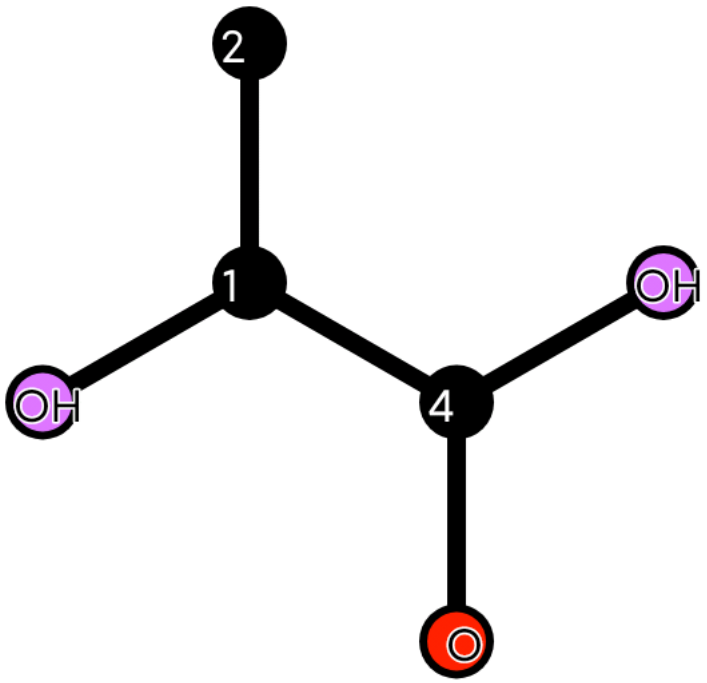
Print calculated values

Report generated by:root, 22.02.2020 - 23:18:55

The following determinant is calculated:

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

It is about this molecule:

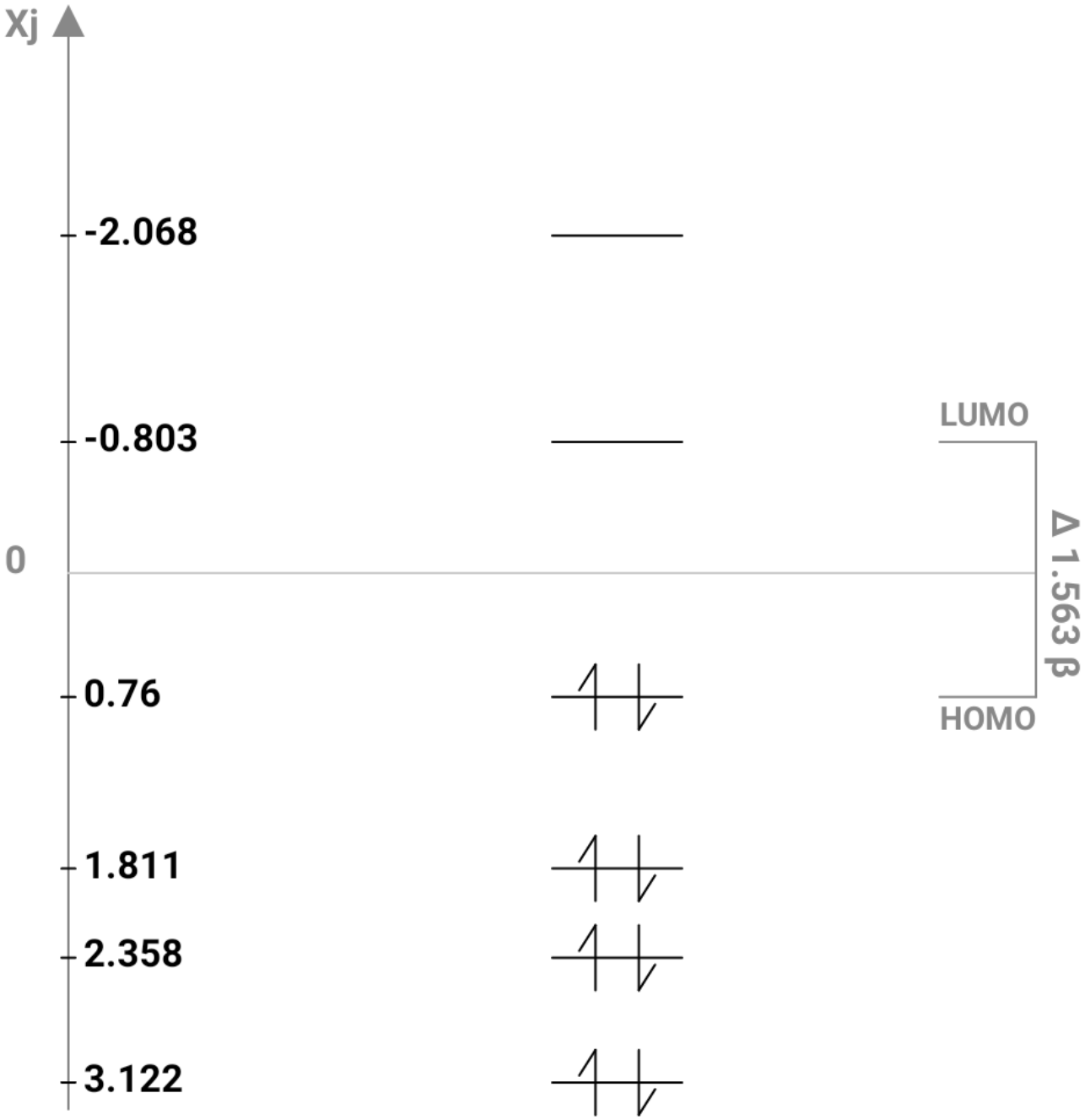


HMO-Energies

x1 = 3.122; x2 = 2.358; x3 = 1.811; x4 = 0.76; x5 = -0.803; x6 = -2.068;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 6α + 16.102β -

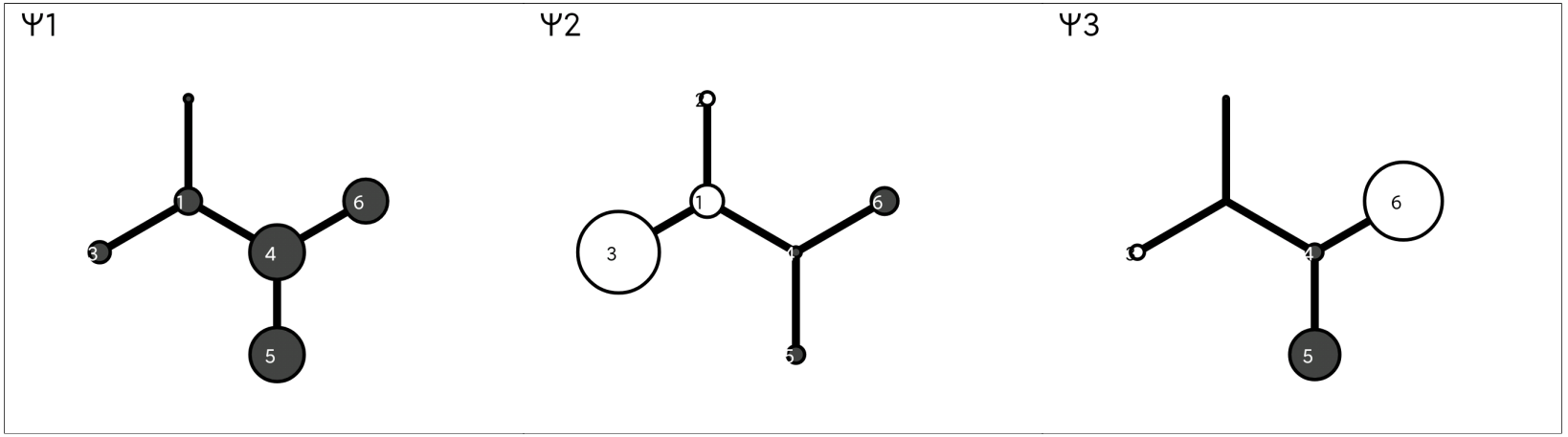
this corresponds to one πelectron: 2.013β

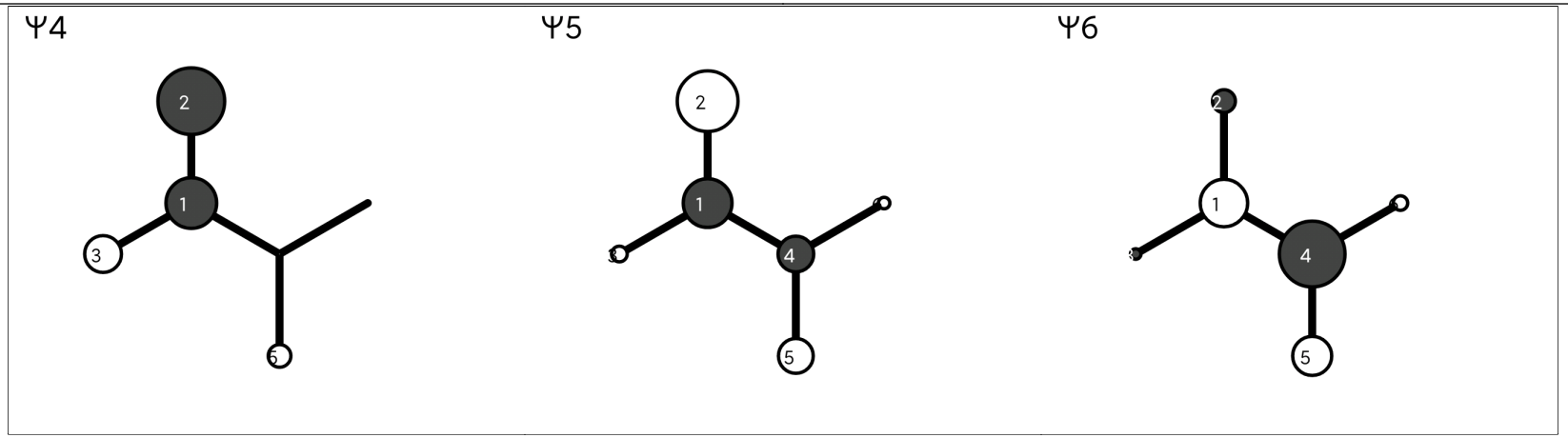
2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6
	x1= 3.122	**x2= 2.358**	**x3= 1.811**	**x4= 0.76**	**x5= -0.803**	**x6= -2.068**
1	-0.276	0.342	-0.031	-0.537	-0.516	0.502
2	-0.088	0.145	-0.017	-0.706	0.643	-0.243
3	-0.222	0.859	0.148	0.389	0.166	-0.111
4	-0.574	-0.112	-0.172	-0.052	-0.378	-0.695
5	-0.57	-0.183	-0.527	0.24	0.368	0.413
6	-0.461	-0.28	0.818	0.038	0.121	0.154

2.2. Molecule orbital presentation:



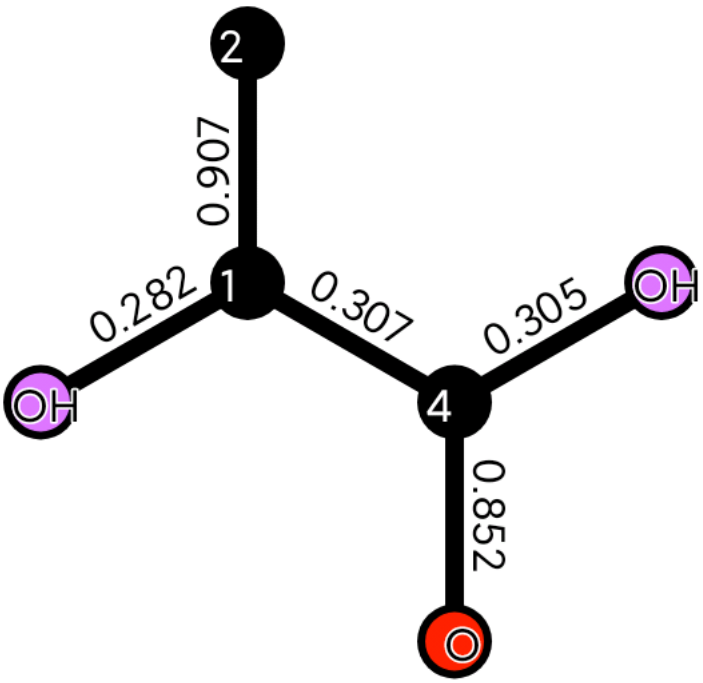

Ψ4
2
1
3
5
Ψ5
2
1
4
5
Ψ6
2
1
4
5

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6
1	0.964					
2	0.907	1.056				
3	0.282	-0.267	1.92			
4	0.307	0.149	-0.029	0.748		
5	-0.035	-0.273	-0.03	0.852	1.388	
6	-0.029	-0.081	-0.006	0.305	-0.216	1.923

3.2. Presentation of bond order:

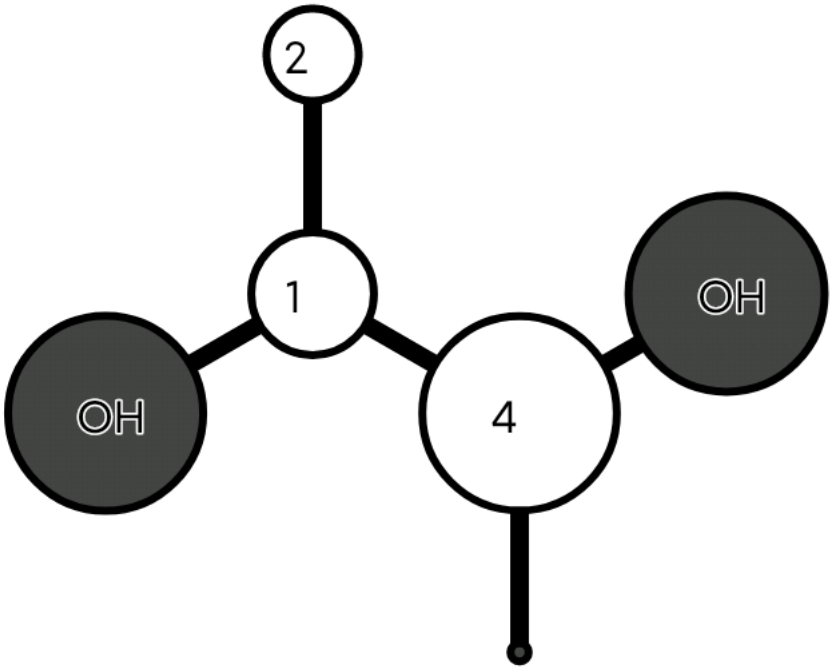


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6
1	0.369					
2		0.278				
3			-0.587			
4				0.585		
5					-0.055	
6						-0.59

4.2. Presentation of molecule:

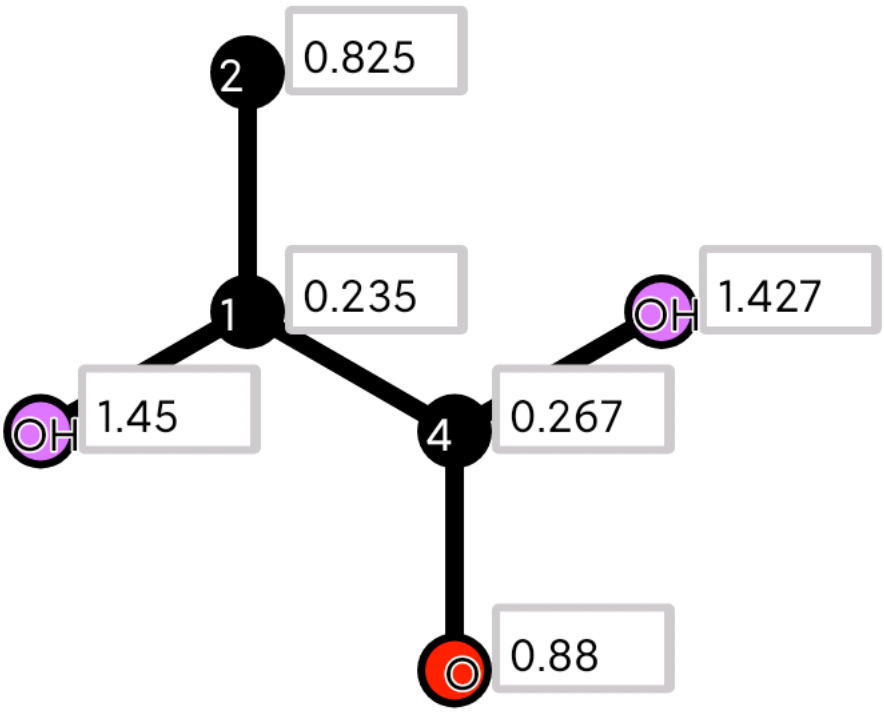


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6
0.235	0.825	1.45	0.267	0.88	1.427

5.2. Presentation of molecule:

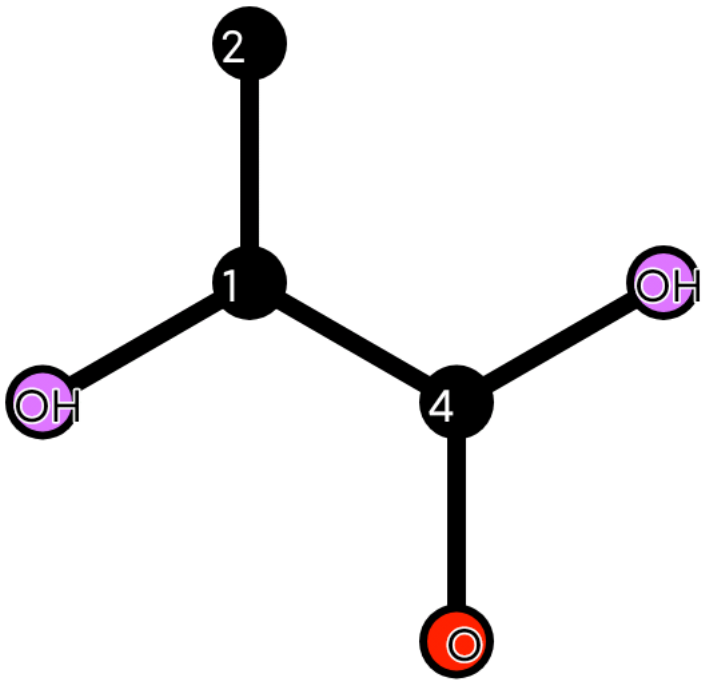


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6
1	0.401					
2	-0.424	0.585				
3	0.009	-0.064	0.05			
4	-0.009	-0.018	0.002	0.202		
5	0.022	-0.073	0.003	-0.164	0.239	
6	0.002	-0.006	0.0	-0.013	-0.025	0.042

6.2. Presentation of molecule:

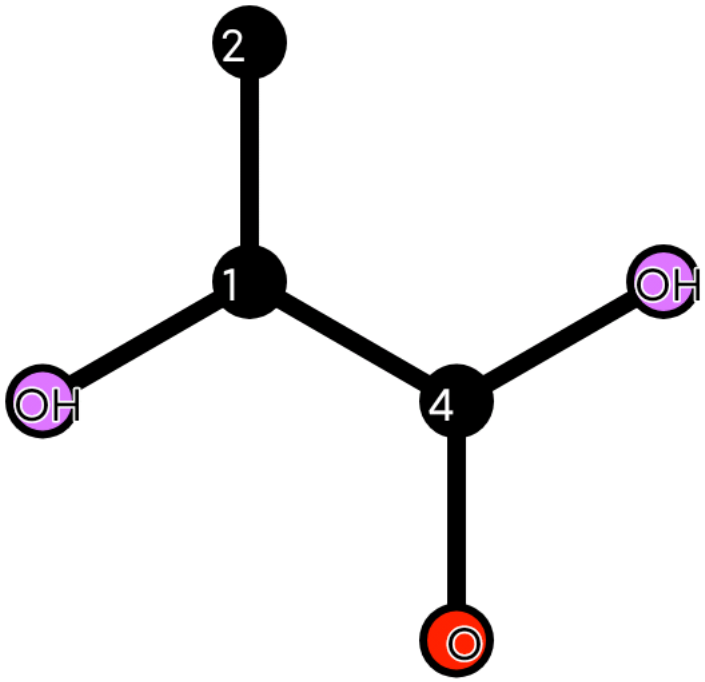


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6
1 2	0.022	-0.026	0.024	-0.013	-0.006	-0.002
1 3	-0.07	0.168	-0.088	-0.001	-0.008	-0.001
1 4	0.037	-0.104	0.009	0.033	0.022	0.005
4 5	-0.009	0.042	-0.003	0.046	-0.098	0.021
4 6	-0.001	0.011	-0.001	0.001	0.069	-0.079

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3	1 4	4 5	4 6
1 2	0.058				
1 3	-0.09	0.331			
1 4	-0.083	-0.049	0.29		
4 5	0.029	0.013	-0.095	0.113	
4 6	0.011	0.004	-0.035	-0.095	0.313

8.2. Presentation of molecule: