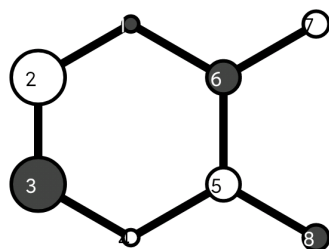
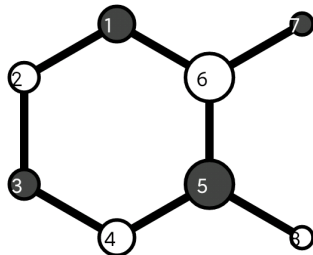
2. Hückel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8
	x1= 2.194	x2= 1.295	x3= 1.194	x4= 0.295	x5= -0.295	x6= -1.194	x7= -1.295	x8= -2.194
1	-0.357	-0.16	-0.484	0.335	0.335	0.484	-0.16	-0.357
2	-0.299	-0.543	-0.221	0.259	-0.259	-0.221	0.543	0.299
3	-0.299	-0.543	0.221	-0.259	-0.259	-0.221	-0.543	-0.299
4	-0.357	-0.16	0.484	-0.335	0.335	0.484	0.16	0.357
5	-0.484	0.335	0.357	0.16	0.16	-0.357	0.335	-0.484
6	-0.484	0.335	-0.357	-0.16	0.16	-0.357	-0.335	0.484
7	-0.221	0.259	-0.299	-0.543	-0.543	0.299	0.259	-0.221
8	-0.221	0.259	0.299	0.543	-0.543	0.299	-0.259	0.221

2.2. Molecule orbital presentation:



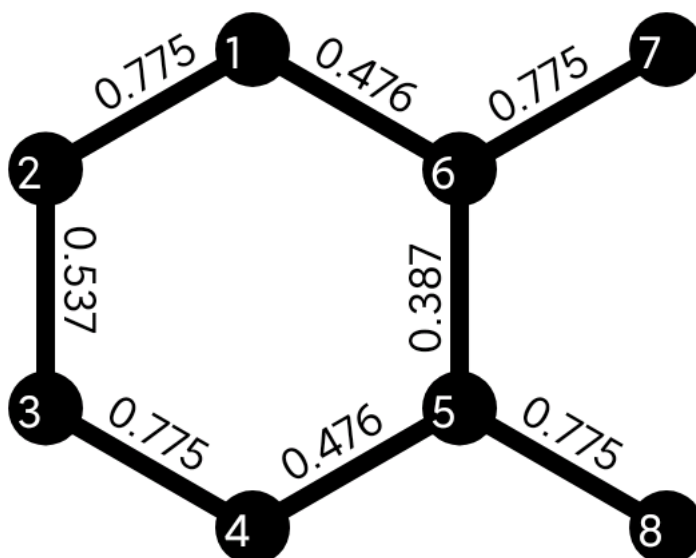
Ψ_4  Ψ_5  Ψ_6  Ψ_7  Ψ_8 

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8
1	1.0							
2	0.775	1.0						
3	0.0	0.537	1.0					
4	-0.387	0.0	0.775	1.0				
5	0.0	-0.149	0.0	0.476	1.0			
6	0.476	0.0	-0.149	0.0	0.387	1.0		
7	0.0	-0.298	0.0	0.149	0.0	0.775	1.0	
8	0.149	0.0	-0.298	0.0	0.775	0.0	-0.537	1.0

3.2. Presentation of bond order:

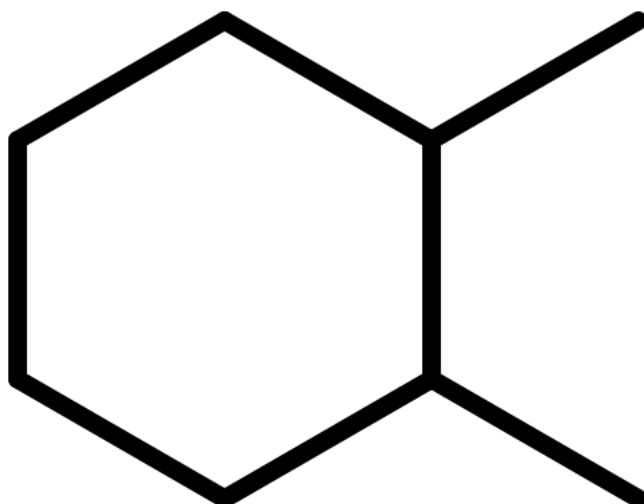


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8
1	0.0							
2		0.0						
3			0.0					
4				0.0				
5					0.0			
6						0.0		
7							0.0	
8								0.0

4.2. Presentation of molecule:

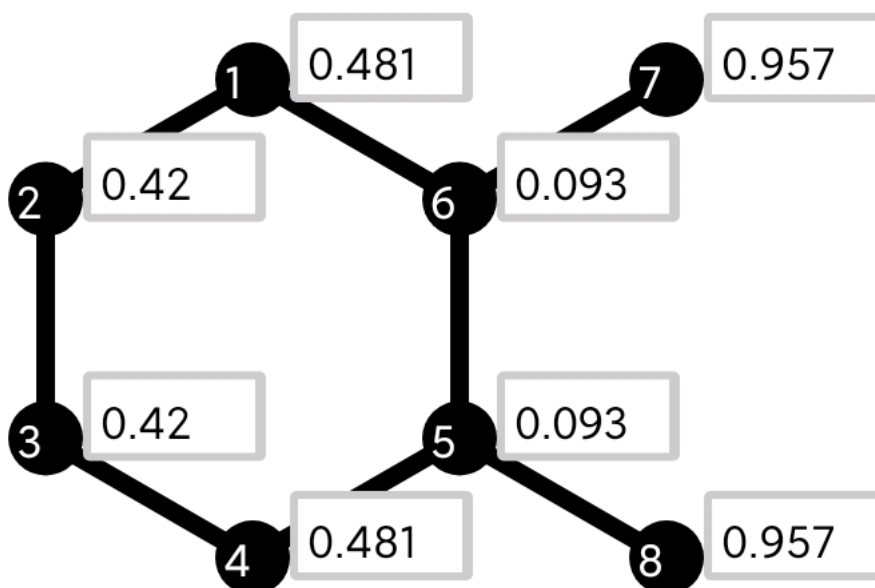


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8
0.481	0.42	0.42	0.481	0.093	0.093	0.957	0.957

5.2. Presentation of molecule:

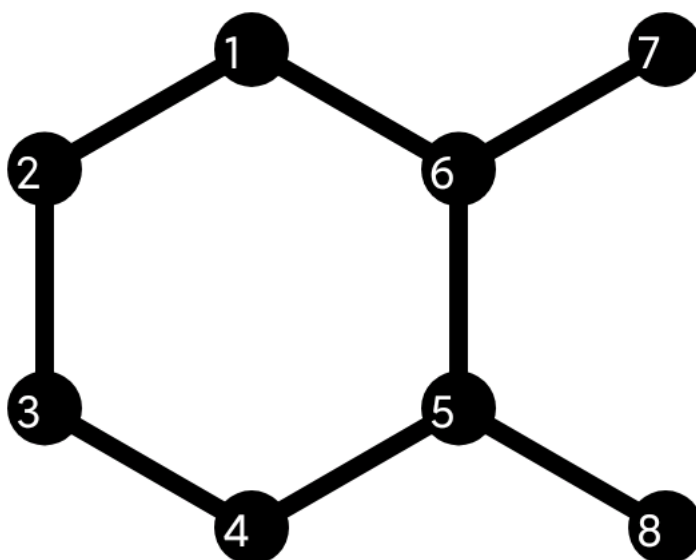


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8
1	0.493							
2	-0.288	0.429						
3	0.039	-0.079	0.429					
4	-0.192	0.039	-0.288	0.493				
5	0.005	-0.015	0.014	-0.055	0.33			
6	-0.055	0.014	-0.015	0.005	-0.029	0.33		
7	0.119	-0.155	0.055	-0.12	0.039	-0.288	0.936	
8	-0.12	0.055	-0.155	0.119	-0.288	0.039	-0.585	0.936

6.2. Presentation of molecule:

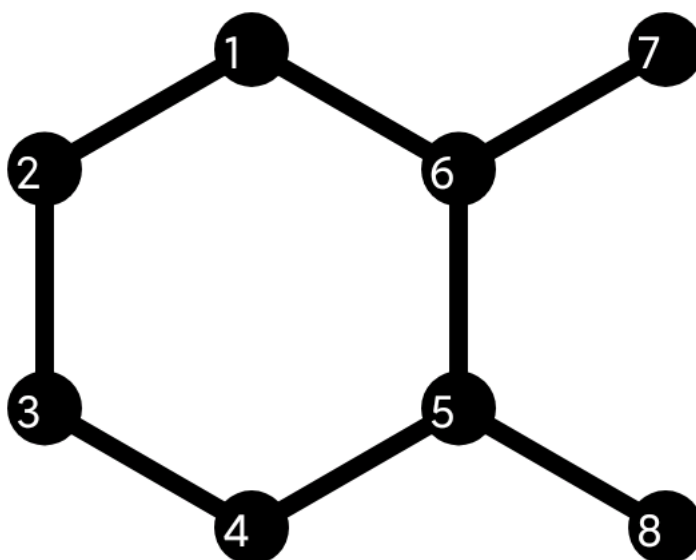


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8
1 2	0.0	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	0.0
2 3	0.0	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	0.0
4 5	0.0	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	0.0
5 8	0.0	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	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	5 8	6 7
1 2	0.17							
1 6	-0.16	0.337						
2 3	-0.199	0.075	0.35					
3 4	0.107	-0.04	-0.199	0.17				
4 5	-0.04	0.038	0.075	-0.16	0.337			
5 6	0.025	-0.05	-0.001	0.025	-0.05	0.301		
5 8	0.02	-0.011	-0.05	0.078	-0.189	-0.125	0.198	
6 7	0.078	-0.189	-0.05	0.02	-0.011	-0.125	0.078	0.198

8.2. Presentation of molecule:

