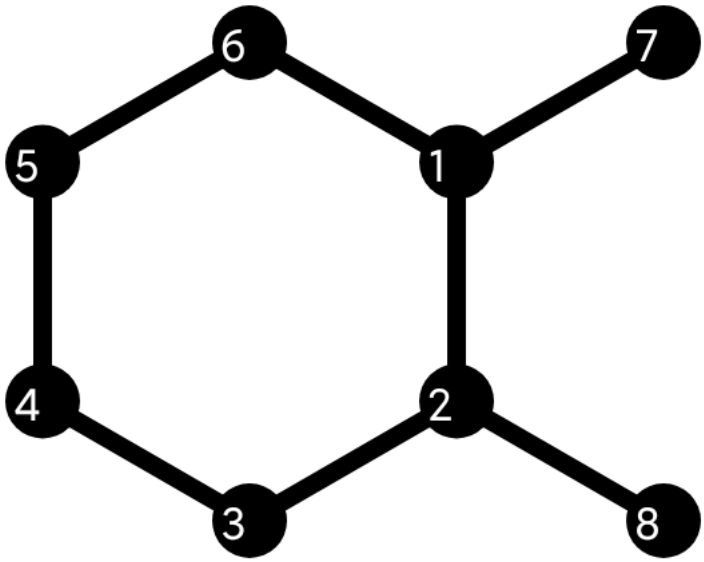
Print calculated values

Report generated by:root, 24.02.2020 - 14:45:02

The following determinant is calculated:

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

It is about this molecule:

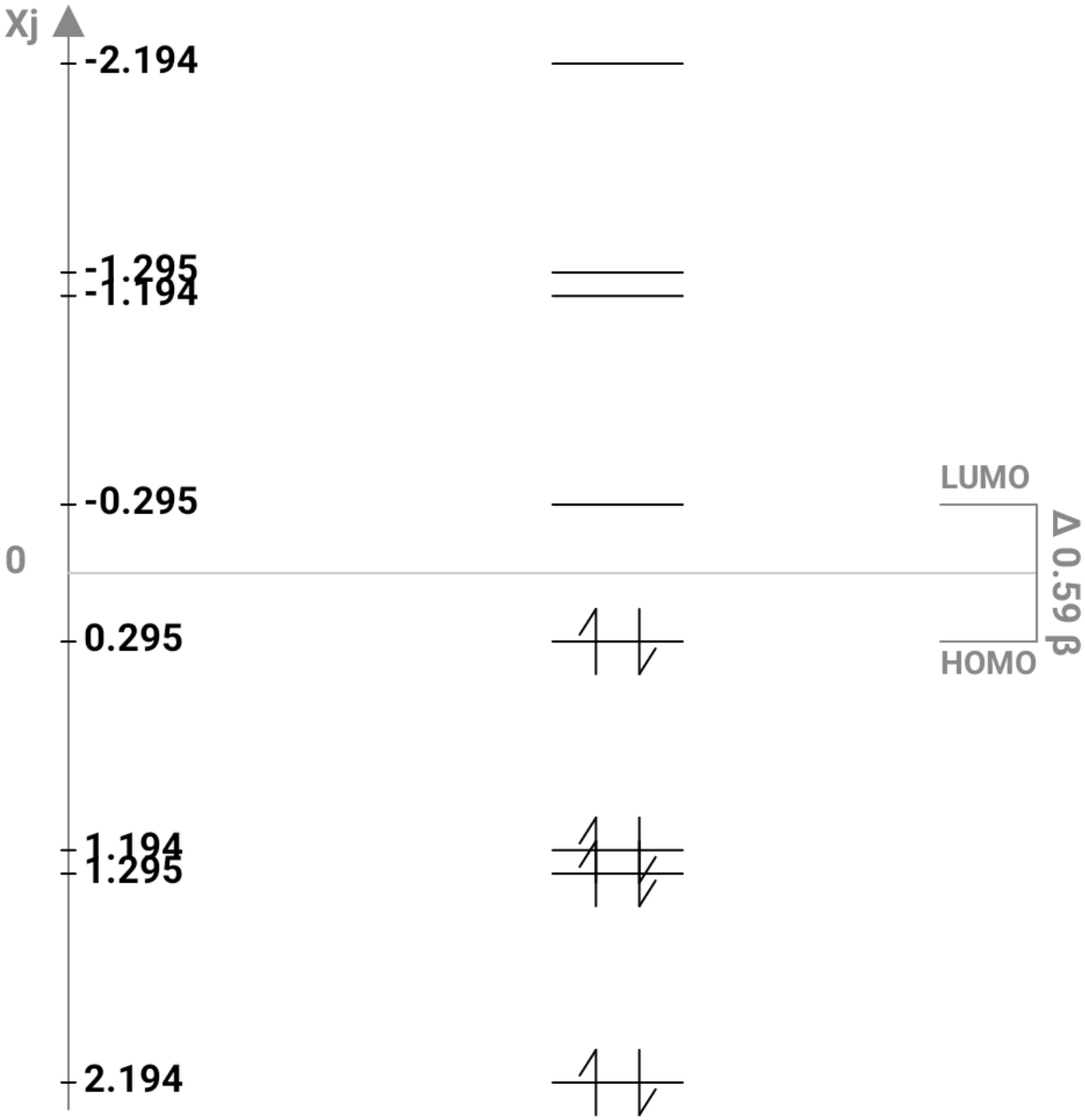


HMO-Energies

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. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 8α + 9.956β -

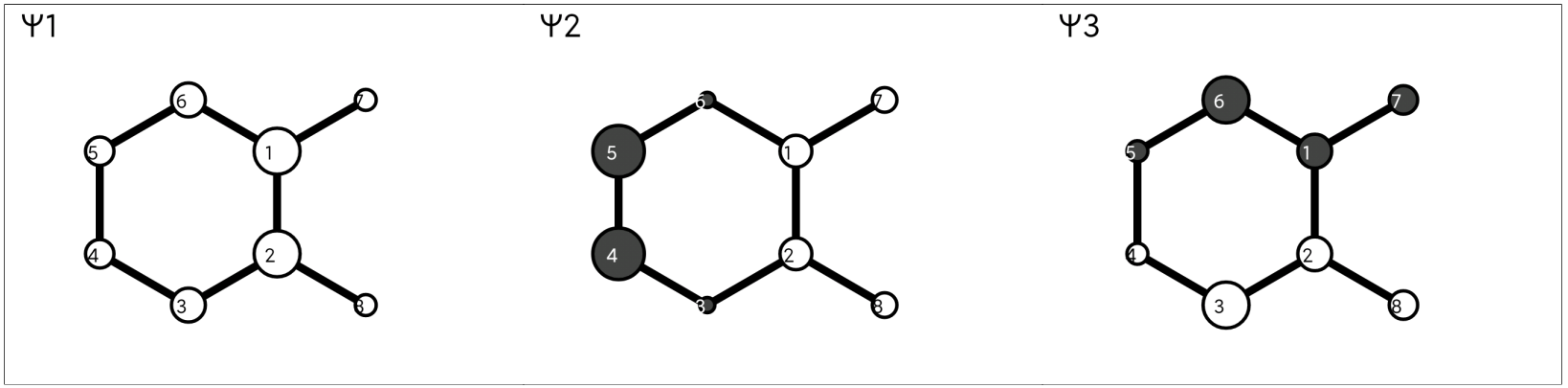
this corresponds to one πelectron: 1.245β

2. Hueckel-coefficient

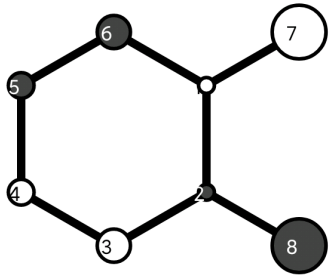
2.1. Calculated values:

	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	0.484	0.335	-0.357	0.16	-0.16	0.357	0.335	0.484
2	0.484	0.335	0.357	-0.16	-0.16	0.357	-0.335	-0.484
3	0.357	-0.16	0.484	0.335	-0.335	-0.484	-0.16	0.357
4	0.299	-0.543	0.221	0.259	0.259	0.221	0.543	-0.299
5	0.299	-0.543	-0.221	-0.259	0.259	0.221	-0.543	0.299
6	0.357	-0.16	-0.484	-0.335	-0.335	-0.484	0.16	-0.357
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

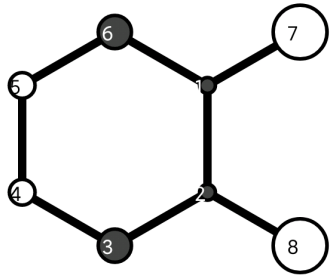
2.2. Molecule orbital presentation:



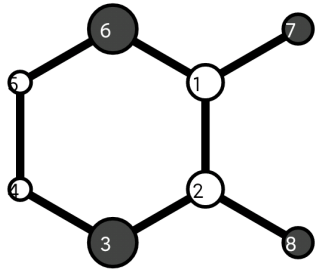
Ψ4



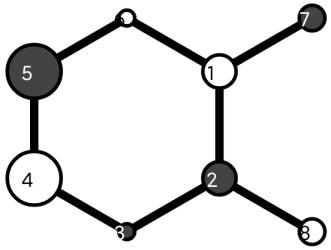
Ψ5



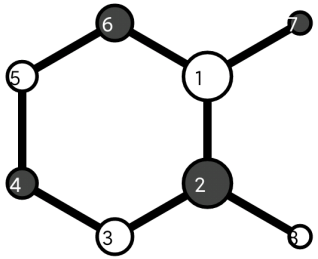
Ψ6



Ψ7



Ψ8

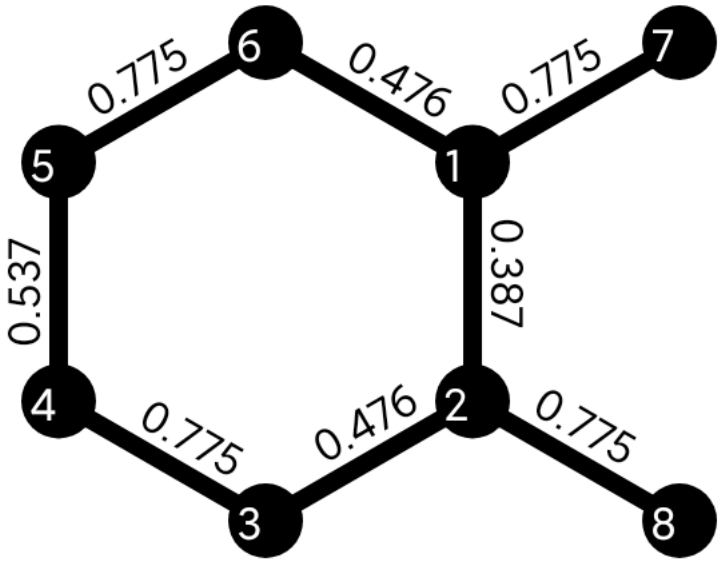


3. Bond Order

3.1. Calculated values:

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

3.2. Presentation of bond order:

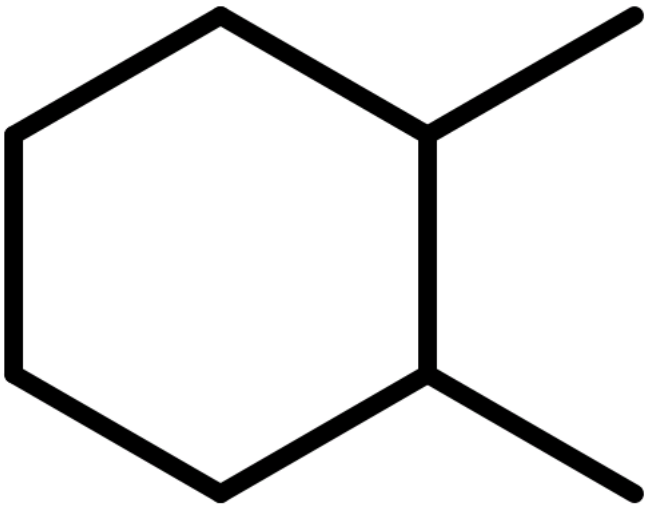


4. Net Charge

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:

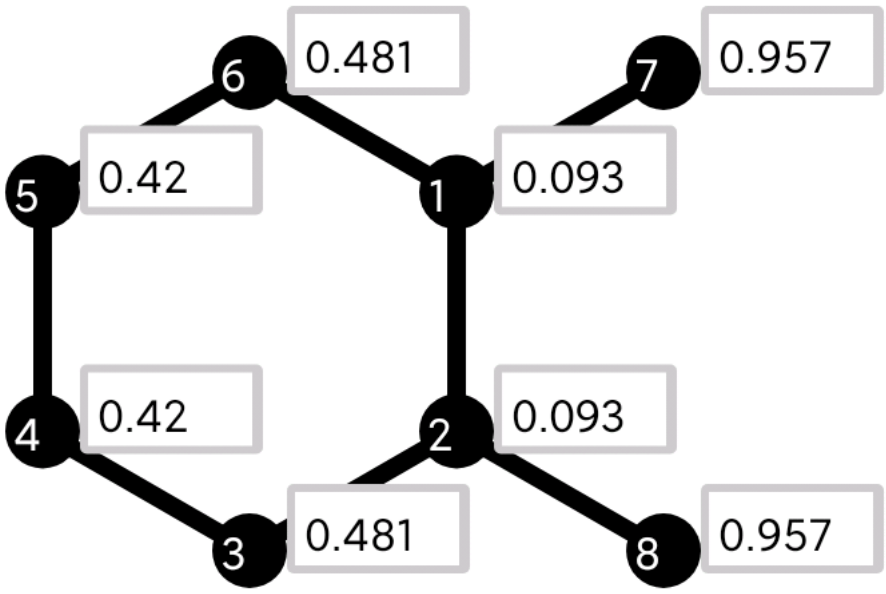


5. Free valences

5.1. Calculated values:

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

5.2. Presentation of molecule:

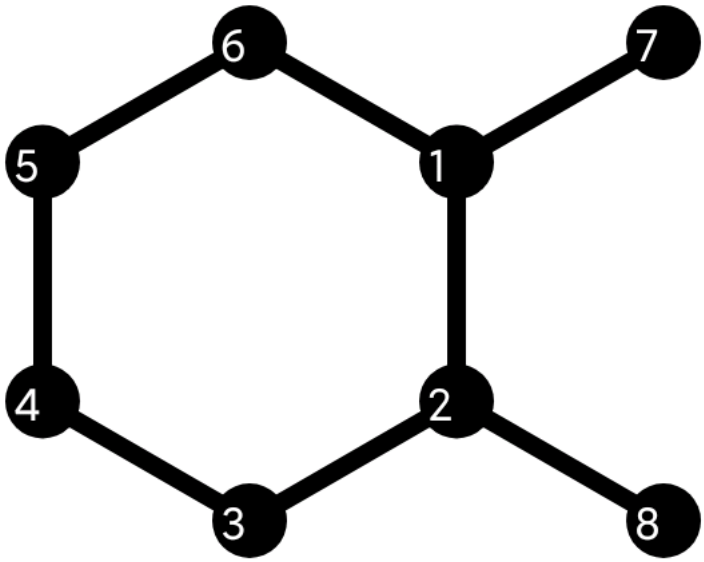


6. Atom-Atom-Polarizability

6.1. Calculated values:

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

6.2. Presentation of molecule:

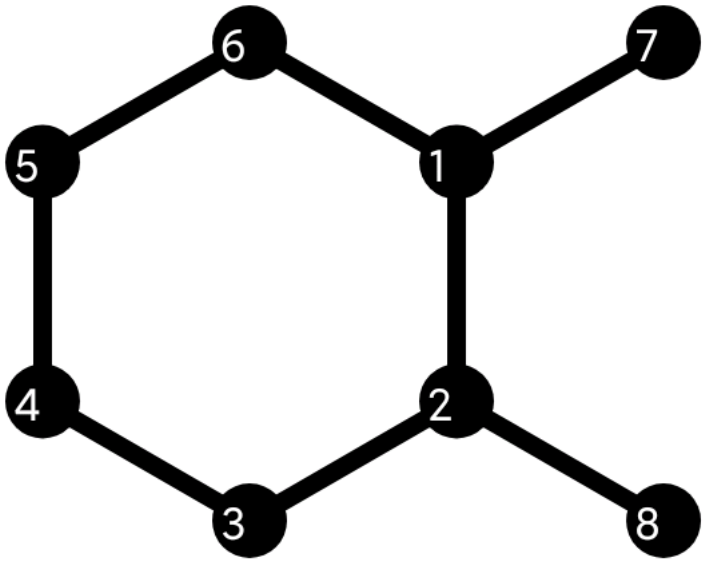


7. Bond-Atom-Polarizability

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
1 7	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
2 8	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

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

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

8.2. Presentation of molecule: