

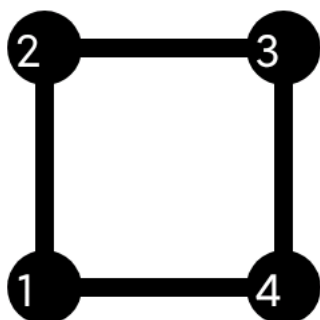
Print calculated values

Report generated by:root, 20.01.2020 - 21:06:27

The following determinant is calculated:

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

It is about this molecule:

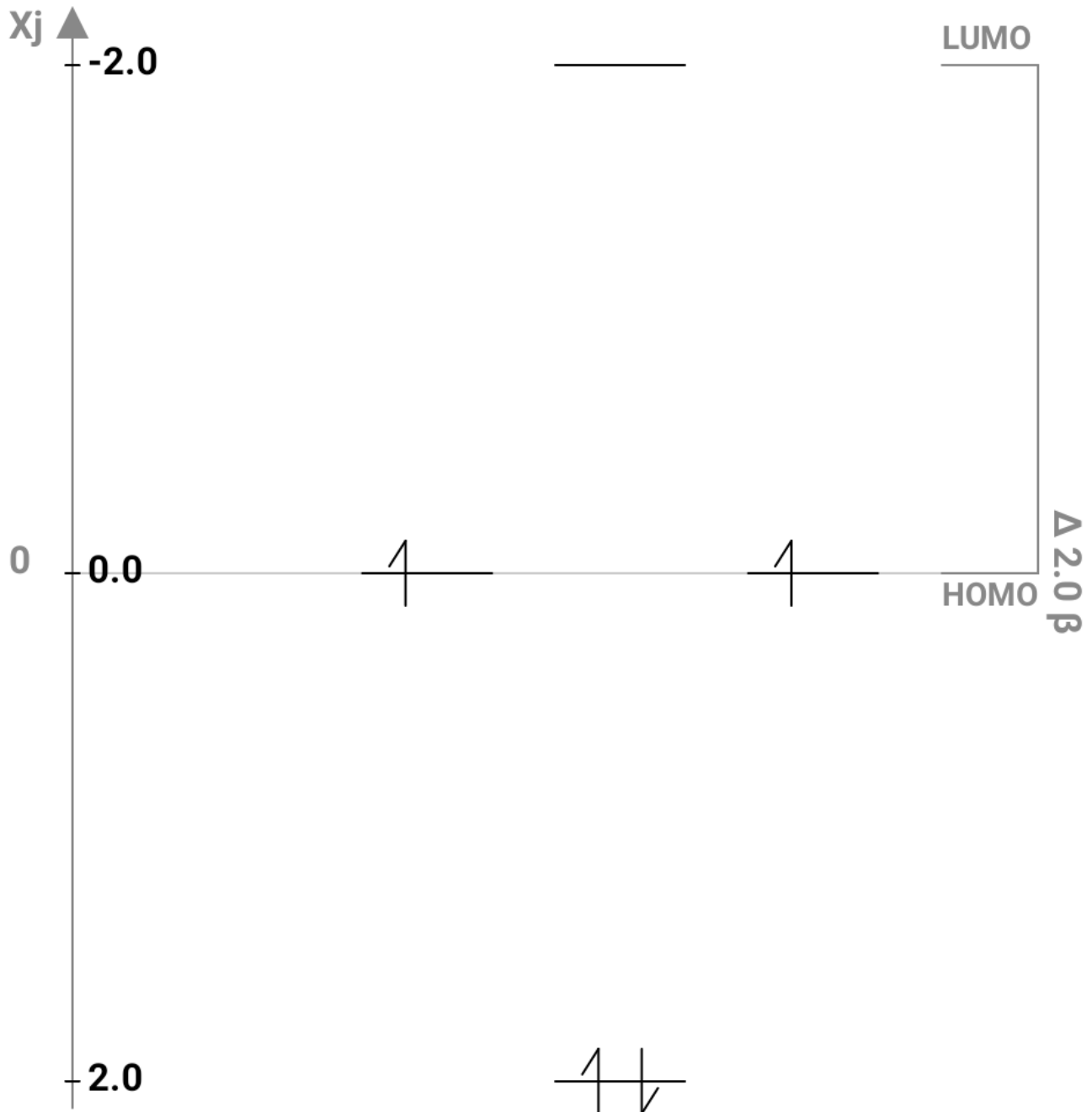


HMO-Energies

$x_1 = 2.0$; $x_2 = 0.0$; $x_3 = 0.0$; $x_4 = -2.0$;

1. Energy-eigenvalues

1.1. Calculated values:



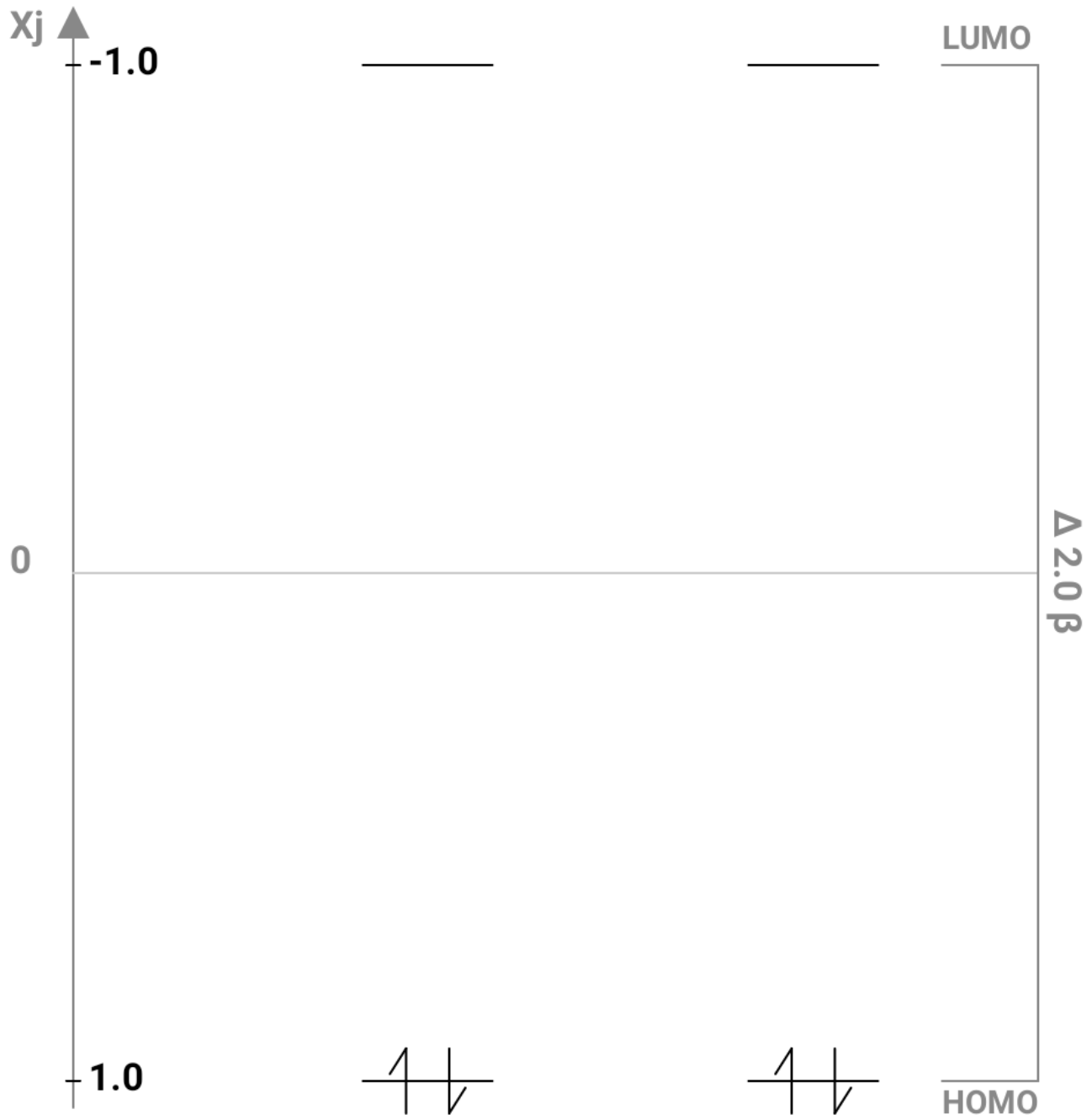
total Power E_π : $4\alpha + 4.0\beta$ -

this corresponds to one π electron: 1.0β

1. Moebius-Energy-eigenvalues

1.1. Calculated values:

$$\beta = \beta * \cos(\pi / n)$$



total Power E_π : $4\alpha + 4.0\beta$ -

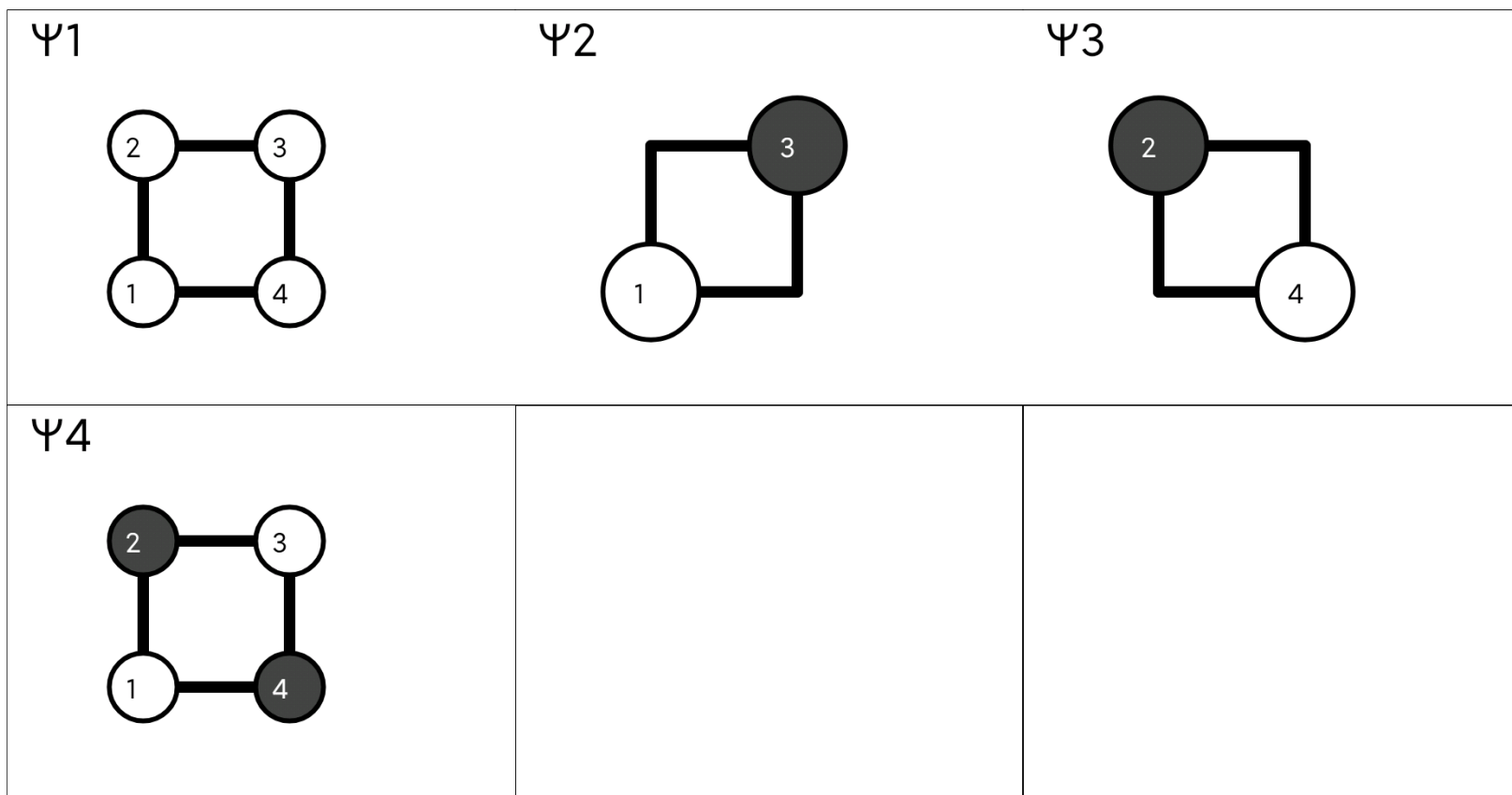
this corresponds to one π electron: 1.0β

2. Hückel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4
	x1= 2.0	x2= 0.0	x3= 0.0	x4= -2.0
1	0.5	0.707	0.0	0.5
2	0.5	0.0	-0.707	-0.5
3	0.5	-0.707	0.0	0.5
4	0.5	0.0	0.707	-0.5

2.2. Molecule orbital presentation:

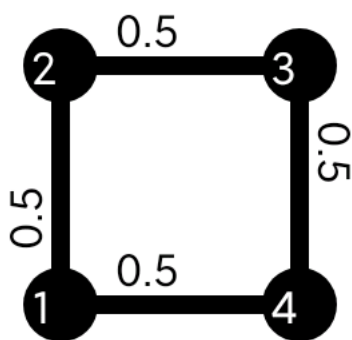


3. Bond Order

3.1. Calculated values:

	1	2	3	4
1	1.0			
2	0.5	1.0		
3	0.0	0.5	1.0	
4	0.5	0.0	0.5	1.0

3.2. Presentation of bond order:

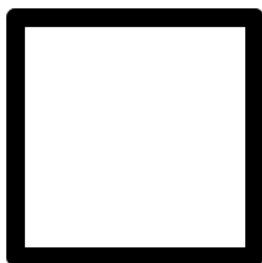


4. Net Charge

4.1. Calculated values:

	1	2	3	4
1	0.0			
2		0.0		
3			0.0	
4				0.0

4.2. Presentation of molecule:

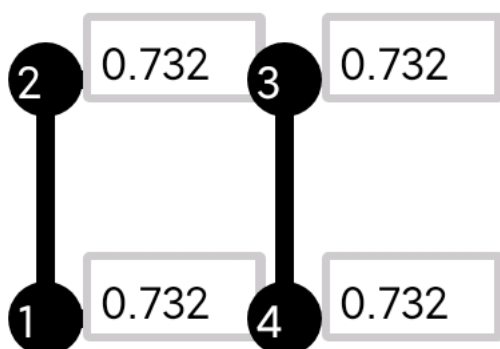


5. Free valences

5.1. Calculated values:

1	2	3	4
0.732	0.732	0.732	0.732

5.2. Presentation of molecule:

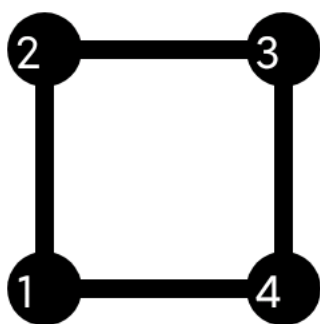


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4
1	0.312			
2	-0.062	0.312		
3	-0.187	-0.062	0.312	
4	-0.062	-0.187	-0.062	0.312

6.2. Presentation of molecule:

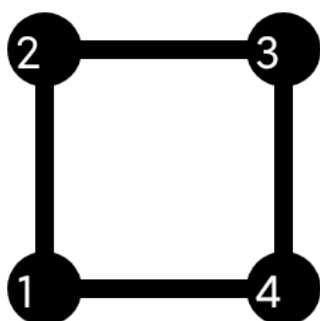


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4
1 2	0.0	0.0	0.0	0.0
1 3	0.062	-0.062	0.062	-0.062
1 4	0.0	0.0	0.0	0.0
2 3	0.0	0.0	0.0	0.0
3 4	0.0	0.0	0.0	0.0

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3	1 4	2 3	3 4
1 2	0.25				
1 3	0.0	0.125			
1 4	0.0	0.0	0.25		
2 3	0.0	0.0	-0.25	0.25	
3 4	-0.25	0.0	0.0	0.0	0.25

8.2. Presentation of molecule:

