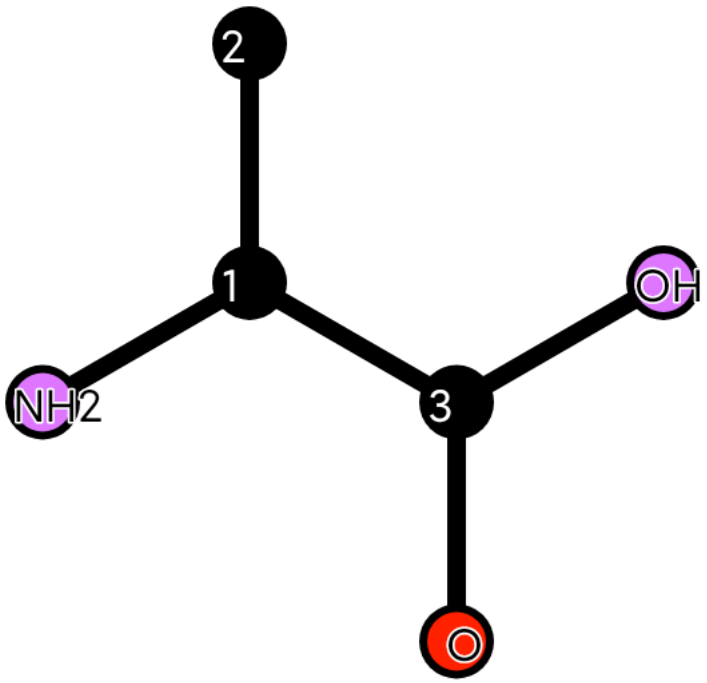
Print calculated values

Report generated by:root, 22.02.2020 - 23:20:15

The following determinant is calculated:

-x	1.0	1.0	0.0	0.0	1.3
1.0	-x	0.0	0.0	0.0	0.0
1.0	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	0.0
1.3	0.0	0.0	0.0	0.0	-x+1.47

It is about this molecule:

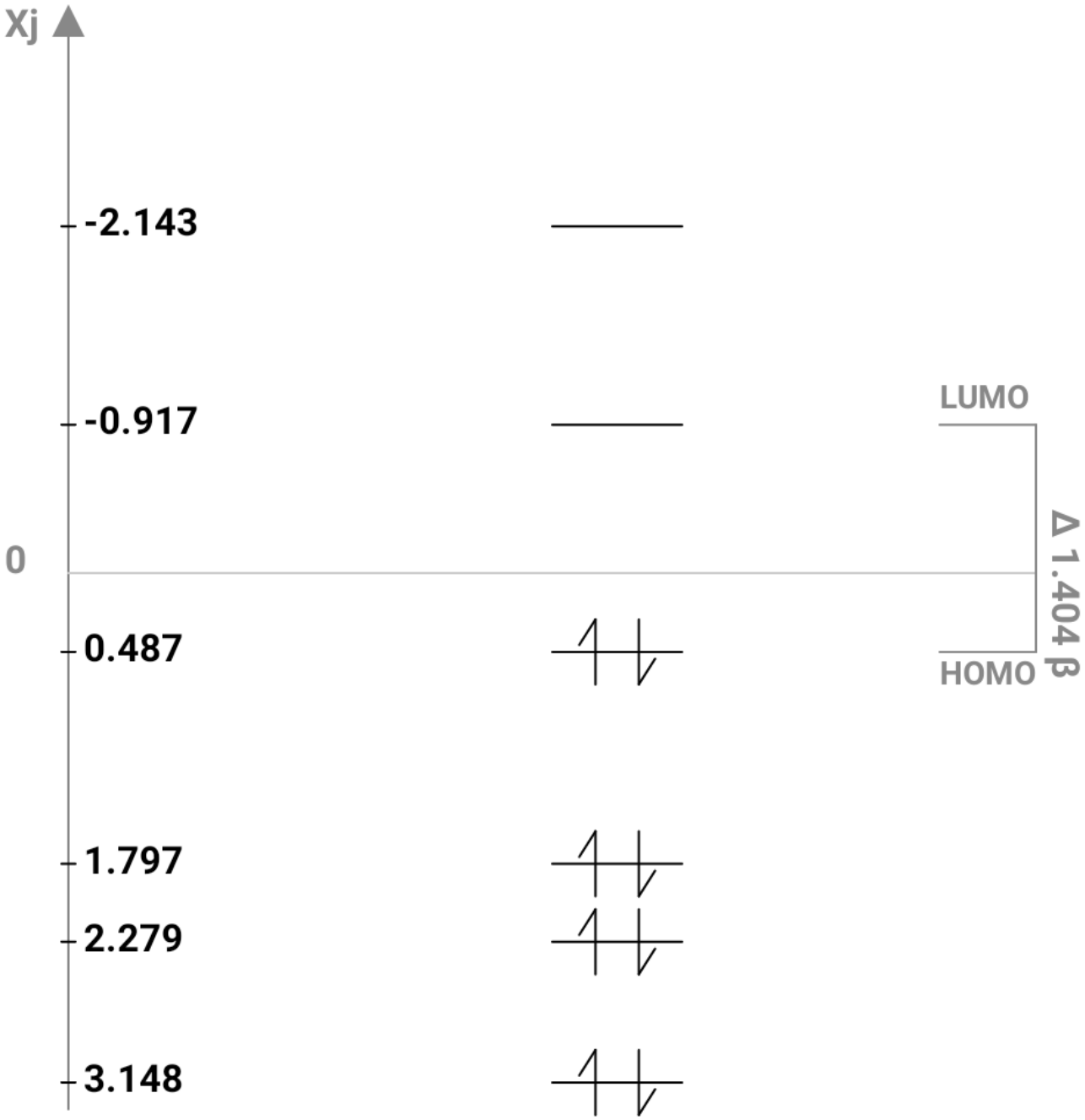


HMO-Energies

x1 = 3.148; x2 = 2.279; x3 = 1.797; x4 = 0.487; x5 = -0.917; x6 = -2.143;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 6α + 15.422β -

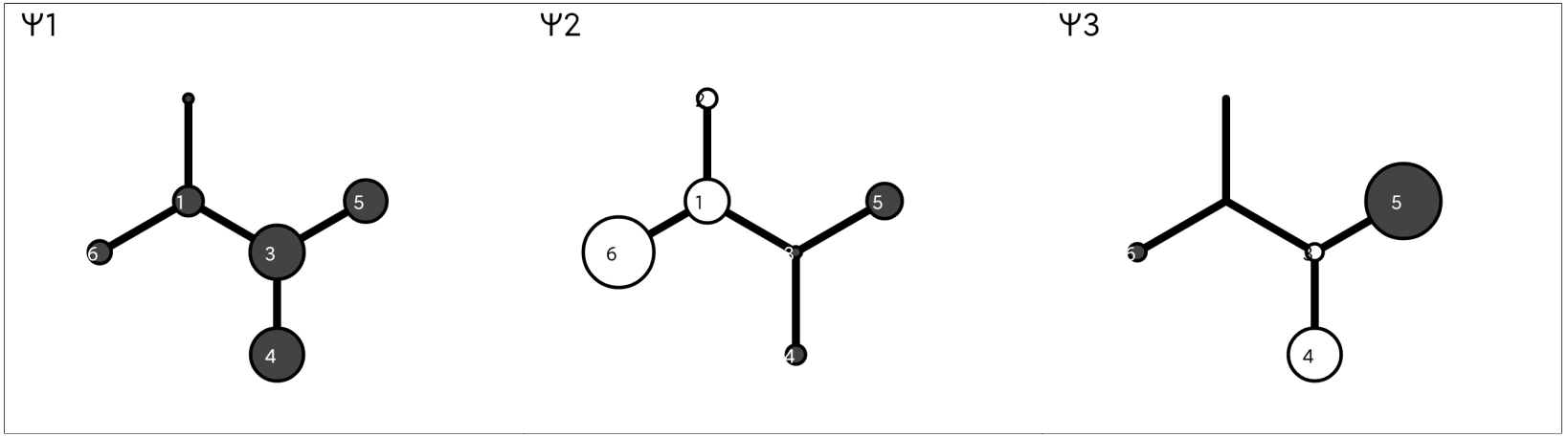
this corresponds to one πelectron: 1.928β

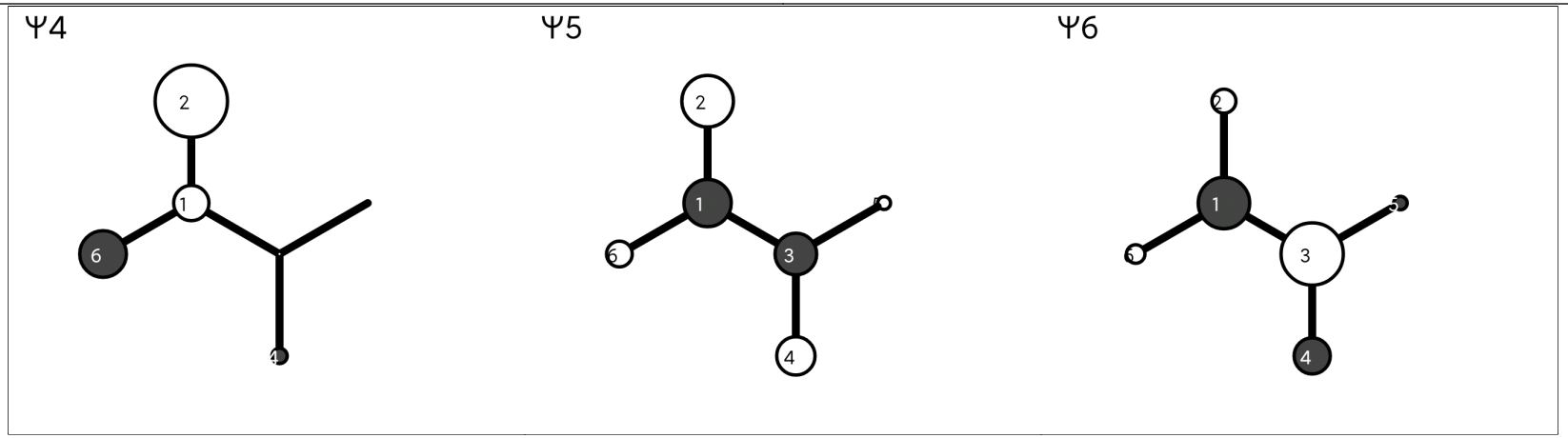
2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6
	x1= 3.148	**x2= 2.279**	**x3= 1.797**	**x4= 0.487**	**x5= -0.917**	**x6= -2.143**
1	-0.312	0.463	-0.045	0.373	-0.501	-0.545
2	-0.099	0.203	-0.025	0.765	0.546	0.254
3	-0.569	-0.115	0.178	0.058	-0.441	0.659
4	-0.558	-0.202	0.557	-0.162	0.406	-0.382
5	-0.446	-0.372	-0.789	-0.035	0.136	-0.143
6	-0.242	0.743	-0.18	-0.494	0.273	0.196

2.2. Molecule orbital presentation:



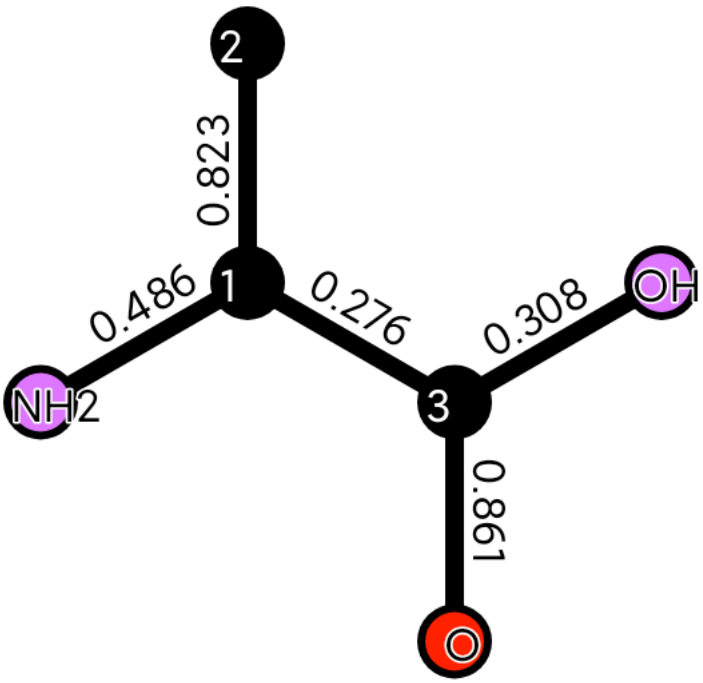

Ψ4
2
1
6
Ψ5
2
1
3
4
Ψ6
2
1
3
4

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6
1	0.905					
2	0.823	1.275				
3	0.276	0.146	0.744			
4	-0.01	-0.248	0.861	1.379		
5	-0.02	-0.076	0.308	-0.22	1.922	
6	0.486	-0.397	-0.018	-0.071	-0.018	1.775

3.2. Presentation of bond order:

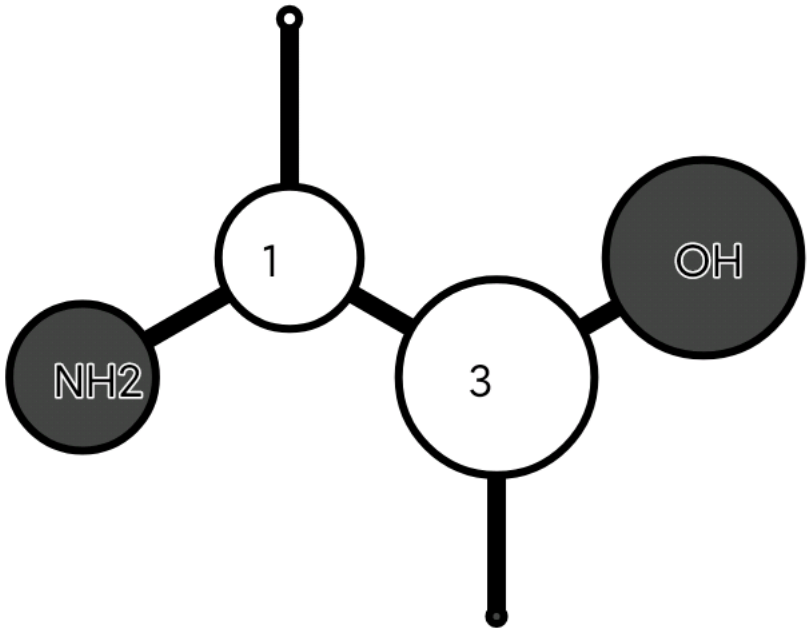


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6
1	0.428					
2		0.058				
3			0.589			
4				-0.045		
5					-0.589	
6						-0.441

4.2. Presentation of molecule:

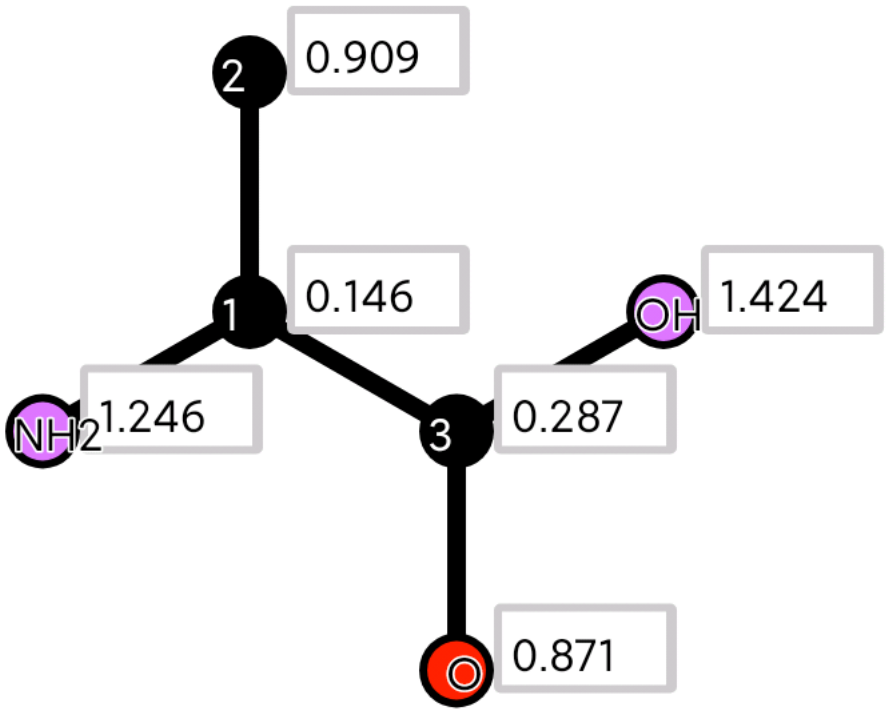


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6
0.146	0.909	0.287	0.871	1.424	1.246

5.2. Presentation of molecule:

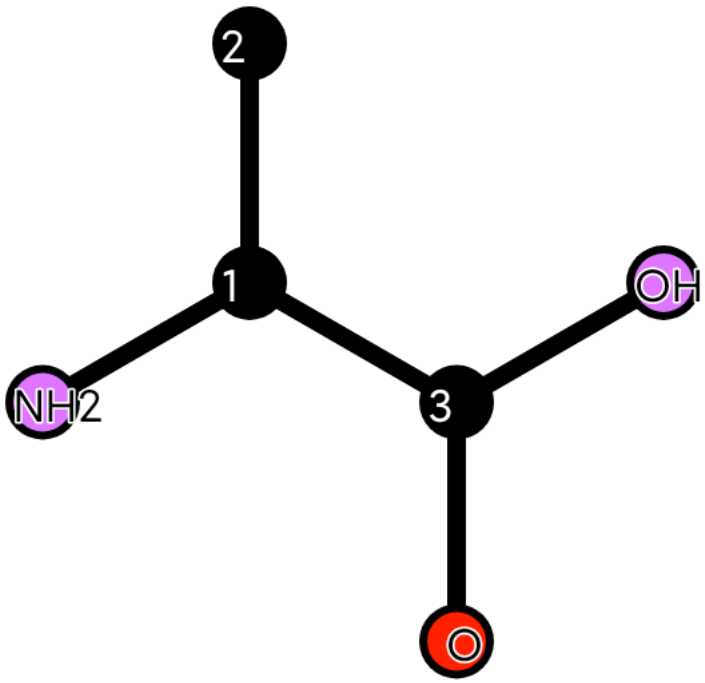


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6
1	0.334					
2	-0.339	0.576				
3	-0.005	-0.021	0.204			
4	0.017	-0.063	-0.17	0.238		
5	0.002	-0.005	-0.013	-0.026	0.042	
6	-0.009	-0.148	0.006	0.004	0.001	0.147

6.2. Presentation of molecule:

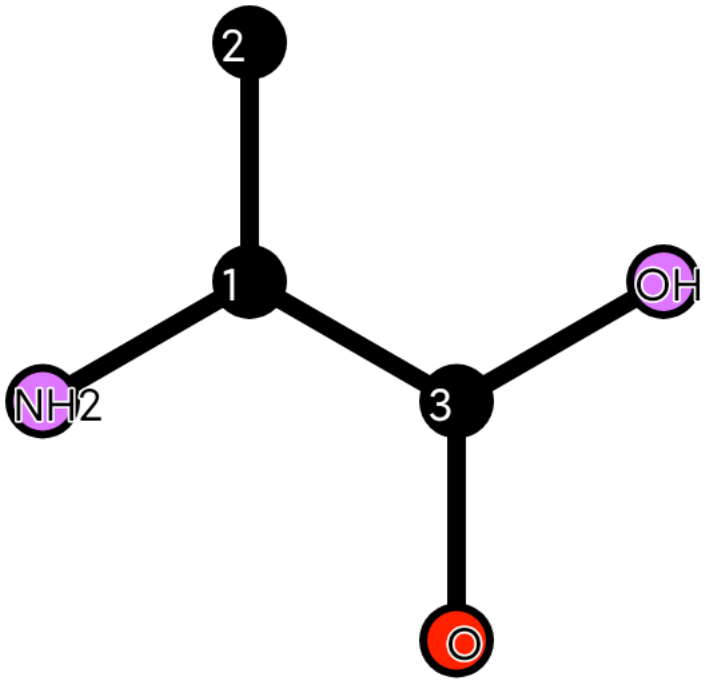


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6
1 2	0.064	-0.14	-0.009	0.003	-0.001	0.082
1 3	0.034	-0.096	0.03	0.012	0.004	0.016
1 6	-0.065	0.231	-0.005	-0.01	-0.001	-0.151
3 4	-0.009	0.04	0.048	-0.095	0.022	-0.006
3 5	-0.002	0.011	0.002	0.071	-0.08	-0.002

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3	1 6	3 4	3 5
1 2	0.147				
1 3	-0.041	0.266			
1 6	-0.201	-0.07	0.356		
3 4	0.013	-0.079	0.02	0.106	
3 5	0.006	-0.03	0.006	-0.098	0.316

8.2. Presentation of molecule: