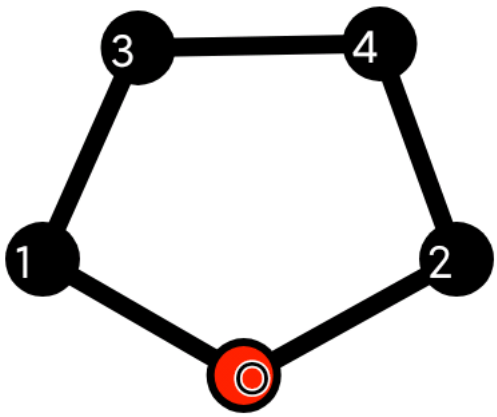
Print calculated values

Report generated by:root, 16.02.2020 - 18:01:21

The following determinant is calculated:

-x	0.0	1.0	0.0	0.19
0.0	-x	0.0	1.0	0.19
1.0	0.0	-x	1.0	0.0
0.0	1.0	1.0	-x	0.0
0.19	0.19	0.0	0.0	-x+2.06

It is about this molecule:

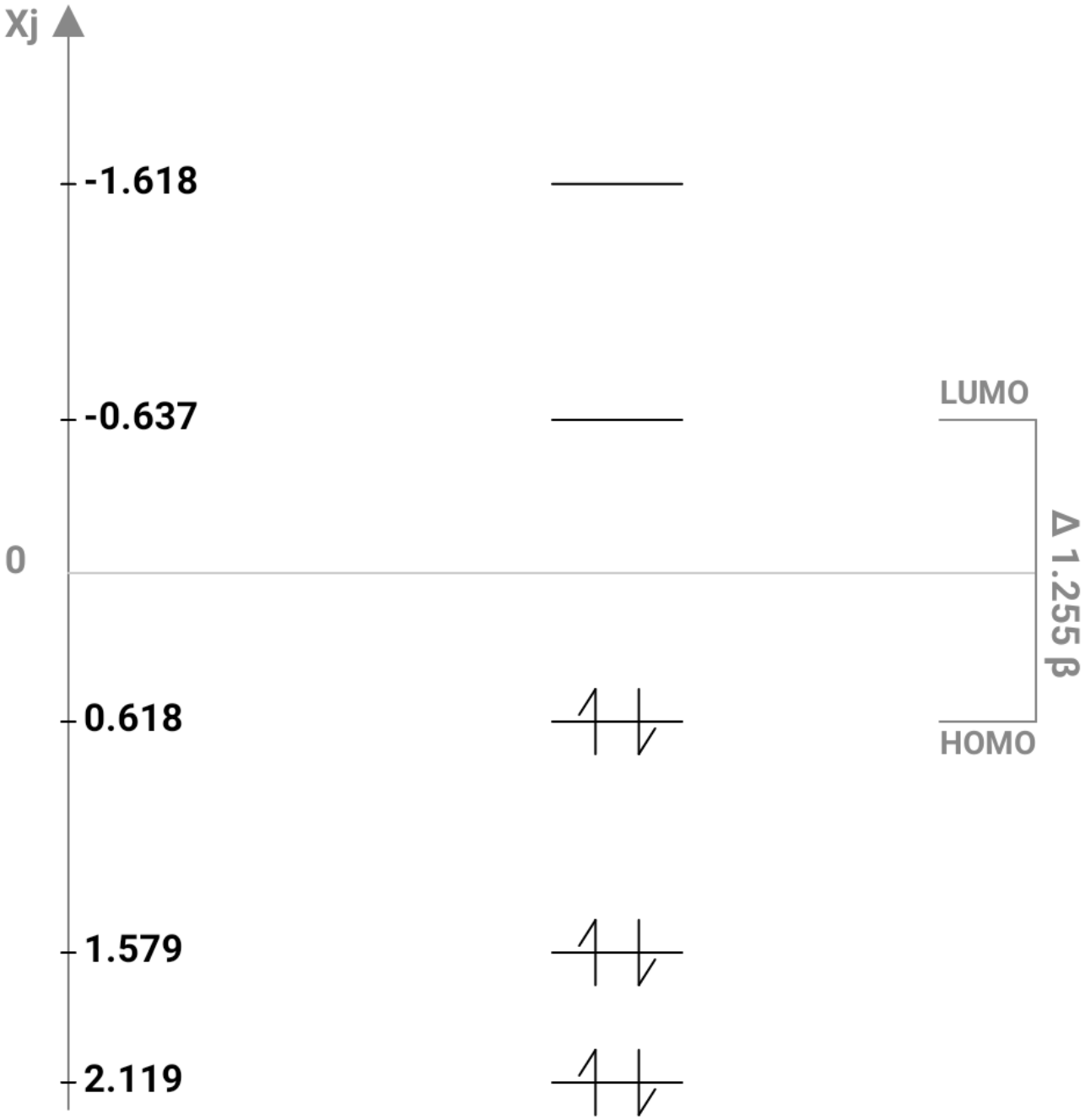


HMO-Energies

x1 = 2.119; x2 = 1.579; x3 = 0.618; x4 = -0.637; x5 = -1.618;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 5α + 8.632β -

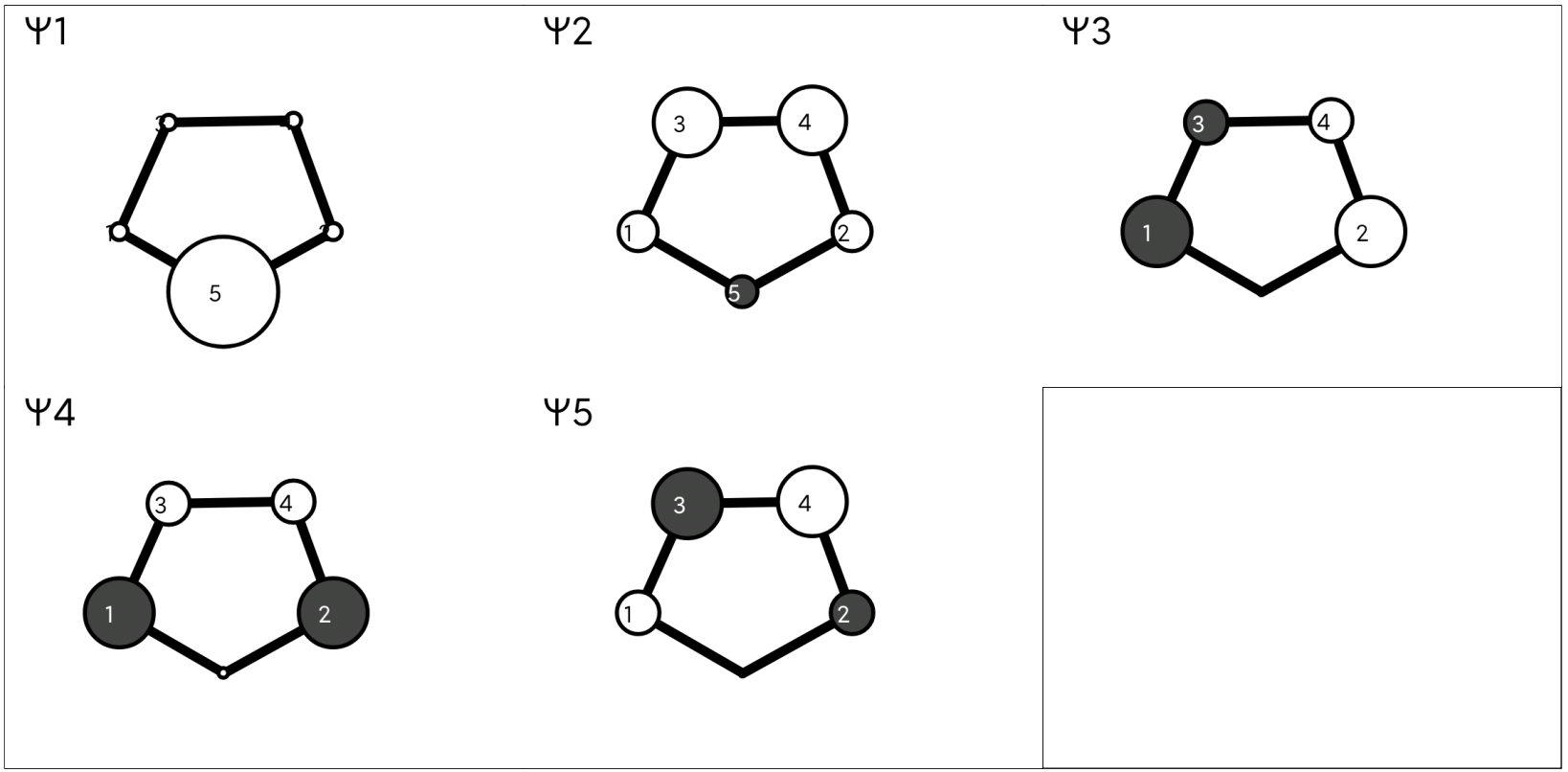
this corresponds to one πelectron: 1.439β

2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5
	x1= 2.119	**x2= 1.579**	**x3= 0.618**	**x4= -0.637**	**x5= -1.618**
1	0.149	0.341	-0.602	-0.601	0.372
2	0.149	0.341	0.602	-0.601	-0.372
3	0.133	0.589	-0.372	0.367	-0.602
4	0.133	0.589	0.372	0.367	0.602
5	0.959	-0.269	0.0	0.085	0.0

2.2. Molecule orbital presentation:

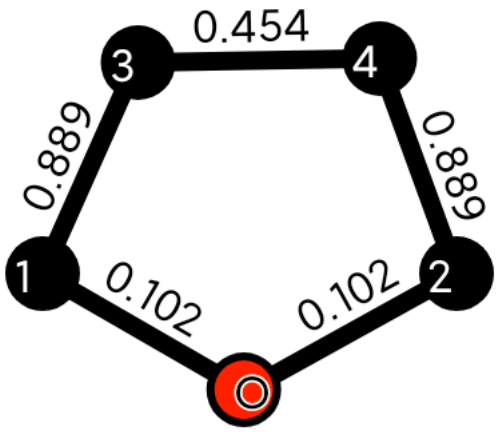


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5
1	1.0				
2	-0.447	1.0			
3	0.889	-0.006	1.007		
4	-0.006	0.889	0.454	1.007	
5	0.102	0.102	-0.062	-0.062	1.986

3.2. Presentation of bond order:

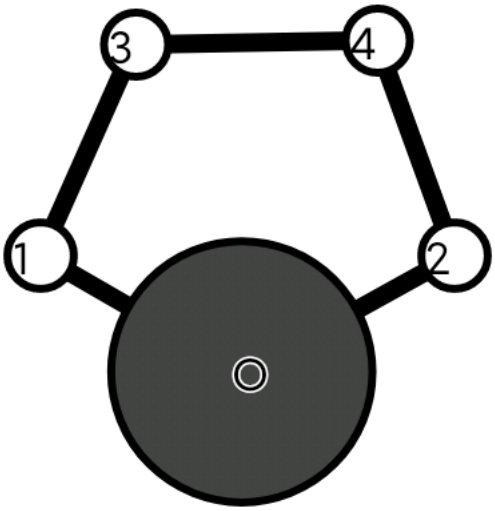


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5
1	0.2				
2		0.2			
3			0.193		
4				0.193	
5					-0.786

4.2. Presentation of molecule:

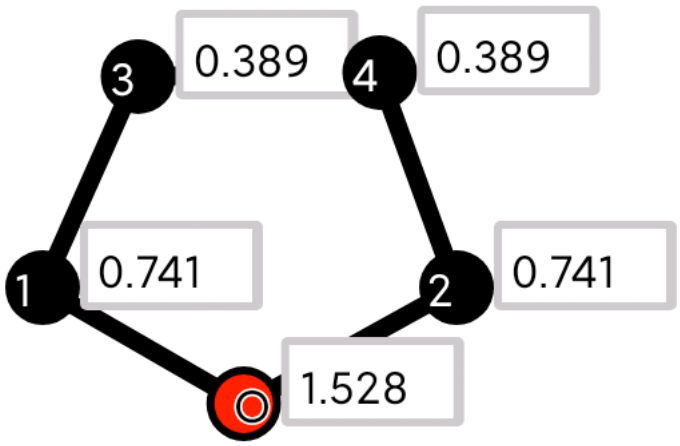


5. Free valences

5.1. Calculated values:

1	2	3	4	5
0.741	0.741	0.389	0.389	1.528

5.2. Presentation of molecule:

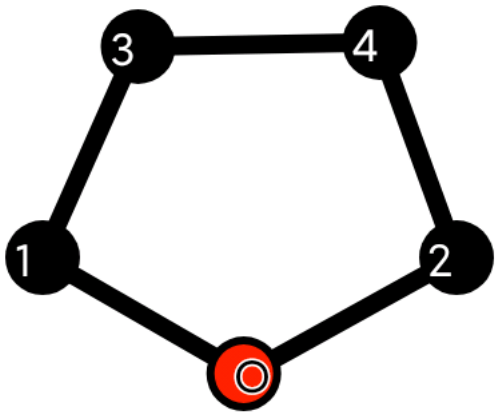


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5
1	0.617				
2	-0.263	0.617			
3	-0.394	0.042	0.401		
4	0.042	-0.394	-0.046	0.401	
5	-0.002	-0.002	-0.003	-0.003	0.011

6.2. Presentation of molecule:

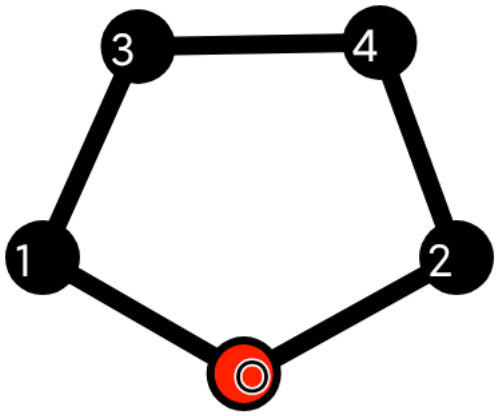


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5
1 3	0.001	-0.002	-0.003	0.001	0.003
1 5	-0.025	0.028	0.035	-0.001	-0.037
2 4	-0.002	0.001	0.001	-0.003	0.003
2 5	0.028	-0.025	-0.001	0.035	-0.037
3 4	0.003	0.003	-0.001	-0.001	-0.003

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 3	1 5	2 4	2 5	3 4
1 3	0.094				
1 5	-0.038	0.342			
2 4	0.092	-0.02	0.094		
2 5	-0.02	0.185	-0.038	0.342	
3 4	-0.181	0.035	-0.181	0.035	0.355

8.2. Presentation of molecule: