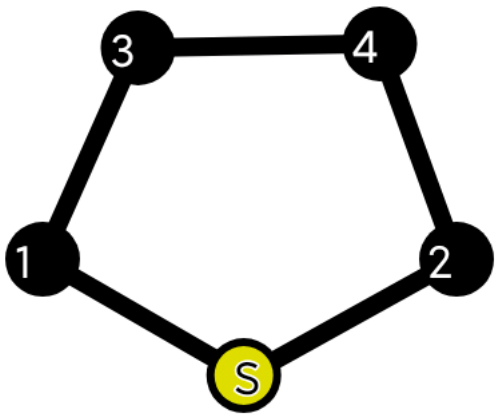
Print calculated values

Report generated by:root, 16.02.2020 - 18:02:03

The following determinant is calculated:

-x	0.0	1.0	0.0	0.8
0.0	-x	0.0	1.0	0.8
1.0	0.0	-x	1.0	0.0
0.0	1.0	1.0	-x	0.0
0.8	0.8	0.0	0.0	-x

It is about this molecule:

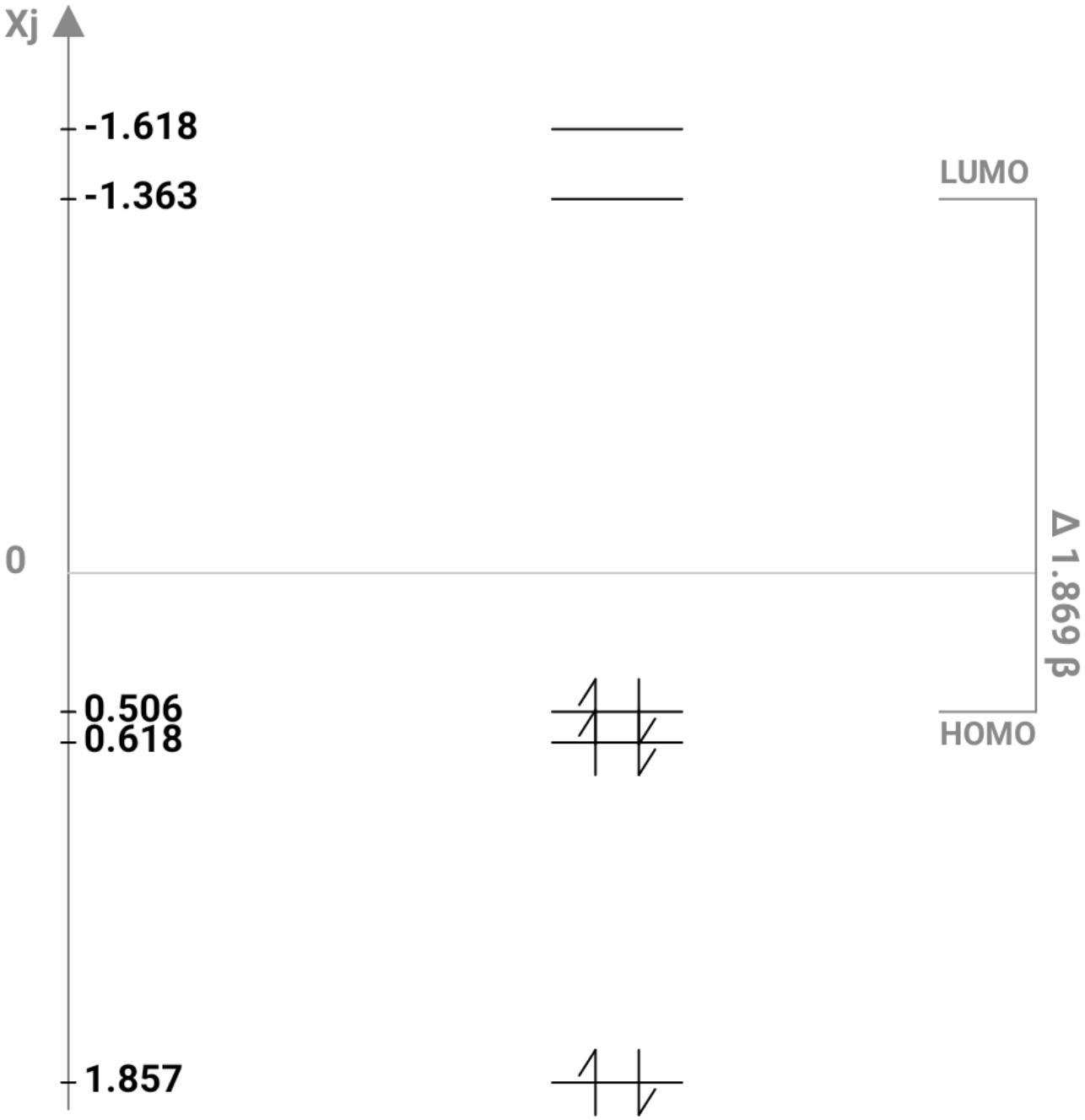


HMO-Energies

x1 = 1.857; x2 = 0.618; x3 = 0.506; x4 = -1.363; x5 = -1.618;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 5α + 5.962β -

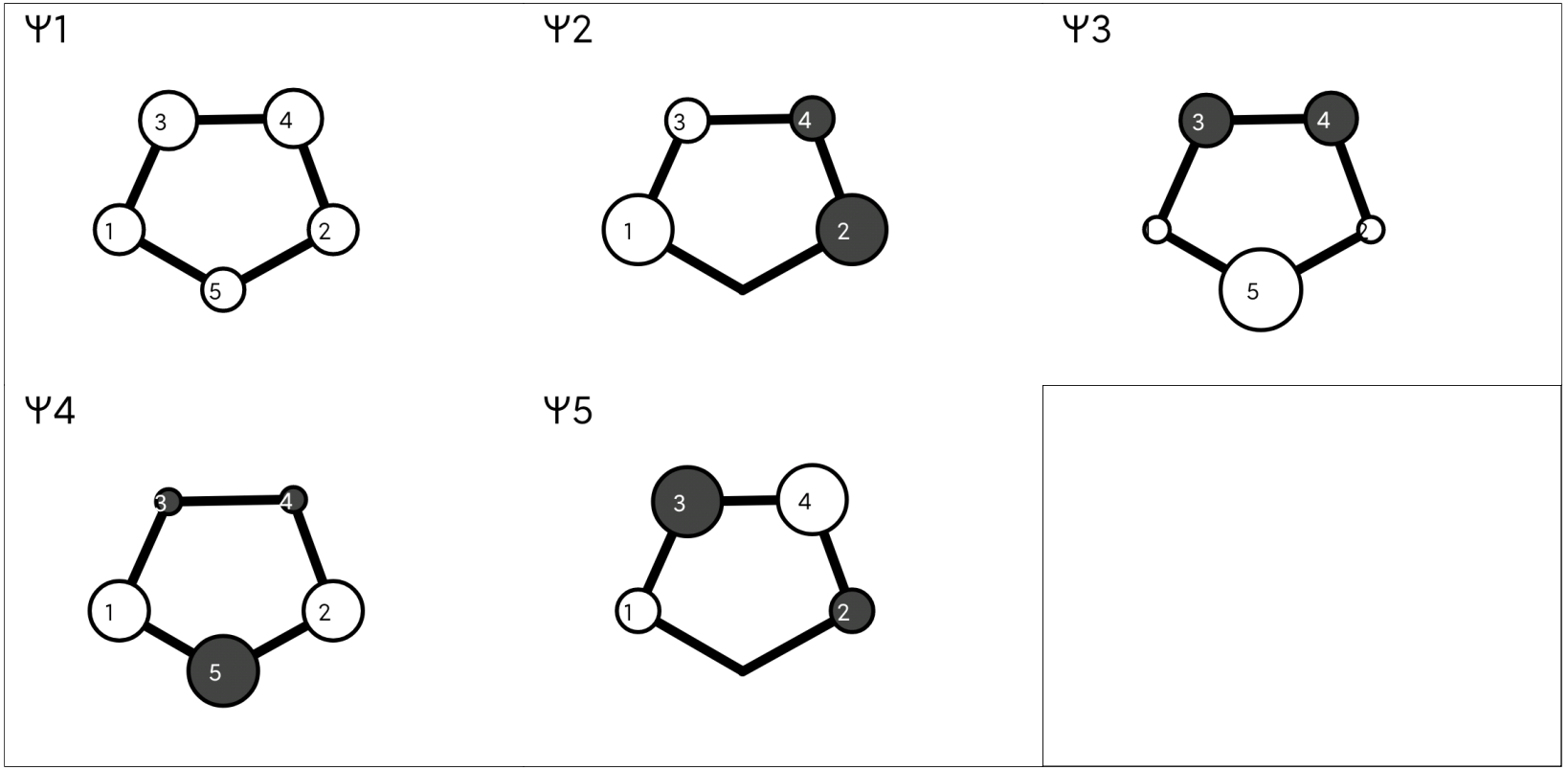
this corresponds to one πelectron: 0.994β

2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5
	x1= 1.857	**x2= 0.618**	**x3= 0.506**	**x4= -1.363**	**x5= -1.618**
1	0.428	0.602	0.223	0.517	0.372
2	0.428	-0.602	0.223	0.517	-0.372
3	0.499	0.372	-0.45	-0.219	-0.602
4	0.499	-0.372	-0.45	-0.219	0.602
5	0.369	0.0	0.704	-0.607	0.0

2.2. Molecule orbital presentation:

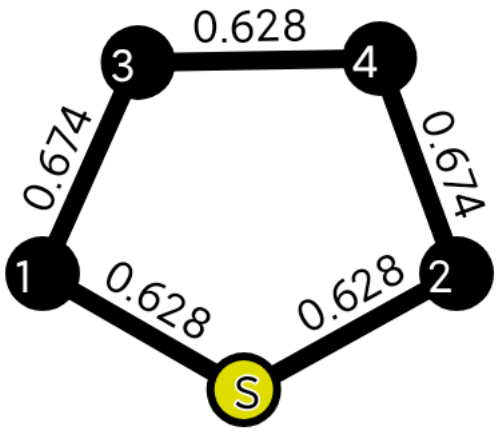


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5
1	1.188				
2	-0.259	1.188			
3	0.674	-0.221	1.181		
4	-0.221	0.674	0.628	1.181	
5	0.628	0.628	-0.266	-0.266	1.262

3.2. Presentation of bond order:

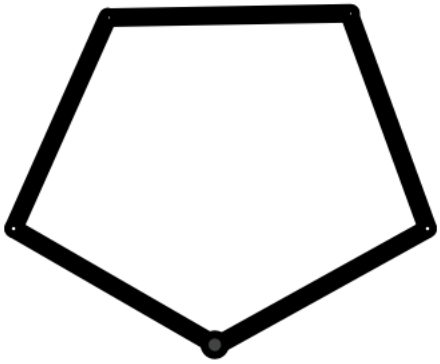


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5
1	0.012				
2		0.012			
3			0.019		
4				0.019	
5					-0.062

4.2. Presentation of molecule:

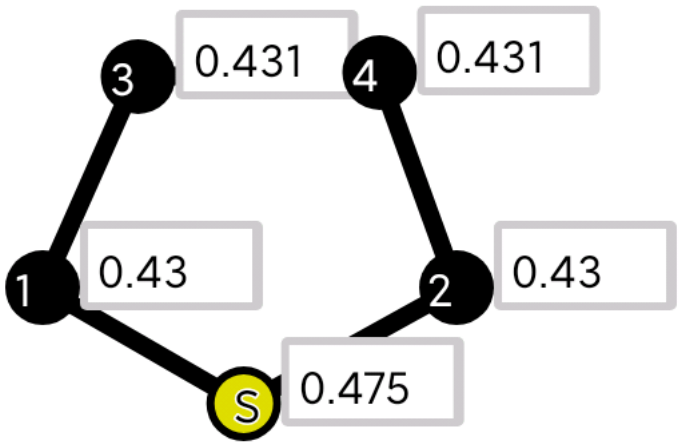


5. Free valences

5.1. Calculated values:

1	2	3	4	5
0.43	0.43	0.431	0.431	0.475

5.2. Presentation of molecule:

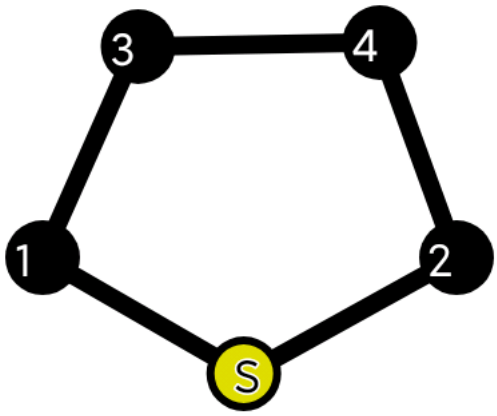


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5
1	0.416				
2	-0.059	0.416			
3	-0.159	-0.031	0.38		
4	-0.031	-0.159	-0.13	0.38	
5	-0.167	-0.167	-0.06	-0.06	0.453

6.2. Presentation of molecule:

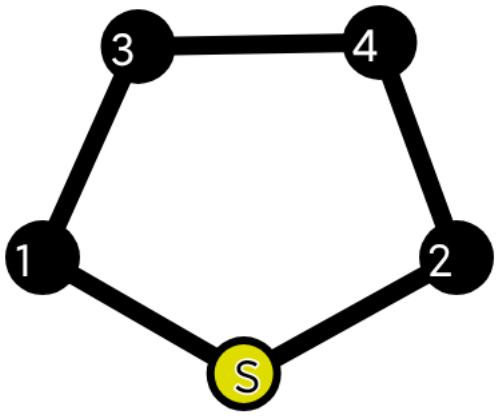


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5
1 3	-0.068	-0.046	-0.066	0.073	0.106
1 5	-0.063	0.101	0.102	-0.044	-0.095
2 4	-0.046	-0.068	0.073	-0.066	0.106
2 5	0.101	-0.063	-0.044	0.102	-0.095
3 4	0.084	0.084	-0.054	-0.054	-0.06

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	0.239				
1 5	-0.178	0.269			
2 4	0.054	0.026	0.239		
2 5	0.026	-0.151	-0.178	0.269	
3 4	-0.171	0.058	-0.171	0.058	0.25

8.2. Presentation of molecule: