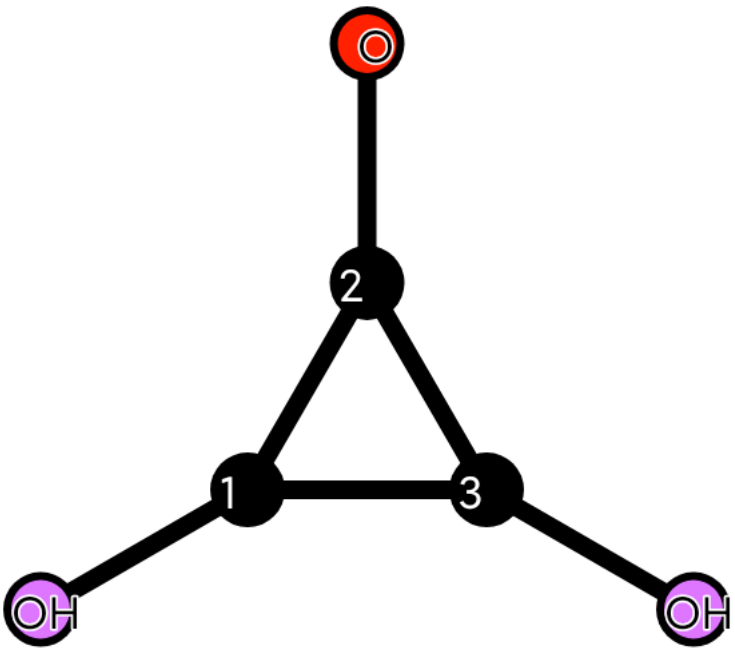
Print calculated values

Report generated by:root, 18.02.2020 - 15:27:33

The following determinant is calculated:

-x	1.0	1.0	0.0	0.9	0.0
1.0	-x	1.0	1.93	0.0	0.0
1.0	1.0	-x	0.0	0.0	0.9
0.0	1.93	0.0	-x+1.18	0.0	0.0
0.9	0.0	0.0	0.0	-x+2.0	0.0
0.0	0.0	0.9	0.0	0.0	-x+2.0

It is about this molecule:

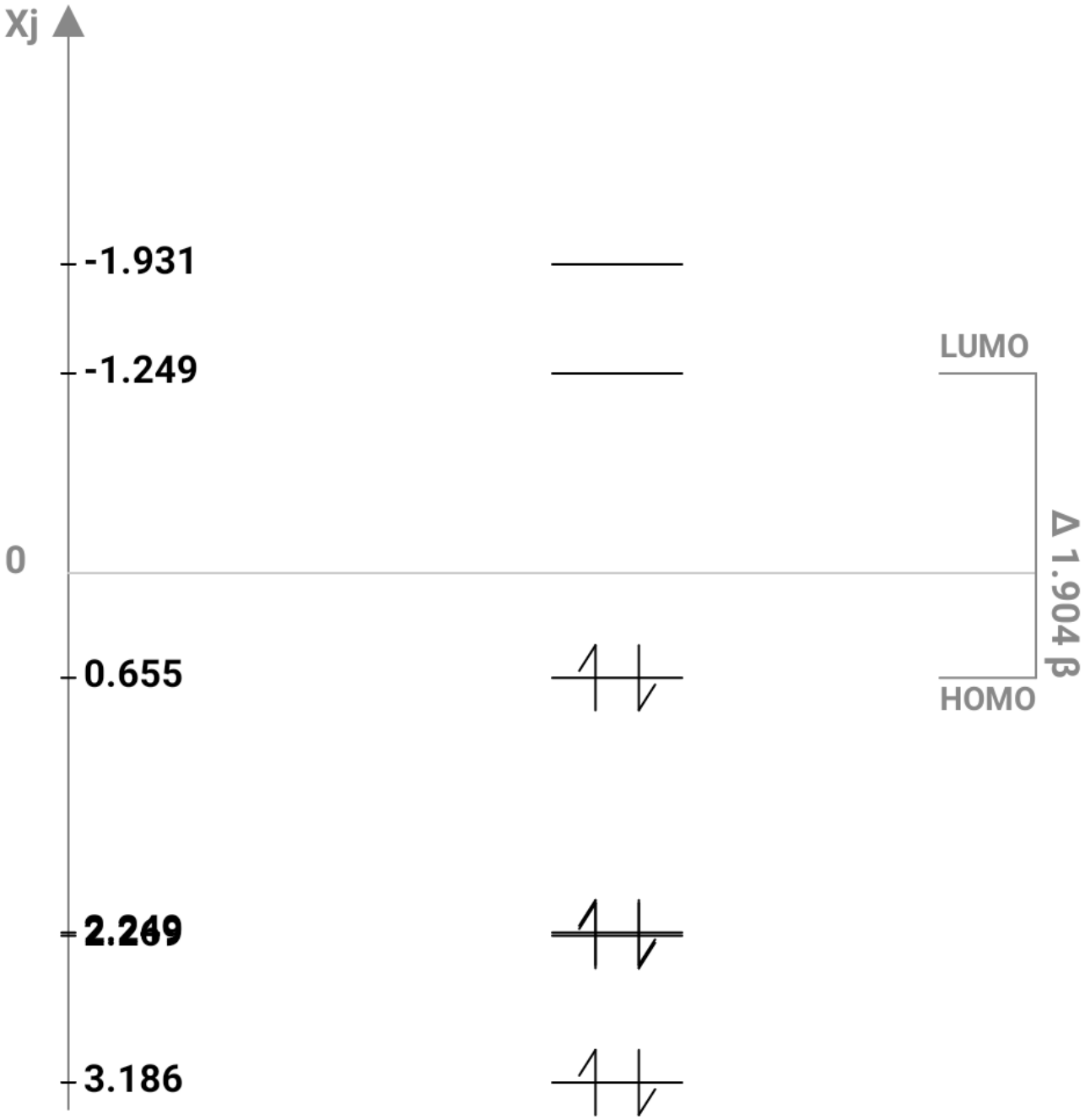


HMO-Energies

x1 = 3.186; x2 = 2.269; x3 = 2.249; x4 = 0.655; x5 = -1.249; x6 = -1.931;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 6α + 16.718β -

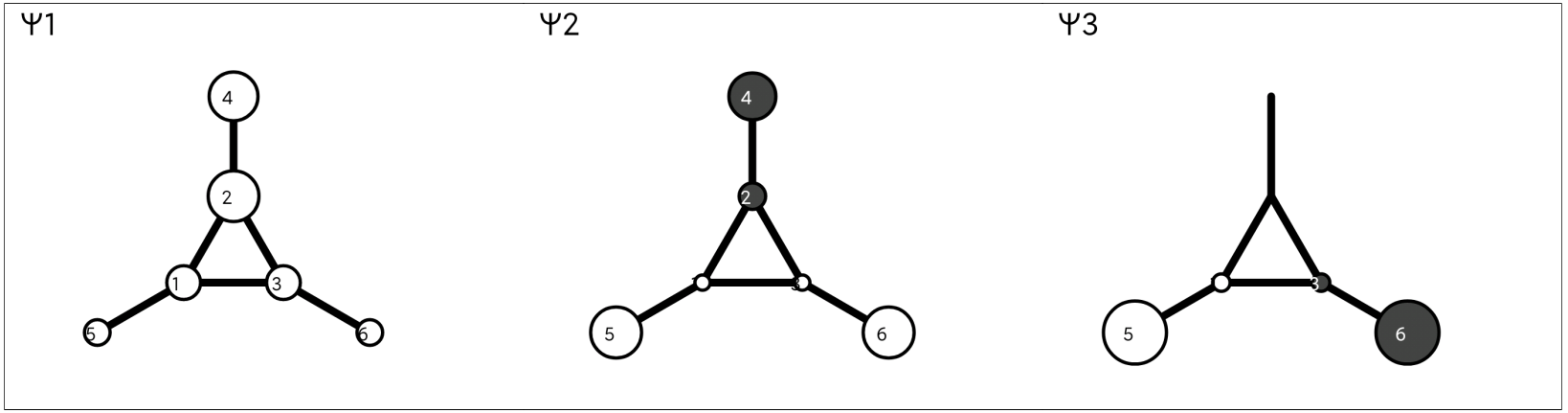
this corresponds to one πelectron: 2.09β

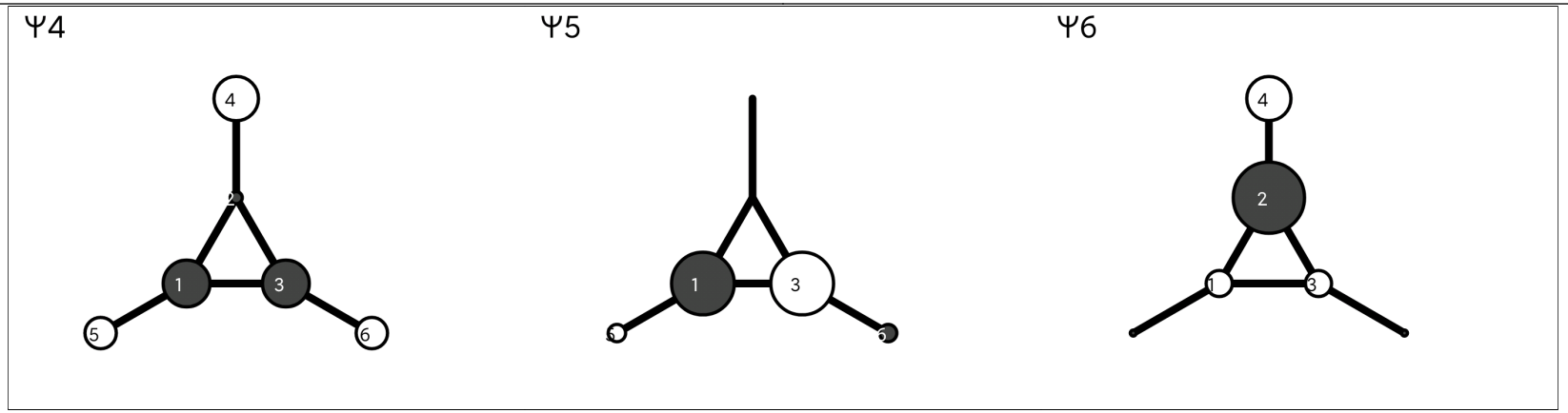
2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6
	x1= 3.186	x2= 2.269	x3= 2.249	x4= 0.655	x5= -1.249	x6= -1.931
1	0.365	0.165	0.189	-0.509	-0.681	0.284
2	0.549	-0.286	0.0	-0.131	0.0	-0.774
3	0.365	0.165	-0.189	-0.509	0.681	0.284
4	0.528	-0.507	0.0	0.483	0.0	0.48
5	0.277	0.551	0.681	0.341	0.189	-0.065
6	0.277	0.551	-0.681	0.341	-0.189	-0.065

2.2. Molecule orbital presentation:



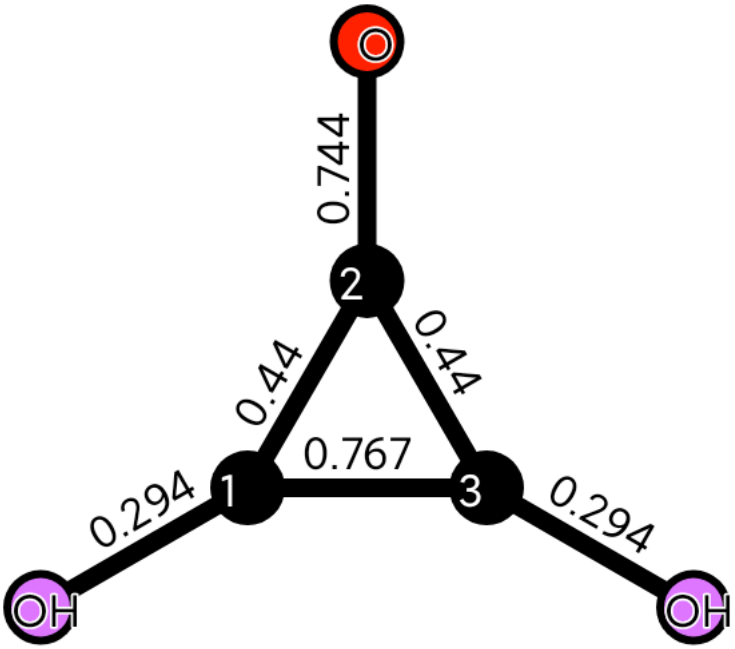

Ψ4
4
2
1
3
5
6
Ψ5
1
3
Ψ6
4
2
1
3

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6
1	0.91					
2	0.44	0.801				
3	0.767	0.44	0.91			
4	-0.273	0.744	-0.273	1.539		
5	0.294	-0.101	-0.22	0.062	1.92	
6	-0.22	-0.101	0.294	0.062	0.063	1.92

3.2. Presentation of bond order:

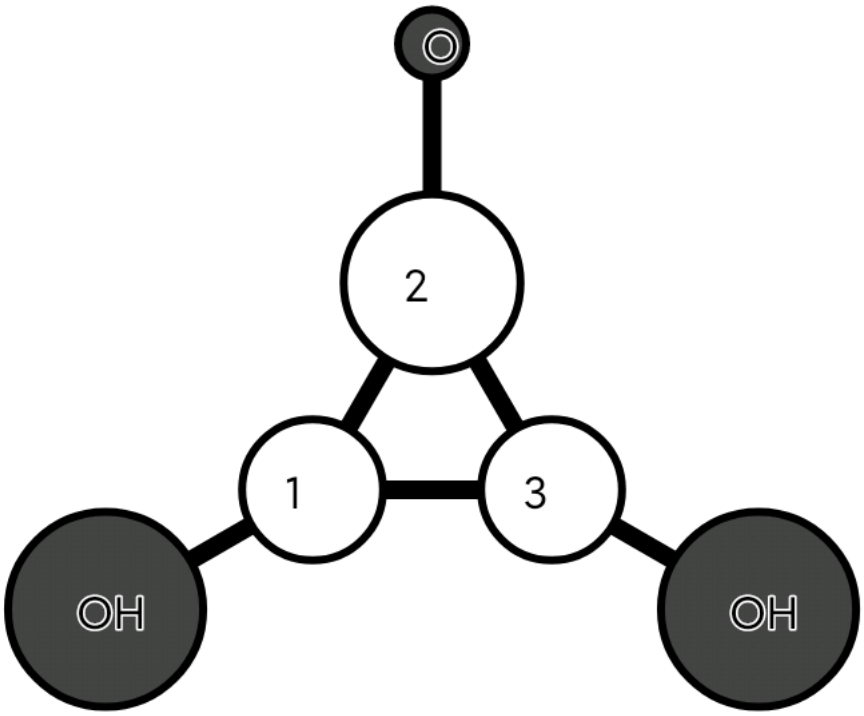


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6
1	0.424					
2		0.532				
3			0.424			
4				-0.205		
5					-0.587	
6						-0.587

4.2. Presentation of molecule:

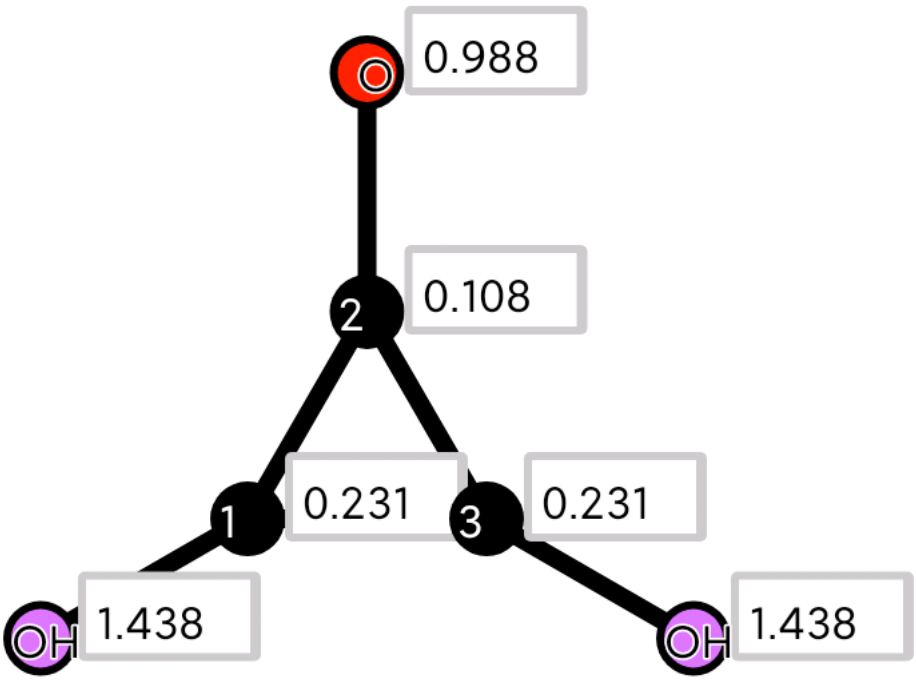


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6
0.231	0.108	0.231	0.988	1.438	1.438

5.2. Presentation of molecule:

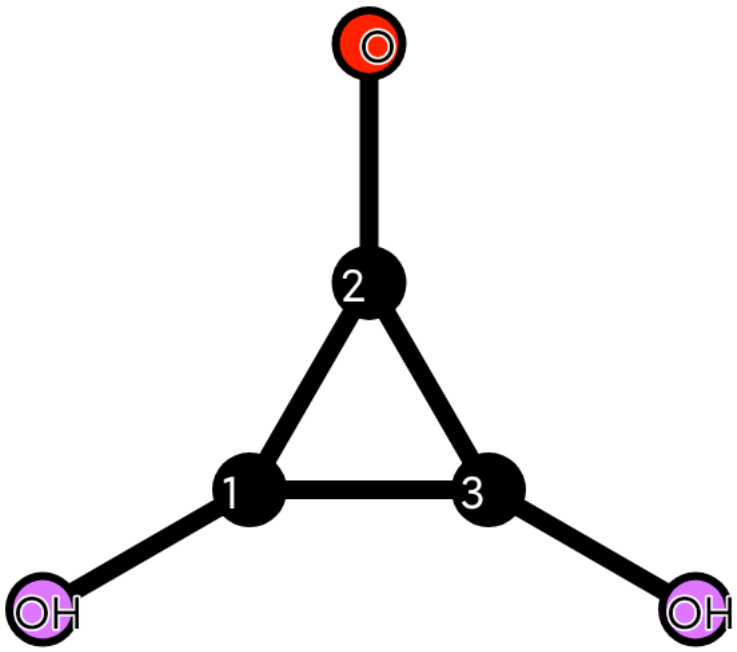


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6
1	0.387					
2	-0.047	0.204				
3	-0.264	-0.047	0.387			
4	-0.042	-0.099	-0.042	0.19		
5	0.003	-0.005	-0.037	-0.003	0.046	
6	-0.037	-0.005	0.003	-0.003	-0.004	0.046

6.2. Presentation of molecule:

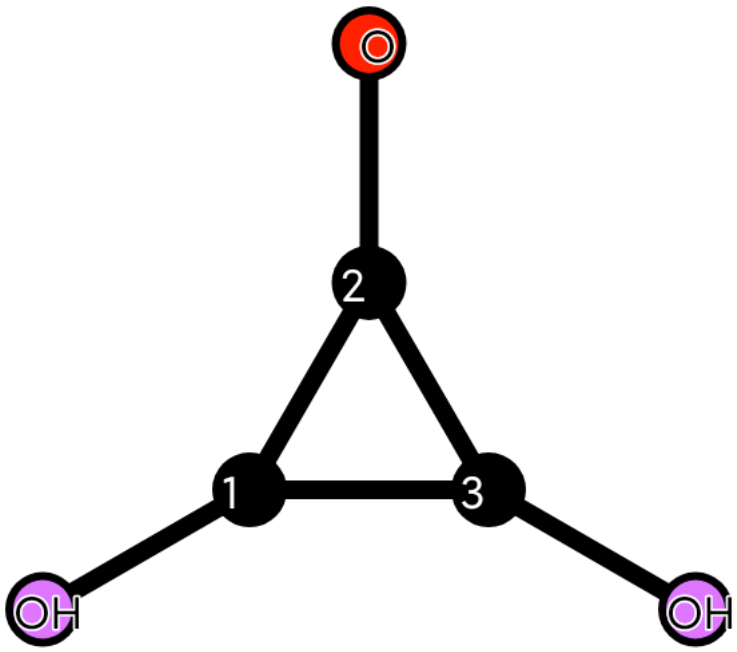


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6
1 2	0.009	0.027	-0.108	0.076	0.01	-0.014
1 3	0.024	-0.047	0.024	-0.042	0.021	0.021
1 5	-0.057	0.016	0.102	0.012	-0.086	0.013
2 3	-0.108	0.027	0.009	0.076	-0.014	0.01
2 4	0.049	0.017	0.049	-0.122	0.004	0.004
3 6	0.102	0.016	-0.057	0.012	0.013	-0.086

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3	1 5	2 3	2 4	3 6
1 2	0.229					
1 3	-0.099	0.123				
1 5	-0.043	-0.081	0.332			
2 3	0.022	-0.099	0.08	0.229		
2 4	-0.139	0.097	-0.029	-0.139	0.187	
3 6	0.08	-0.081	-0.073	-0.043	-0.029	0.332

8.2. Presentation of molecule: