Print calculated values

Report generated by:root, 19.02.2020 - 14:06:03

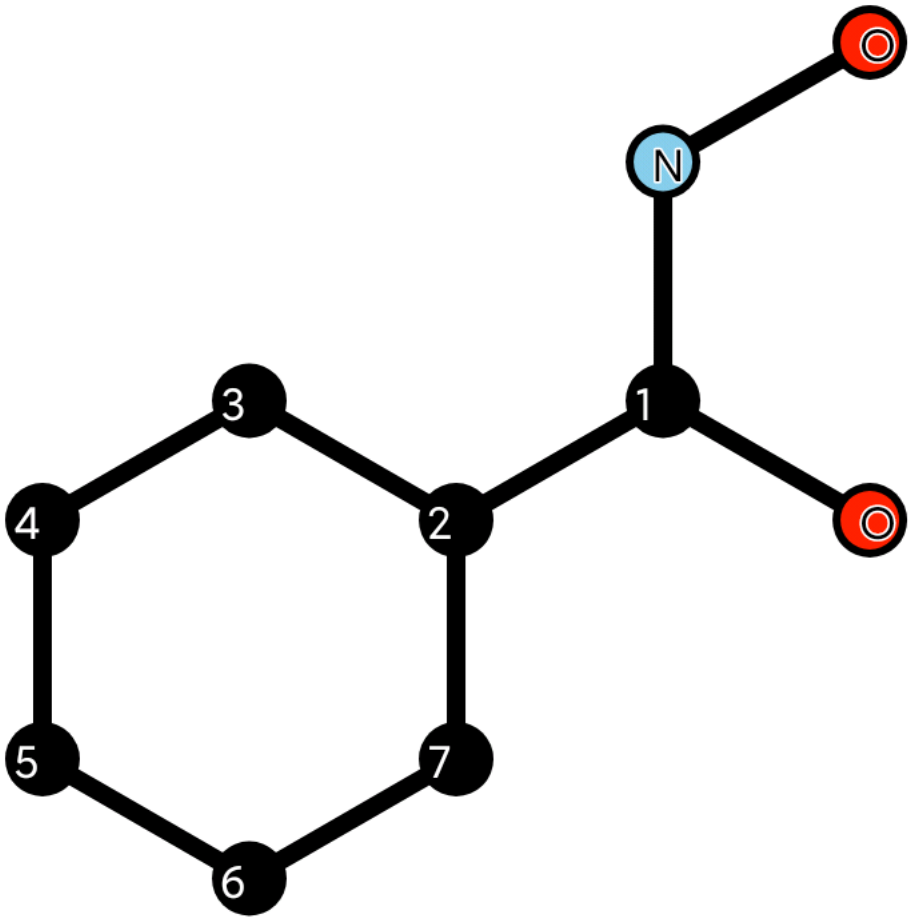
The following determinant is calculated:

-x	1.0	0.0	0.0	0.0	0.0	0.0	1.06	0.0	1.93
1.0	-x	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
0.0	1.0	-x	1.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	1.0	-x	1.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	1.0	-x	1.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1.0	-x	1.0	0.0	0.0	0.0
0.0	1.0	0.0	0.0	0.0	1.0	-x	0.0	0.0	0.0
1.06	0.0	0.0	0.0	0.0	0.0	0.0	-x+0.83	1.95	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.95	-x+1.18	0.0
1.93	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-x+1.18

It is about this molecule:

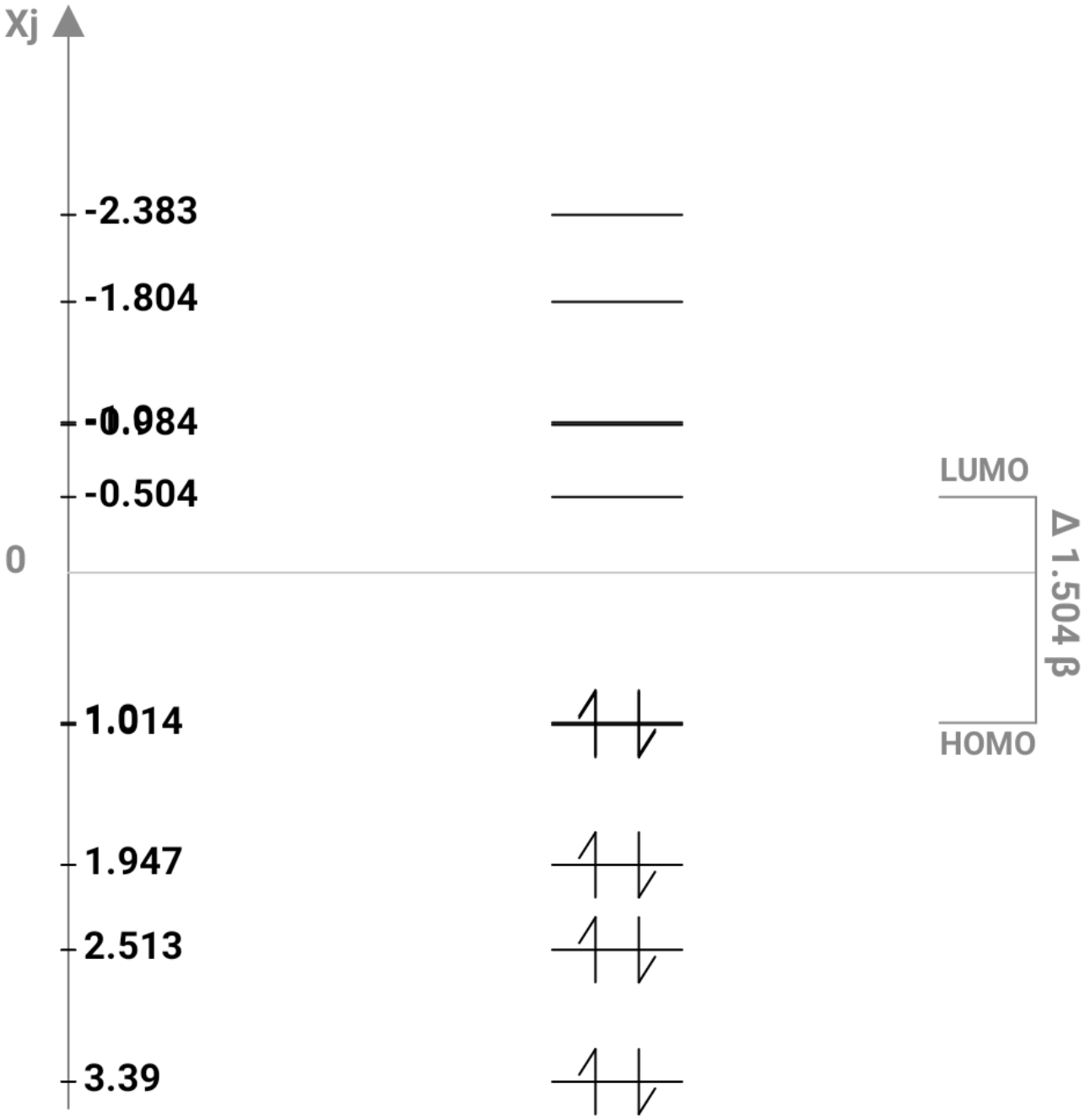
HMO-Energies

x1 = 3.39; x2 = 2.513; x3 = 1.947; x4 = 1.014; x5 = 1.0; x6 = -0.504; x7 = -0.984; x8 = -1.0;
x9 = -1.804; x10 = -2.383;


N
1
2
3
4
5
6
7

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 10α + 19.728β -

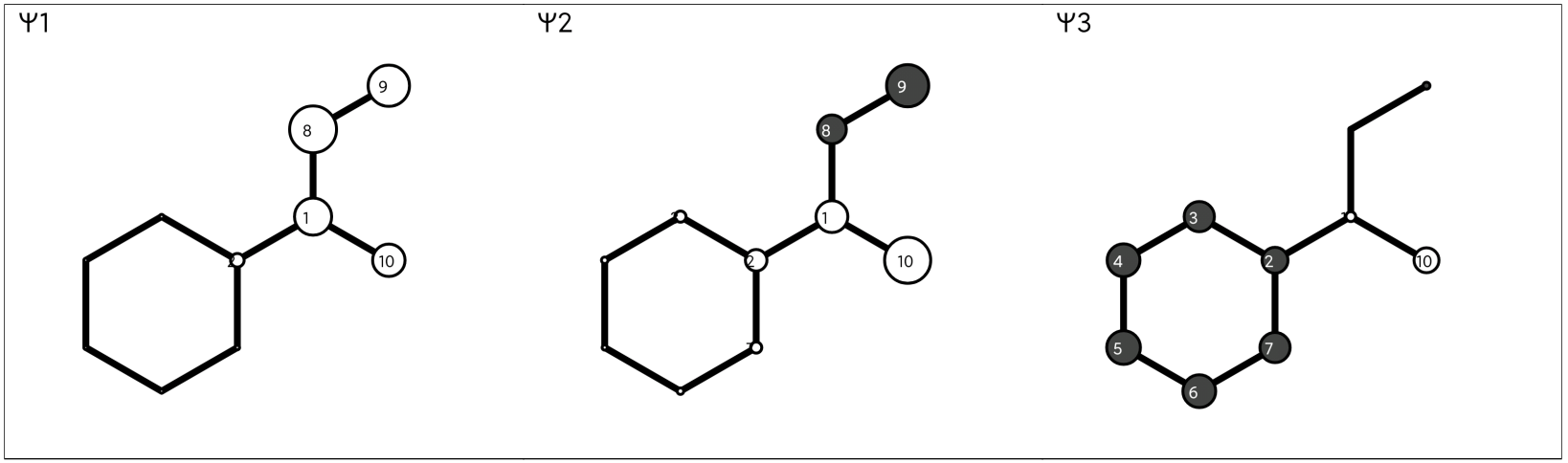
this corresponds to one πelectron: 1.973β

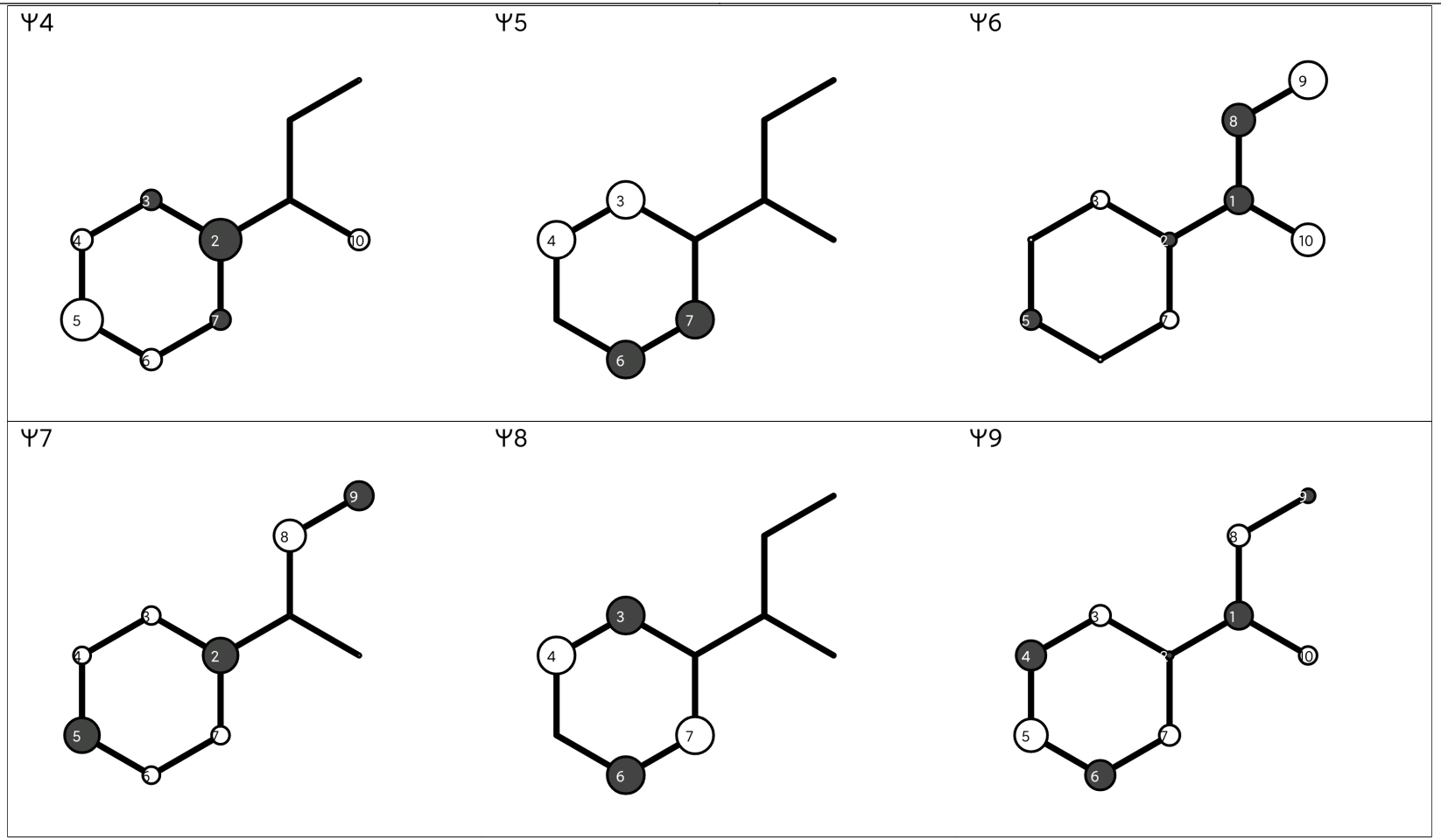
2. Hueckel-coefficient

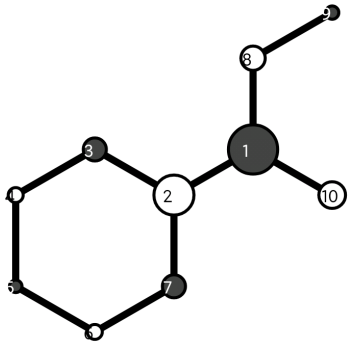
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10
	x1= 3.39	x2= 2.513	x3= 1.947	x4= 1.014	x5= 1.0	x6= -0.504	x7= -0.984	x8= -1.0	x9= -1.804	x10= -2.383
1	0.458	0.393	0.122	-0.024	0.0	-0.378	-0.023	0.0	-0.373	-0.581
2	0.168	0.266	-0.32	-0.556	0.0	-0.187	-0.47	0.0	-0.101	0.473
3	0.055	0.138	-0.373	-0.27	0.5	0.236	0.243	-0.5	0.278	-0.272
4	0.02	0.08	-0.405	0.282	0.5	0.068	0.231	0.5	-0.4	0.177
5	0.012	0.064	-0.416	0.556	0.0	-0.271	-0.47	0.0	0.444	-0.148
6	0.02	0.08	-0.405	0.282	-0.5	0.068	0.231	-0.5	-0.4	0.177
7	0.055	0.138	-0.373	-0.27	-0.5	0.236	0.243	0.5	0.278	-0.272
8	0.578	-0.355	-0.034	-0.001	0.0	-0.433	0.428	0.0	0.291	0.287
9	0.51	-0.52	-0.086	0.013	0.0	0.502	-0.385	0.0	-0.19	-0.157
10	0.4	0.569	0.308	0.276	0.0	0.434	0.02	0.0	0.241	0.315

2.2. Molecule orbital presentation:




Ψ4
Ψ5
Ψ6
Ψ7
Ψ8
Ψ9

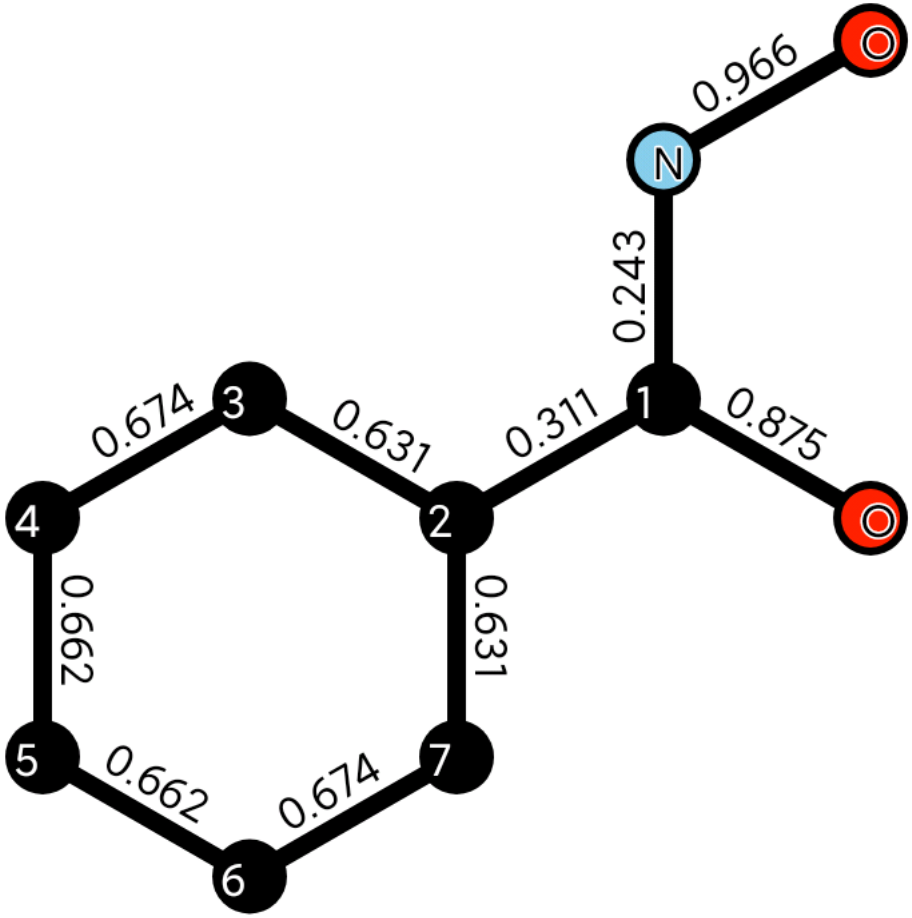
Ψ10 		

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.759									
2	0.311	1.021								
3	0.081	0.631	0.968							
4	-0.031	-0.005	0.674	1.001						
5	-0.067	-0.314	0.029	0.662	0.974					
6	-0.031	-0.005	-0.326	0.001	0.662	1.001				
7	0.081	0.631	-0.032	-0.326	0.029	0.674	0.968			
8	0.243	0.028	-0.008	-0.008	-0.005	-0.008	-0.008	0.924		
9	0.038	-0.065	-0.03	0.013	0.031	0.013	-0.03	0.966	1.077	
10	0.875	-0.067	-0.177	0.013	0.133	0.013	-0.177	0.037	-0.229	1.308

3.2. Presentation of bond order:

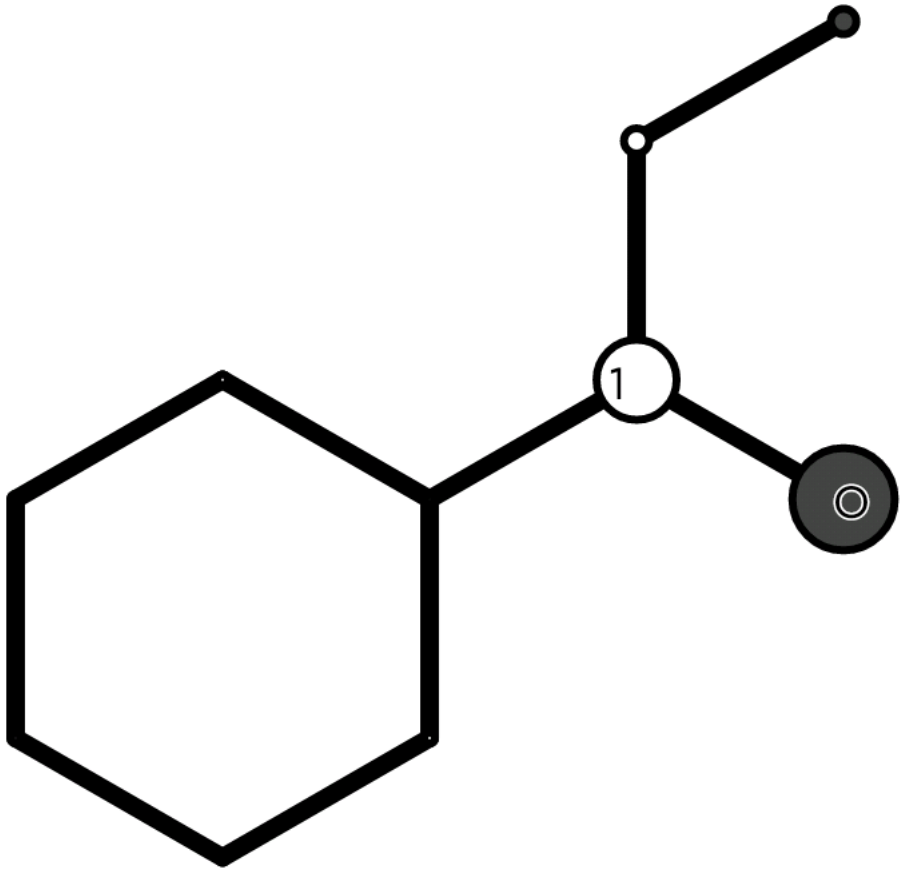

0.966
N
0.243
0.674
3
0.631
0.311
1
0.875
4
2
0.662
0.631
5
0.662
0.674
7
6

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.241									
2		-0.021								
3			0.032							
4				-0.001						
5					0.026					
6						-0.001				
7							0.032			
8								0.076		
9									-0.077	
10										-0.308

4.2. Presentation of molecule:

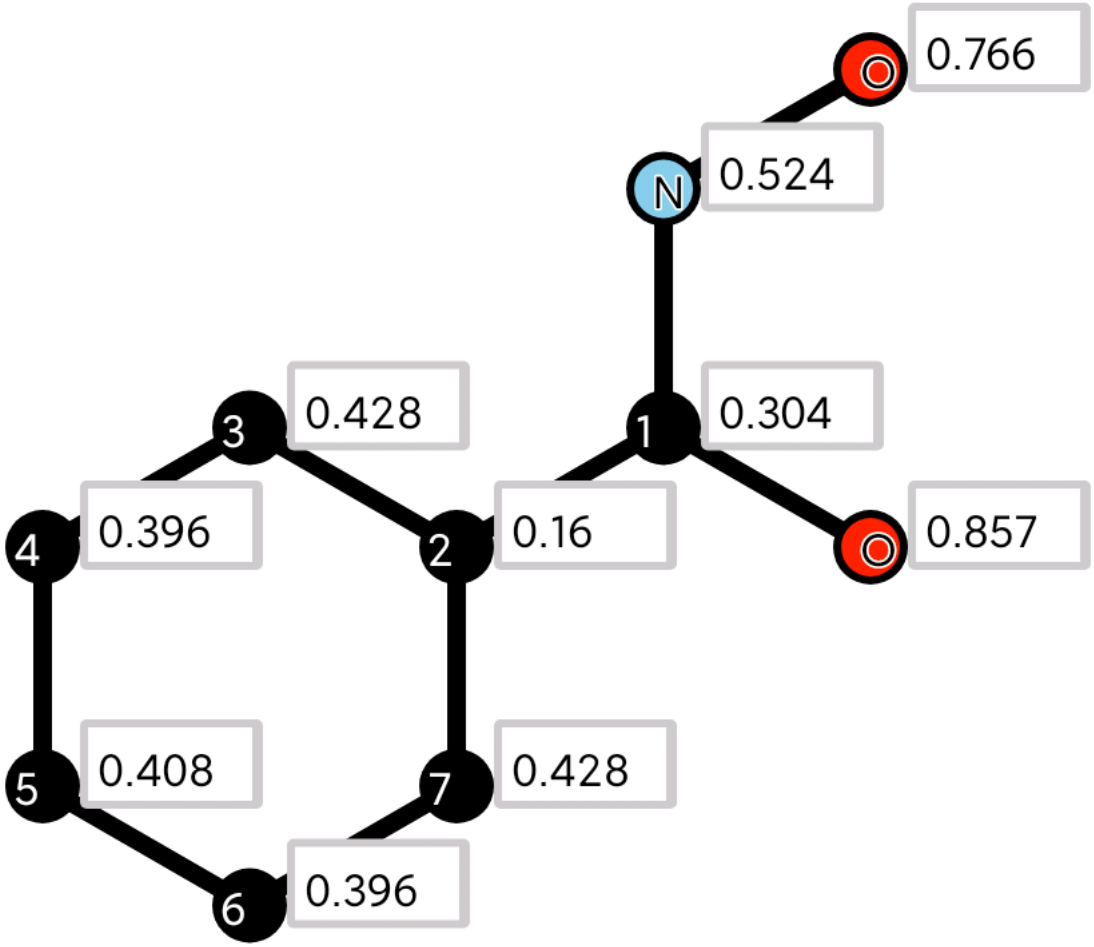

1

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10
0.304	0.16	0.428	0.396	0.408	0.396	0.428	0.524	0.766	0.857

5.2. Presentation of molecule:

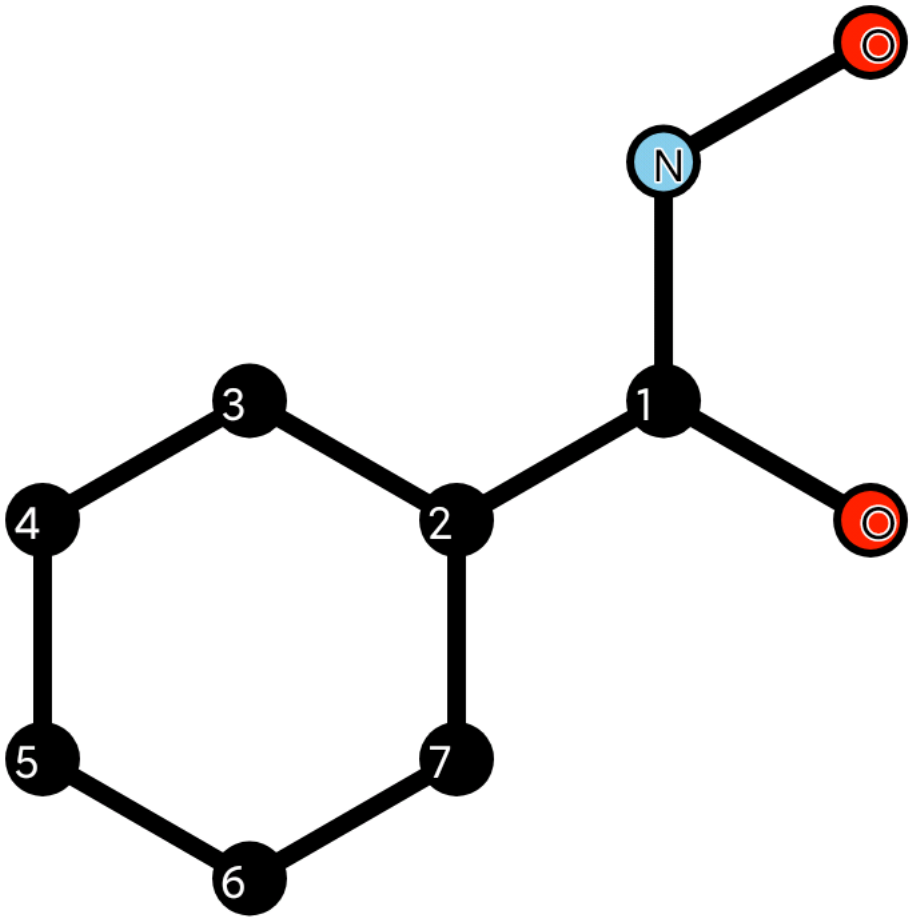

0.766
N
0.524
3
0.428
1
0.304
4
0.396
2
0.16
0.857
5
0.408
7
0.428
6
0.396

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1	0.205									
2	-0.012	0.356								
3	-0.003	-0.14	0.415							
4	0.0	0.008	-0.162	0.397						
5	-0.005	-0.093	0.011	-0.154	0.406					
6	0.0	0.008	-0.099	0.01	-0.154	0.397				
7	-0.003	-0.14	0.004	-0.099	0.011	-0.162	0.415			
8	-0.006	0.0	0.0	0.0	0.0	0.0	0.0	0.239		
9	0.006	-0.002	-0.001	0.0	-0.001	0.0	-0.001	-0.239	0.271	
10	-0.183	0.014	-0.027	0.001	-0.023	0.001	-0.027	0.006	-0.033	0.27

6.2. Presentation of molecule:

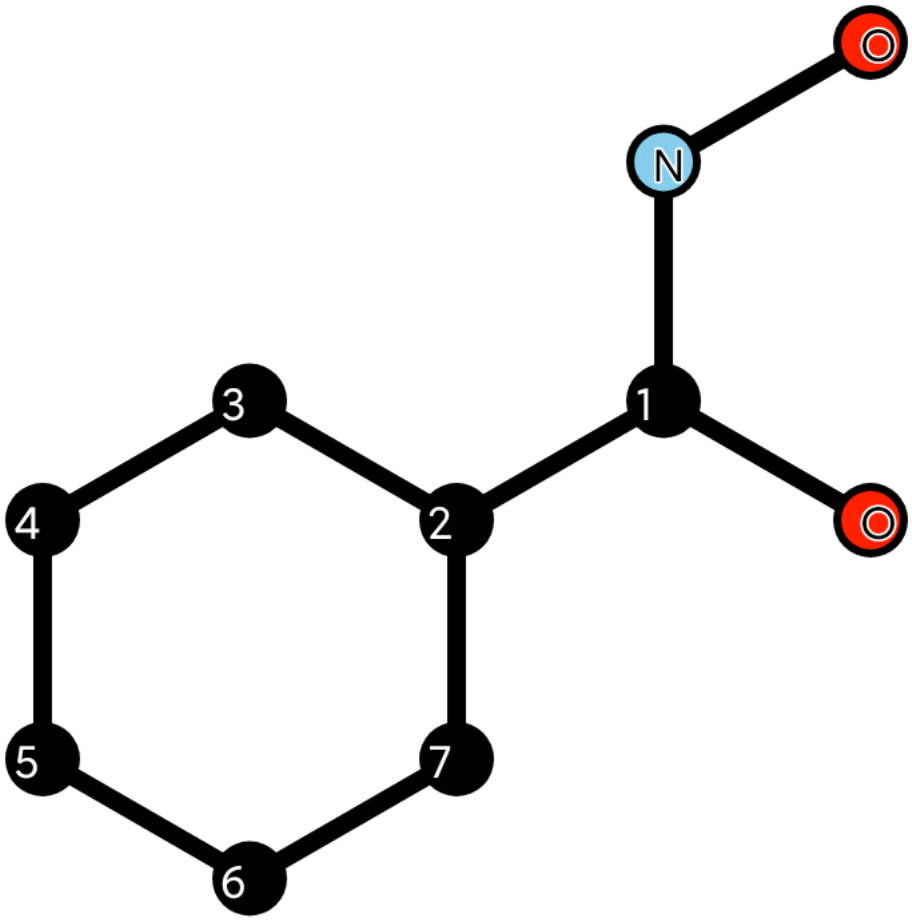

O
N
3
1
4
2
O
5
7
6

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10
1 2	0.027	0.017	-0.03	0.001	-0.025	0.001	-0.03	-0.002	0.003	0.036
1 8	0.015	-0.003	0.0	0.0	-0.001	0.0	0.0	0.012	-0.011	-0.013
1 10	0.044	-0.001	0.012	0.0	0.011	0.0	0.012	-0.003	0.005	-0.079
2 3	-0.008	-0.011	0.007	0.001	0.01	-0.002	0.015	0.0	-0.001	-0.011
2 7	-0.008	-0.011	0.015	-0.002	0.01	0.001	0.007	0.0	-0.001	-0.011
3 4	0.002	0.003	0.016	0.001	-0.012	0.0	-0.013	0.0	0.0	0.003
4 5	-0.002	-0.002	-0.014	-0.002	0.011	0.0	0.011	0.0	0.0	-0.002
5 6	-0.002	-0.002	0.011	0.0	0.011	-0.002	-0.014	0.0	0.0	-0.002
6 7	0.002	0.003	-0.013	0.0	-0.012	0.001	0.016	0.0	0.0	0.003
8 9	-0.003	0.001	0.0	0.0	0.0	0.0	0.0	0.017	-0.02	0.005

7.2. Presentation of molecule:

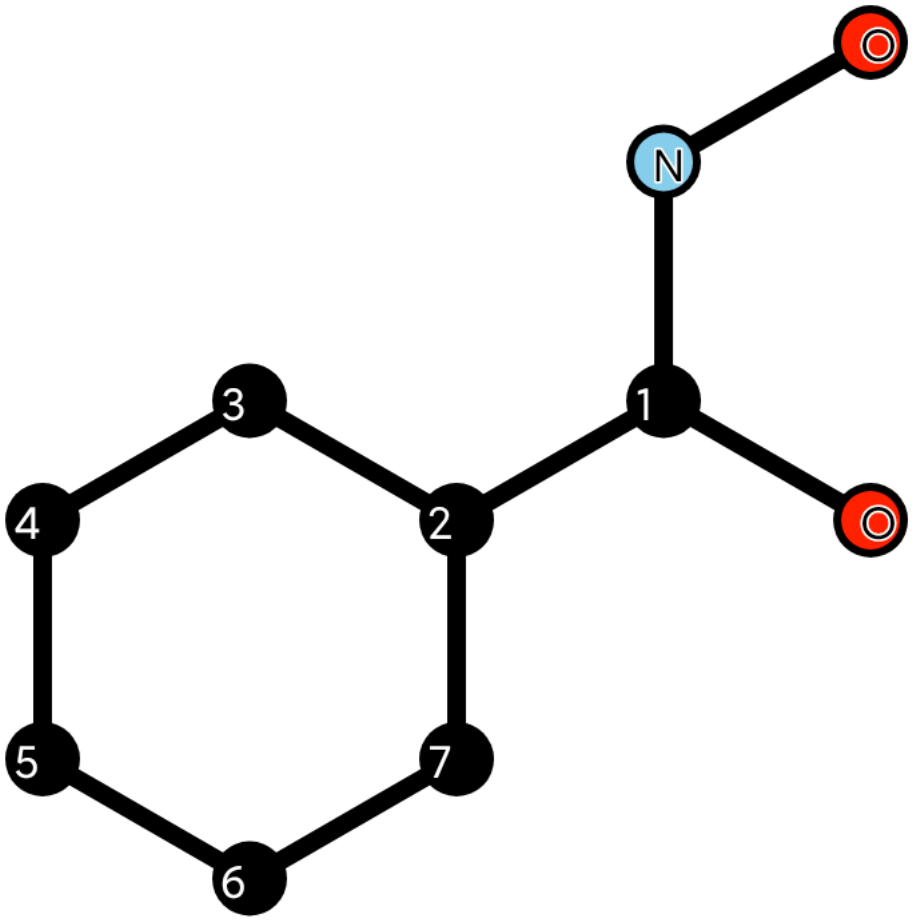

O
N
3
1
4
2
O
5
7
6

8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 8	1 10	2 3	2 7	3 4	4 5	5 6	6 7	8 9
1 2	0.286									
1 8	-0.014	0.216								
1 10	-0.1	-0.047	0.088							
2 3	-0.069	0.0	0.025	0.246						
2 7	-0.069	0.0	0.025	-0.174	0.246					
3 4	0.014	0.001	-0.006	-0.195	0.118	0.244				
4 5	-0.009	-0.001	0.005	0.126	-0.085	-0.21	0.248			
5 6	-0.009	-0.001	0.005	-0.085	0.126	0.128	-0.202	0.248		
6 7	0.014	0.001	-0.006	0.118	-0.195	-0.091	0.128	-0.21	0.244	
8 9	0.003	-0.055	0.012	0.0	0.0	0.0	0.0	0.0	0.0	0.018

8.2. Presentation of molecule:


O
N
3
1
4
2
O
5
7
6