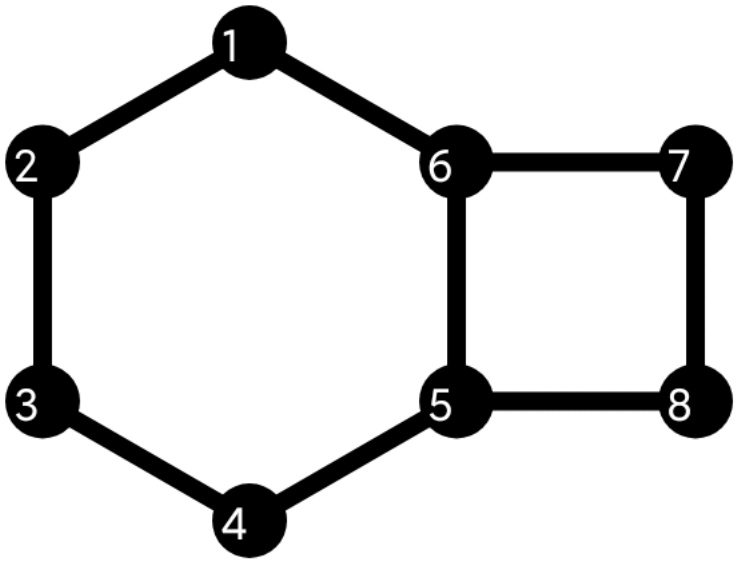
Print calculated values

Report generated by:root, 14.03.2020 - 21:24:23

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	1.0
0.0	0.0	0.0	0.0	1.0	0.0	1.0	-x

It is about this molecule:

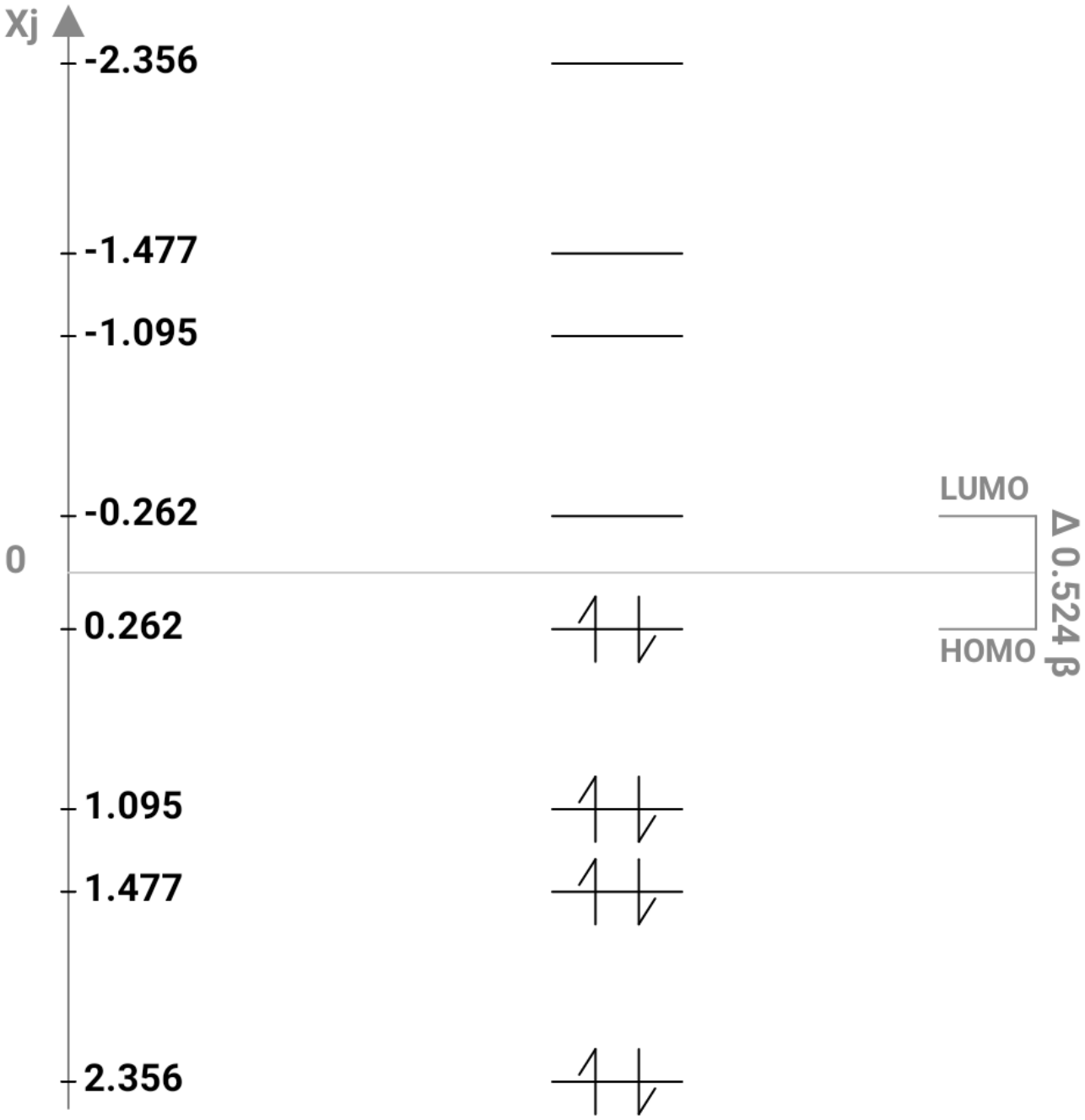


HMO-Energies

x1 = 2.356; x2 = 1.477; x3 = 1.095; x4 = 0.262; x5 = -0.262; x6 = -1.095; x7 = -1.477; x8 = -2.356;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 8α + 10.38β -

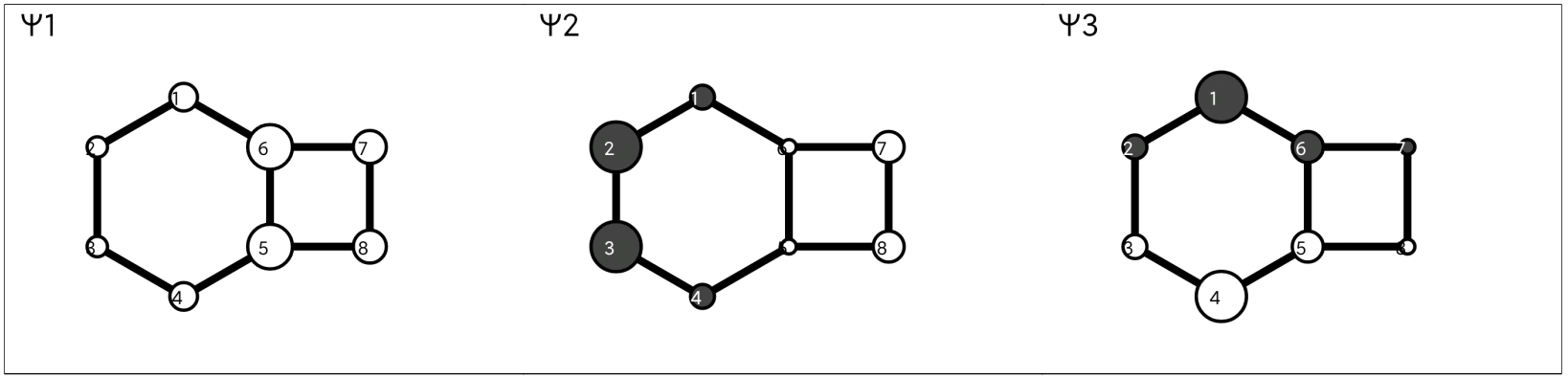
this corresponds to one πelectron: 1.297β

2. Hueckel-coefficient

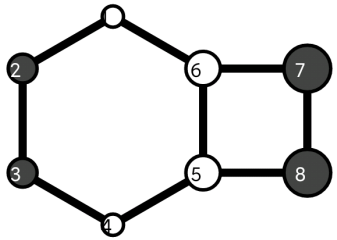
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8
	x1= 2.356	x2= 1.477	x3= 1.095	x4= 0.262	x5= -0.262	x6= -1.095	x7= -1.477	x8= -2.356
1	0.299	-0.259	-0.543	0.221	0.221	-0.543	-0.259	0.299
2	0.221	-0.543	-0.259	-0.299	0.299	0.259	0.543	-0.221
3	0.221	-0.543	0.259	-0.299	-0.299	0.259	-0.543	0.221
4	0.299	-0.259	0.543	0.221	-0.221	-0.543	0.259	-0.299
5	0.484	0.16	0.335	0.357	0.357	0.335	0.16	0.484
6	0.484	0.16	-0.335	0.357	-0.357	0.335	-0.16	-0.484
7	0.357	0.335	-0.16	-0.484	-0.484	-0.16	0.335	0.357
8	0.357	0.335	0.16	-0.484	0.484	-0.16	-0.335	-0.357

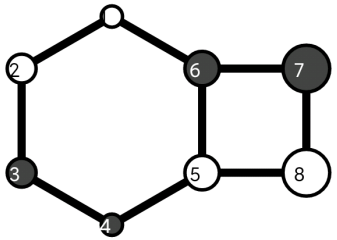
2.2. Molecule orbital presentation:



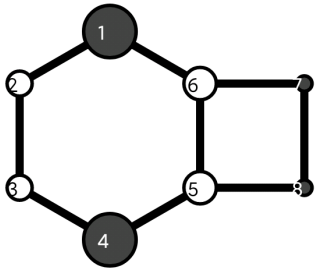
Ψ4



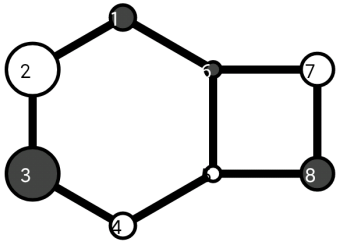
Ψ5



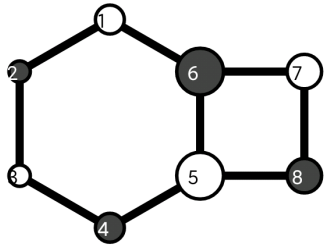
Ψ6



Ψ7



Ψ8

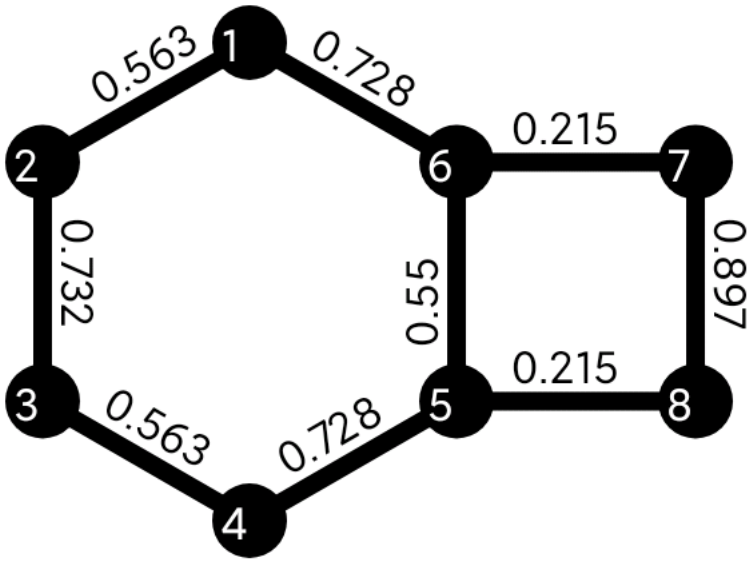


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8
1	1.0							
2	0.563	1.0						
3	0.0	0.732	1.0					
4	-0.179	0.0	0.563	1.0				
5	0.0	-0.348	0.0	0.728	1.0			
6	0.728	0.0	-0.348	0.0	0.55	1.0		
7	0.0	0.166	0.0	-0.348	0.0	0.215	1.0	
8	-0.348	0.0	0.166	0.0	0.215	0.0	0.897	1.0

3.2. Presentation of bond order:

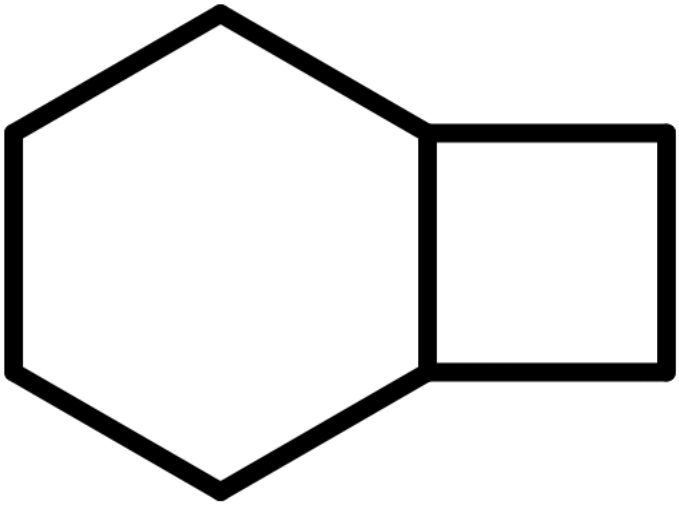


4. Net Charge

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:

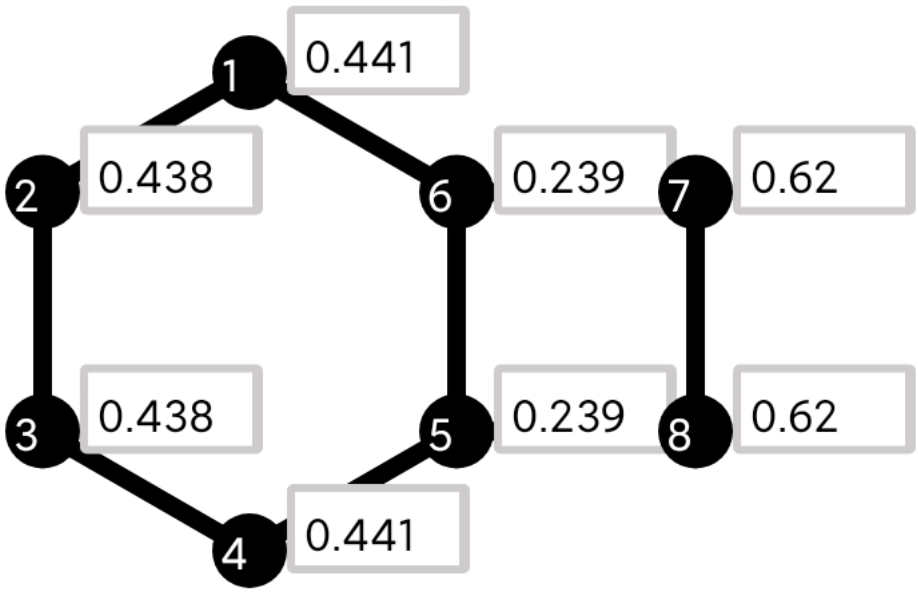


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8
0.441	0.438	0.438	0.441	0.239	0.239	0.62	0.62

5.2. Presentation of molecule:

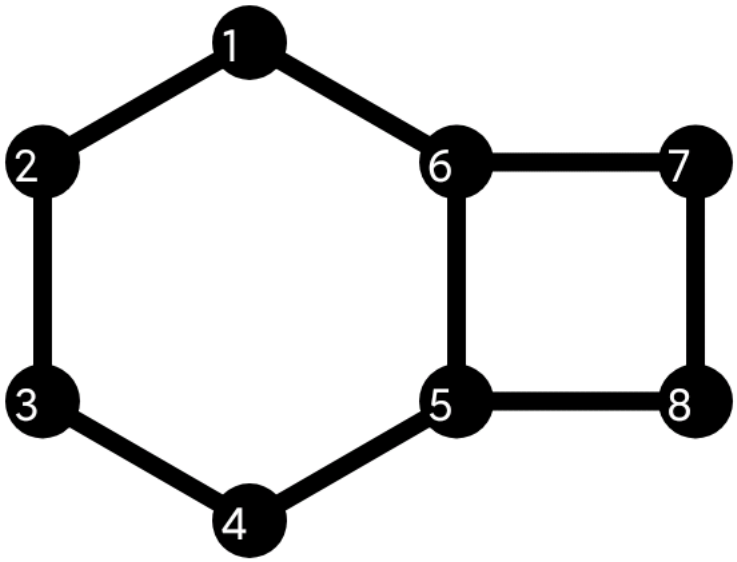


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8
1	0.438							
2	-0.092	0.458						
3	0.035	-0.249	0.458					
4	-0.023	0.035	-0.092	0.438				
5	0.013	-0.166	0.053	-0.258	0.468			
6	-0.258	0.053	-0.166	0.013	-0.159	0.468		
7	0.053	-0.116	0.078	-0.166	0.172	-0.124	0.746	
8	-0.166	0.078	-0.116	0.053	-0.124	0.172	-0.642	0.746

6.2. Presentation of molecule:

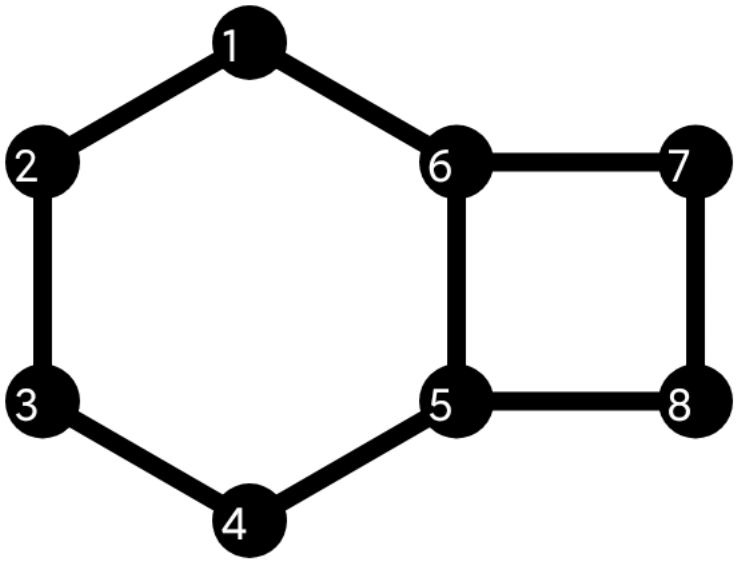


7. Bond-Atom-Polarizability

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 8	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	7 8
1 2	0.355								
1 6	-0.208	0.189							
2 3	-0.205	0.109	0.209						
3 4	0.094	-0.054	-0.205	0.355					
4 5	-0.054	0.051	0.109	-0.208	0.189				
5 6	0.177	-0.175	-0.113	0.177	-0.175	0.309			
5 8	-0.138	0.123	0.068	-0.089	-0.031	-0.125	0.457		
6 7	-0.089	-0.031	0.068	-0.138	0.123	-0.125	-0.145	0.457	
7 8	0.068	-0.004	-0.039	0.068	-0.004	0.048	-0.12	-0.12	0.104

8.2. Presentation of molecule: