Print calculated values

Report generated by:root, 18.02.2020 - 12:02:51

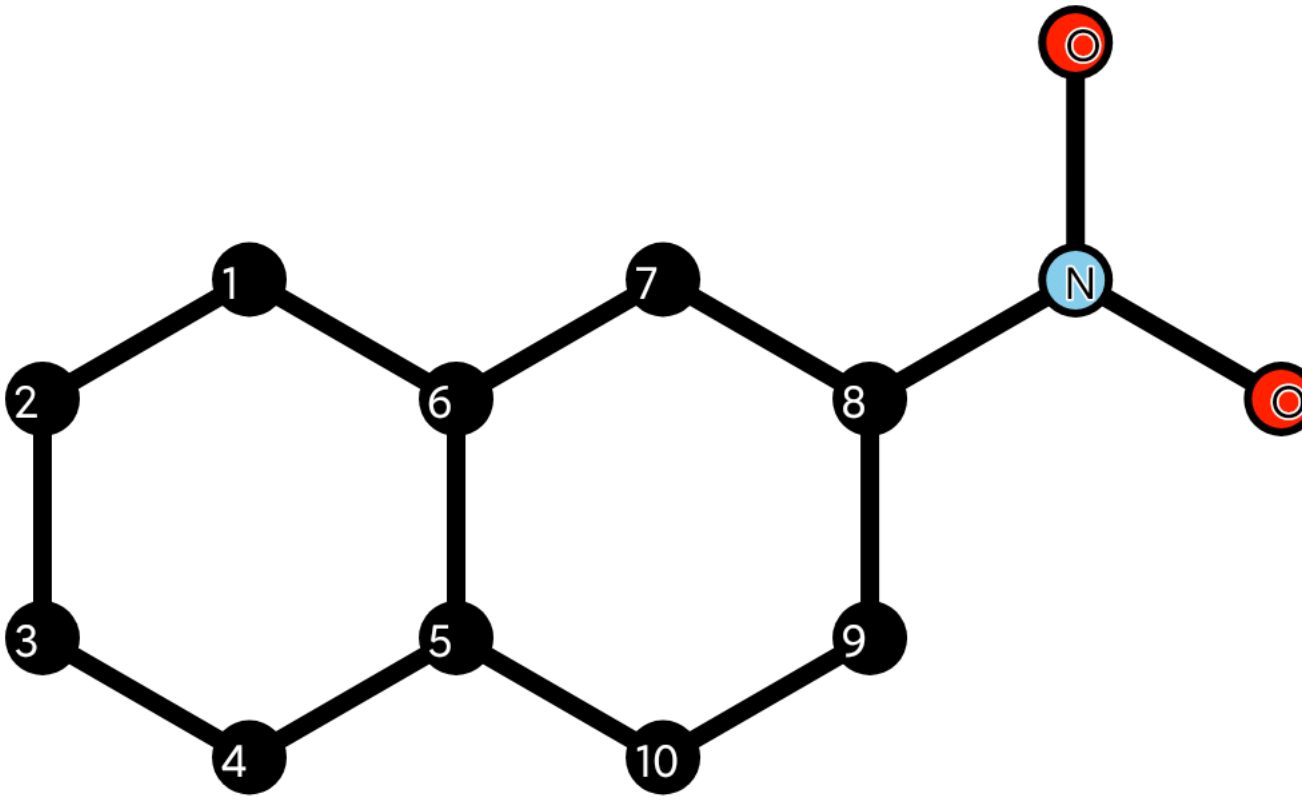
The following determinant is calculated:

-x	1.0	0.0	0.0	0.0	1.0	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	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	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
0.0	0.0	0.0	1.0	-x	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
1.0	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	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	0.0	0.0	0.0	1.0	-x	1.0	0.0	1.3	0.0	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	1.0	0.0	0.0	0.0	1.0	-x	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.3	0.0	0.0	-x+1.47	1.95	1.95
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.95	-x+1.18	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.95	0.0	-x+1.18

It is about this molecule:

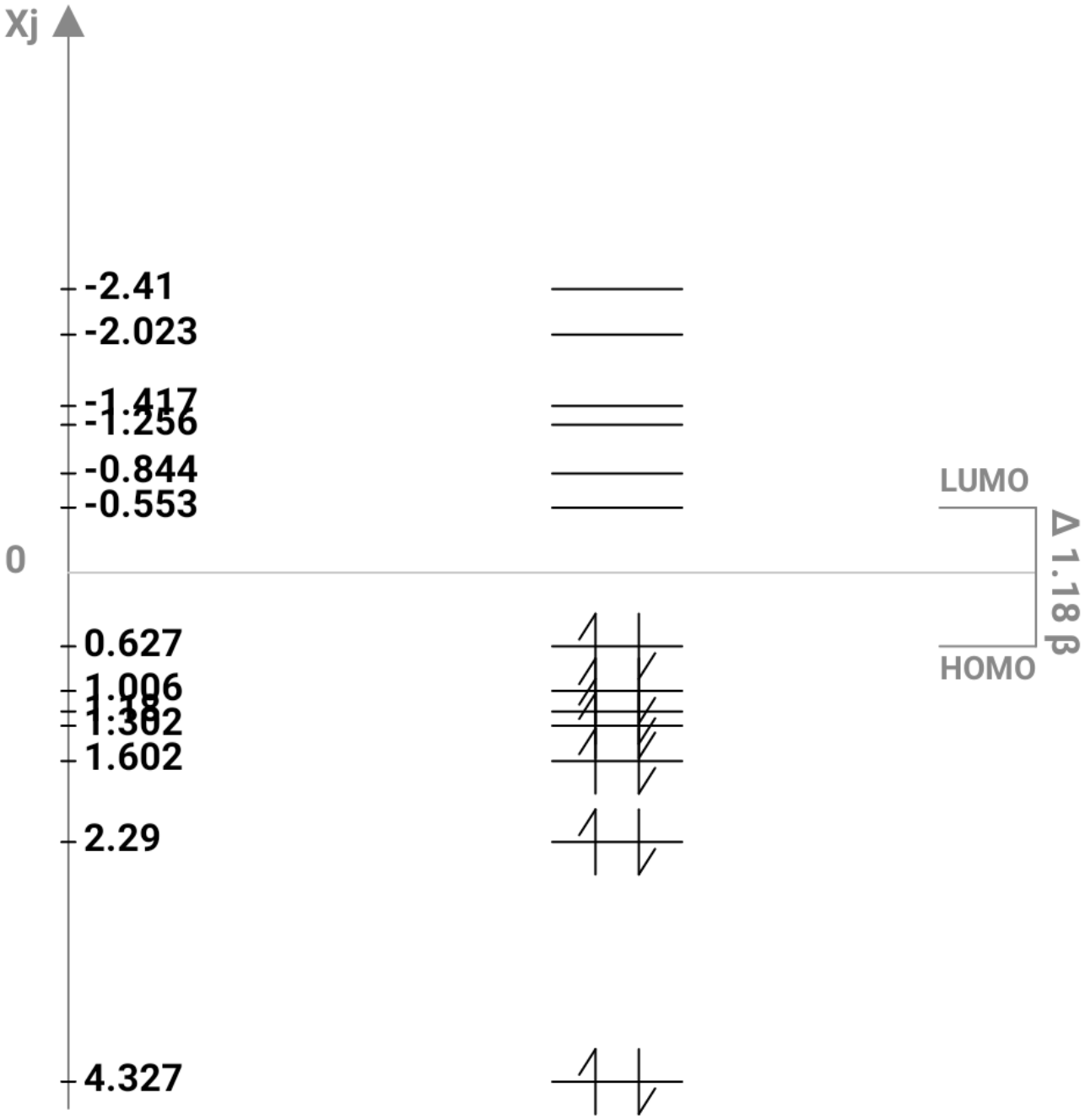
HMO-Energies

x1 = 4.327; x2 = 2.29; x3 = 1.602; x4 = 1.302; x5 = 1.18; x6 = 1.006; x7 = 0.627; x8 = -0.553;
x9 = -0.844; x10 = -1.256; x11 = -1.417; x12 = -2.023; x13 = -2.41;


1
2
3
4
5
6
7
8
9
10
N
O
O

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 13α + 24.668β -

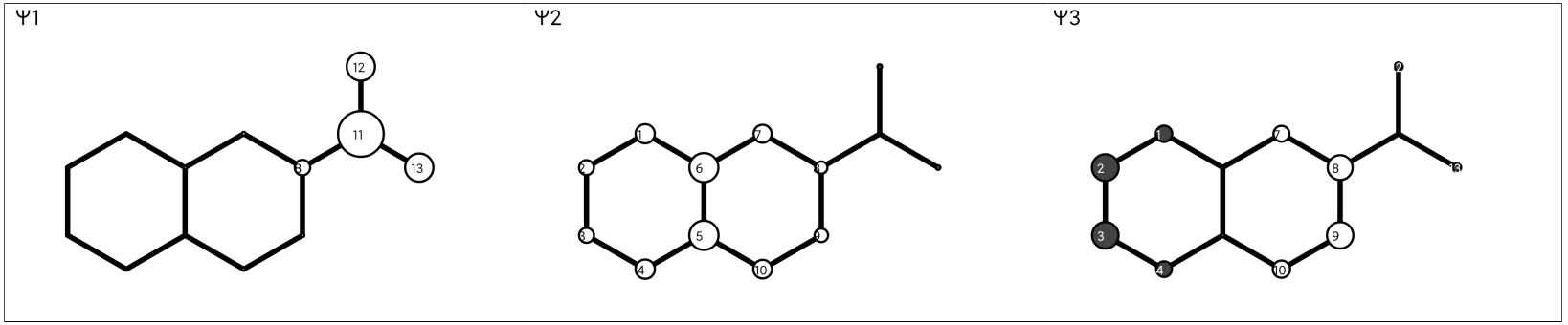
this corresponds to one πelectron: 1.762β

2. Hueckel-coefficient

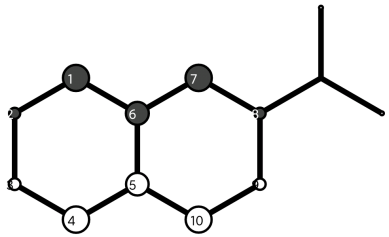
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11	Psi 12	Psi 13
	x1= 4.327	x2= 2.29	x3= 1.602	x4= 1.302	x5= 1.18	x6= 1.006	x7= 0.627	x8= -0.553	x9= -0.844	x10= -1.256	x11= -1.417	x12= -2.023	x13= -2.41
1	0.004	0.306	-0.26	-0.397	0.0	-0.005	0.42	0.401	-0.149	0.31	0.326	0.267	0.218
2	0.001	0.237	-0.426	-0.168	0.0	0.4	0.272	-0.178	0.383	0.079	-0.466	-0.272	-0.153
3	0.001	0.238	-0.422	0.178	0.0	0.408	-0.25	-0.302	-0.175	-0.41	0.334	0.284	0.149
4	0.002	0.307	-0.25	0.4	0.0	0.01	-0.428	0.346	-0.236	0.435	-0.008	-0.303	-0.208
5	0.008	0.466	0.021	0.343	0.0	-0.398	-0.018	0.111	0.374	-0.137	-0.323	0.328	0.351
6	0.017	0.462	0.009	-0.349	0.0	-0.405	-0.008	-0.044	-0.258	-0.469	0.004	-0.268	-0.374
7	0.061	0.287	0.253	-0.4	0.0	-0.005	-0.407	-0.488	-0.007	0.416	-0.008	-0.053	0.332
8	0.246	0.196	0.397	-0.172	0.0	0.4	-0.247	0.314	0.264	-0.053	0.008	0.375	-0.426
9	0.061	0.215	0.42	0.172	0.0	0.392	0.285	0.09	-0.524	-0.121	-0.332	-0.139	0.286
10	0.016	0.298	0.275	0.395	0.0	-0.005	0.425	-0.364	0.178	0.205	0.462	-0.093	-0.264
11	0.726	-0.042	-0.029	0.004	0.0	0.012	-0.025	0.173	0.238	-0.175	0.253	-0.436	0.314
12	0.45	-0.074	-0.133	0.057	0.707	-0.135	0.088	-0.194	-0.229	0.14	-0.19	0.265	-0.171
13	0.45	-0.074	-0.133	0.057	-0.707	-0.135	0.088	-0.194	-0.229	0.14	-0.19	0.265	-0.171

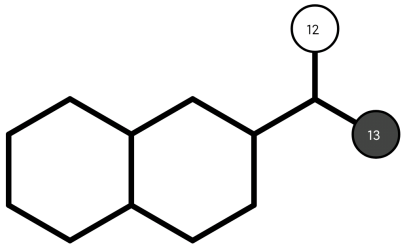
2.2. Molecule orbital presentation:



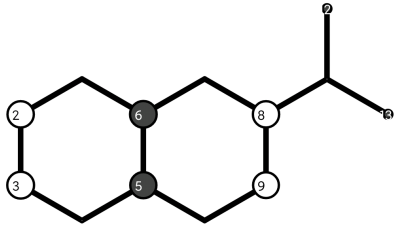
Ψ4



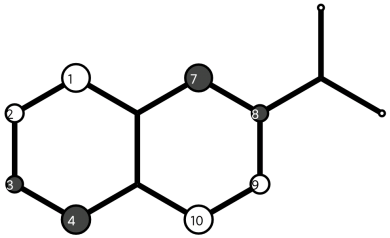
Ψ5



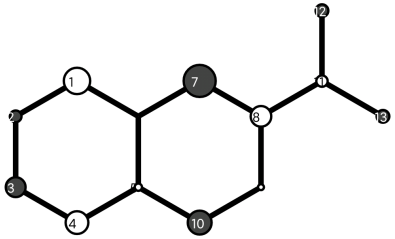
Ψ6



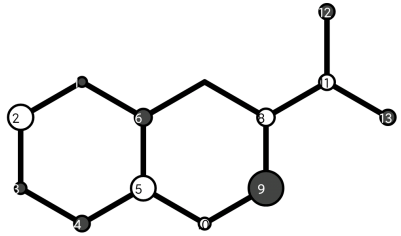
Ψ7



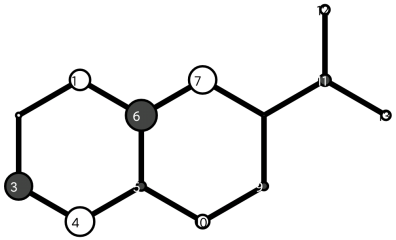
Ψ8



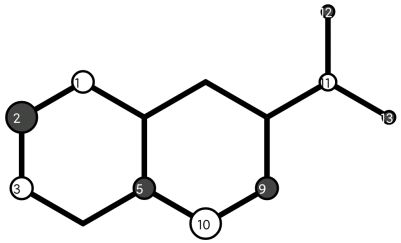
Ψ9



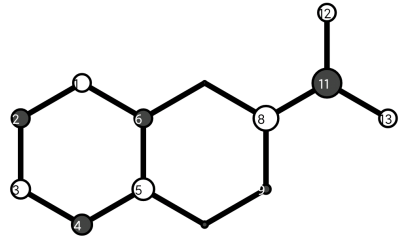
Ψ10



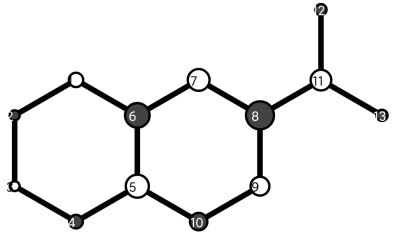
Ψ11



Ψ12



Ψ13

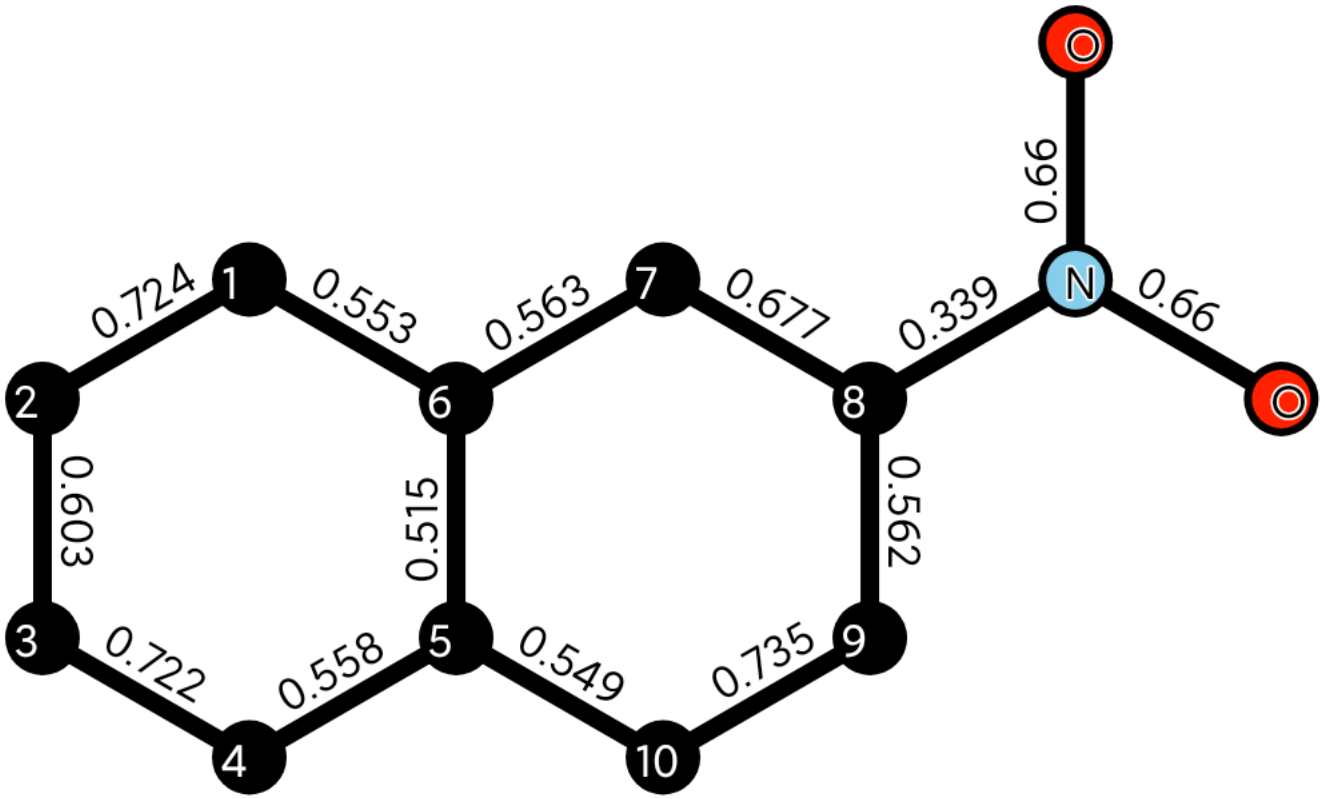


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13
1	0.991												
2	0.724	1.0											
3	0.009	0.603	0.991										
4	-0.36	0.0	0.722	1.001									
5	-0.01	-0.241	0.011	0.558	0.988								
6	0.553	0.0	-0.239	-0.001	0.515	1.001							
7	0.021	-0.17	-0.021	0.078	0.024	0.563	0.952						
8	-0.16	0.0	0.147	0.005	-0.224	-0.004	0.677	1.013					
9	0.012	0.156	-0.012	-0.175	0.015	-0.234	-0.03	0.562	0.981				
10	0.081	0.0	-0.166	-0.002	0.549	0.002	-0.35	-0.007	0.735	1.003			
11	-0.029	0.001	0.029	0.016	-0.035	-0.027	0.067	0.339	0.042	-0.036	1.061		
12	0.057	0.0	-0.056	-0.009	0.076	0.012	-0.171	-0.084	-0.126	0.018	0.66	1.509	
13	0.057	0.0	-0.056	-0.009	0.076	0.012	-0.171	-0.084	-0.126	0.018	0.66	-0.491	1.509

3.2. Presentation of bond order:

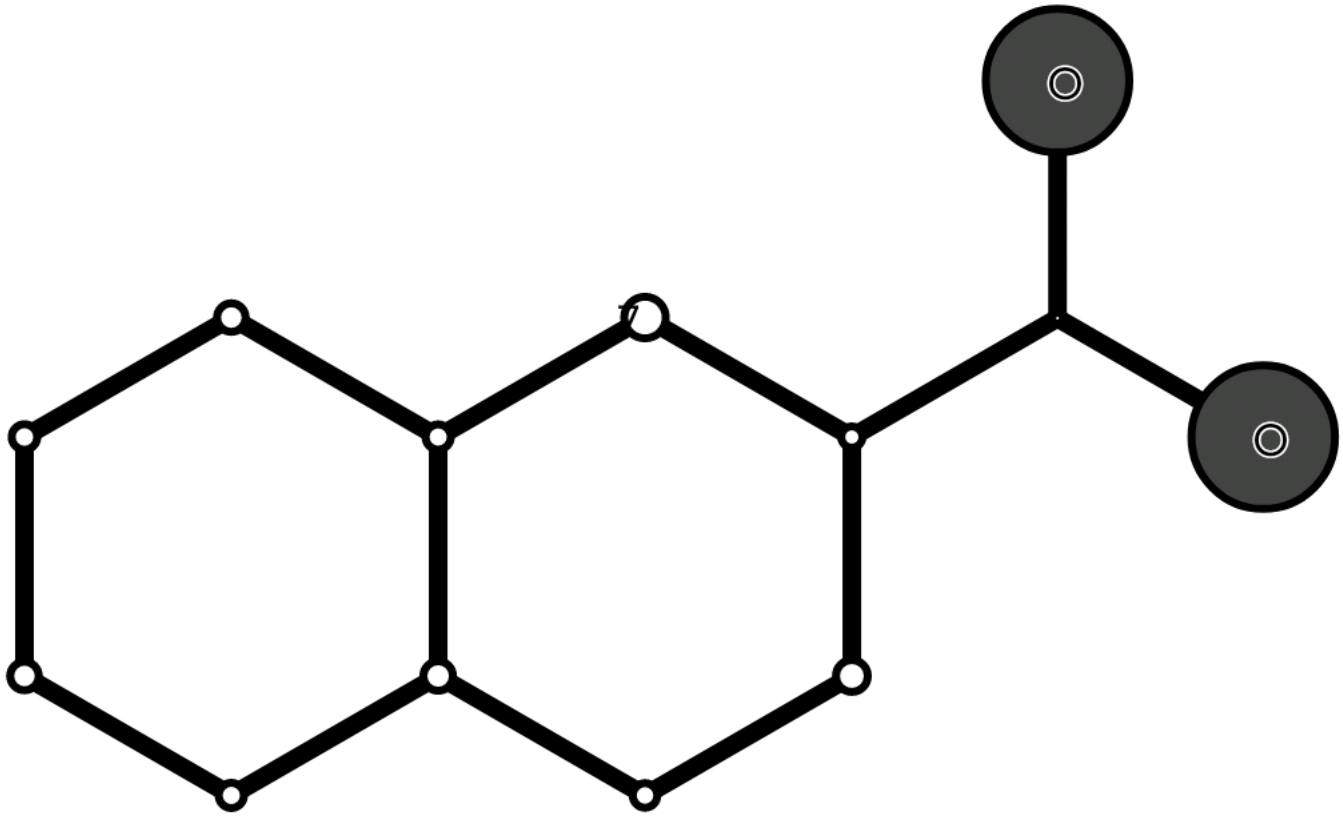

0.724
0.553
0.563
0.677
0.339
0.66
0.99
0.603
0.515
0.562
0.722
0.558
0.549
0.735
1
2
3
4
5
6
7
8
9
10
N
O
O

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13
1	0.086												
2		0.077											
3			0.086										
4				0.076									
5					0.089								
6						0.076							
7							0.125						
8								0.064					
9									0.096				
10										0.074			
11											0.016		
12												-0.432	
13													-0.432

4.2. Presentation of molecule:

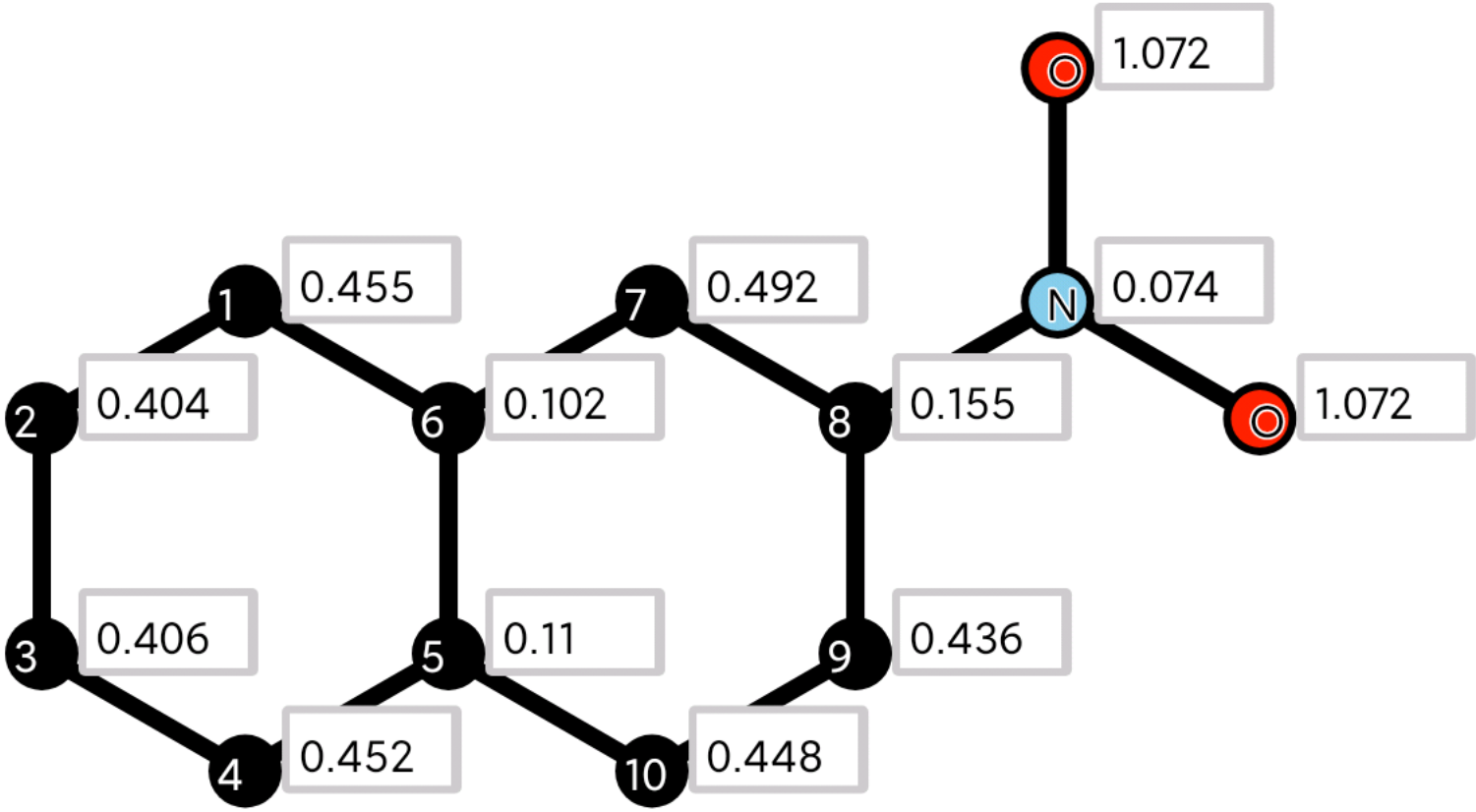


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11	12	13
0.455	0.404	0.406	0.452	0.11	0.102	0.492	0.155	0.436	0.448	0.074	1.072	1.072

5.2. Presentation of molecule:

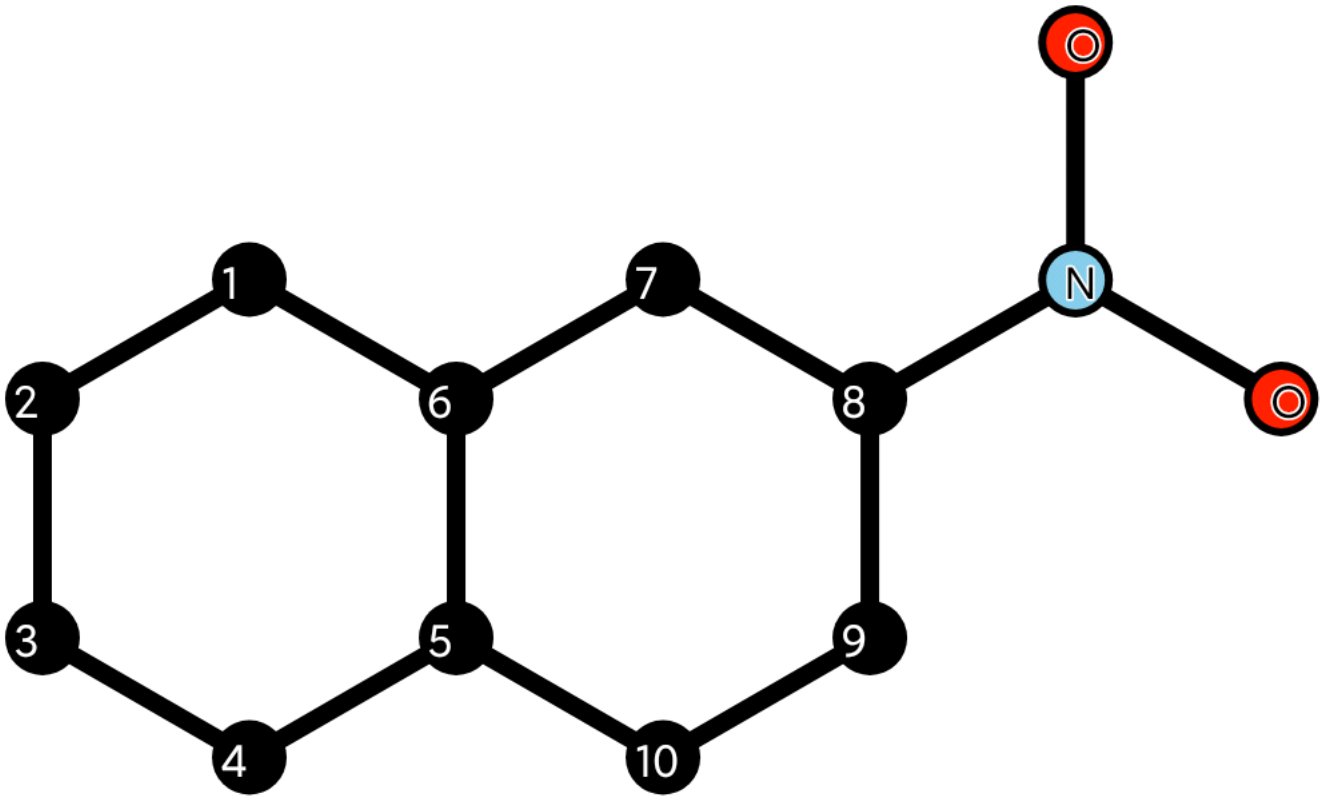

1.072
0.455
1
7
0.492
N
0.074
2
0.404
6
0.102
8
0.155
1.072
3
0.406
5
0.11
9
0.436
4
0.452
10
0.448

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13
1	0.446												
2	-0.213	0.405											
3	0.019	-0.11	0.407										
4	-0.138	0.018	-0.211	0.442									
5	0.003	-0.049	0.008	-0.091	0.333								
6	-0.088	0.007	-0.048	0.003	-0.075	0.329							
7	0.03	-0.032	0.008	-0.022	0.004	-0.093	0.468						
8	-0.03	0.0	-0.03	0.005	-0.043	0.006	-0.189	0.35					
9	0.005	-0.033	0.0	-0.034	0.009	-0.047	0.01	-0.093	0.422				
10	-0.023	0.006	-0.031	0.026	-0.086	0.004	-0.133	0.015	-0.22	0.439			
11	-0.001	0.0	-0.001	0.0	-0.001	0.0	-0.003	-0.013	0.001	0.0	0.167		
12	-0.005	0.0	-0.005	0.001	-0.006	0.0	-0.025	0.011	-0.01	0.001	-0.074	0.255	
13	-0.005	0.0	-0.005	0.001	-0.006	0.0	-0.025	0.011	-0.01	0.001	-0.074	-0.144	0.255

6.2. Presentation of molecule:

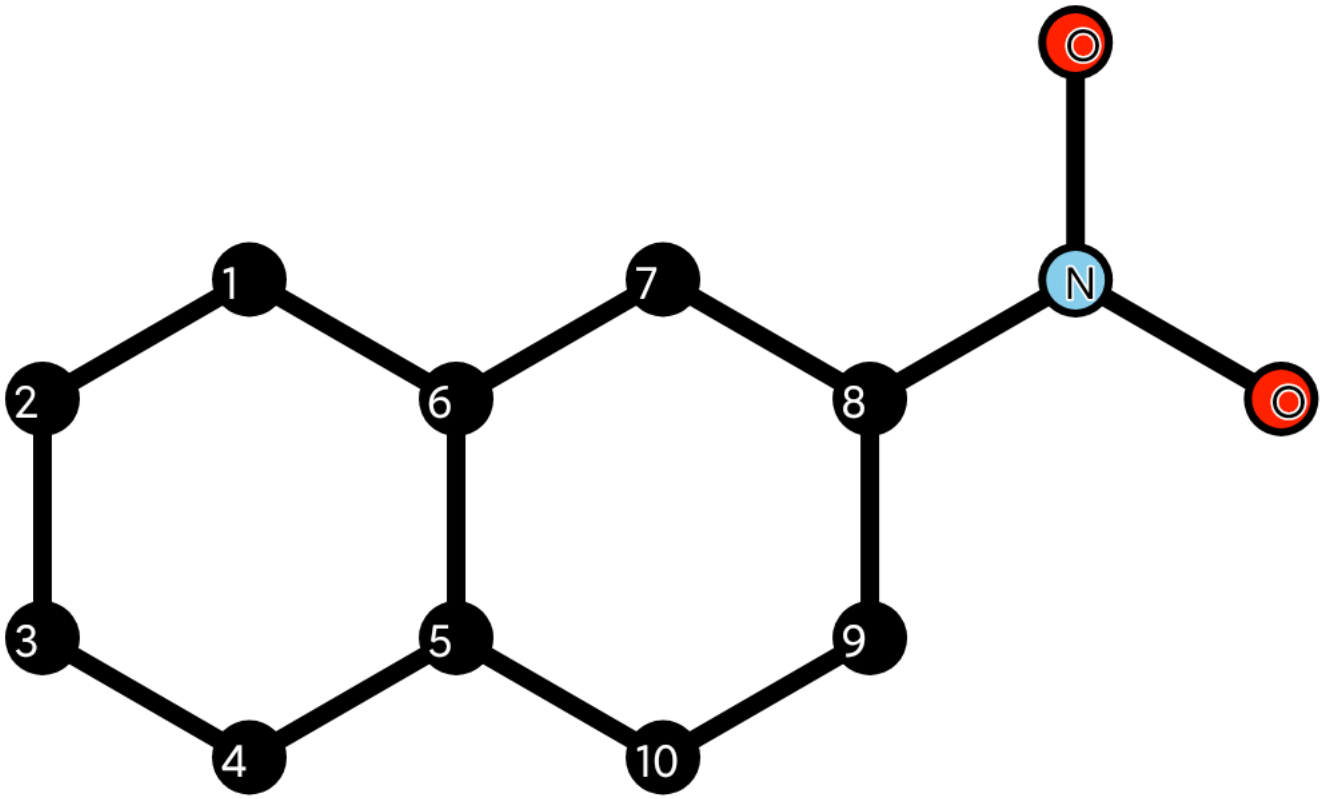

O
1
7
N
2
6
8
O
3
5
9
4
10

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13
1 2	0.005	0.0	-0.003	0.0	-0.003	0.0	0.005	0.0	-0.003	0.0	0.0	0.0	0.0
1 6	0.002	0.0	0.002	0.0	0.003	-0.001	-0.008	-0.001	0.004	0.0	0.0	-0.001	-0.001
2 3	-0.005	0.0	0.003	0.0	0.003	0.0	-0.005	0.0	0.003	0.0	0.0	0.0	0.0
3 4	0.005	0.0	0.005	-0.002	-0.004	0.0	0.004	-0.001	-0.003	-0.001	-0.001	-0.001	-0.001
4 5	-0.006	0.0	-0.006	0.001	0.005	0.0	-0.005	0.002	0.004	0.001	0.001	0.001	0.001
5 6	0.003	0.0	0.003	0.0	0.003	-0.001	-0.008	-0.002	0.004	0.0	-0.001	-0.001	-0.001
5 10	0.003	0.0	0.002	0.0	0.003	0.0	0.012	-0.003	-0.009	-0.003	-0.001	-0.002	-0.002
6 7	-0.006	0.0	-0.006	0.0	-0.007	0.001	0.017	0.003	-0.008	0.0	0.001	0.002	0.002
7 8	0.004	0.0	0.004	-0.001	0.006	0.001	0.016	-0.013	0.011	-0.004	-0.005	-0.01	-0.01
8 9	0.004	0.0	0.003	0.0	0.003	-0.001	0.018	-0.009	0.0	0.002	-0.004	-0.008	-0.008
8 11	-0.007	0.0	-0.007	0.001	-0.009	0.001	-0.034	0.008	-0.013	0.002	0.005	0.026	0.026
9 10	-0.003	0.0	-0.003	0.0	-0.004	0.0	-0.015	0.004	0.012	0.001	0.002	0.003	0.003
11 12	0.002	0.0	0.003	0.0	0.003	0.0	0.011	0.002	0.003	0.0	-0.009	-0.133	0.118
11 13	0.002	0.0	0.003	0.0	0.003	0.0	0.011	0.002	0.003	0.0	-0.009	0.118	-0.133

7.2. Presentation of molecule:

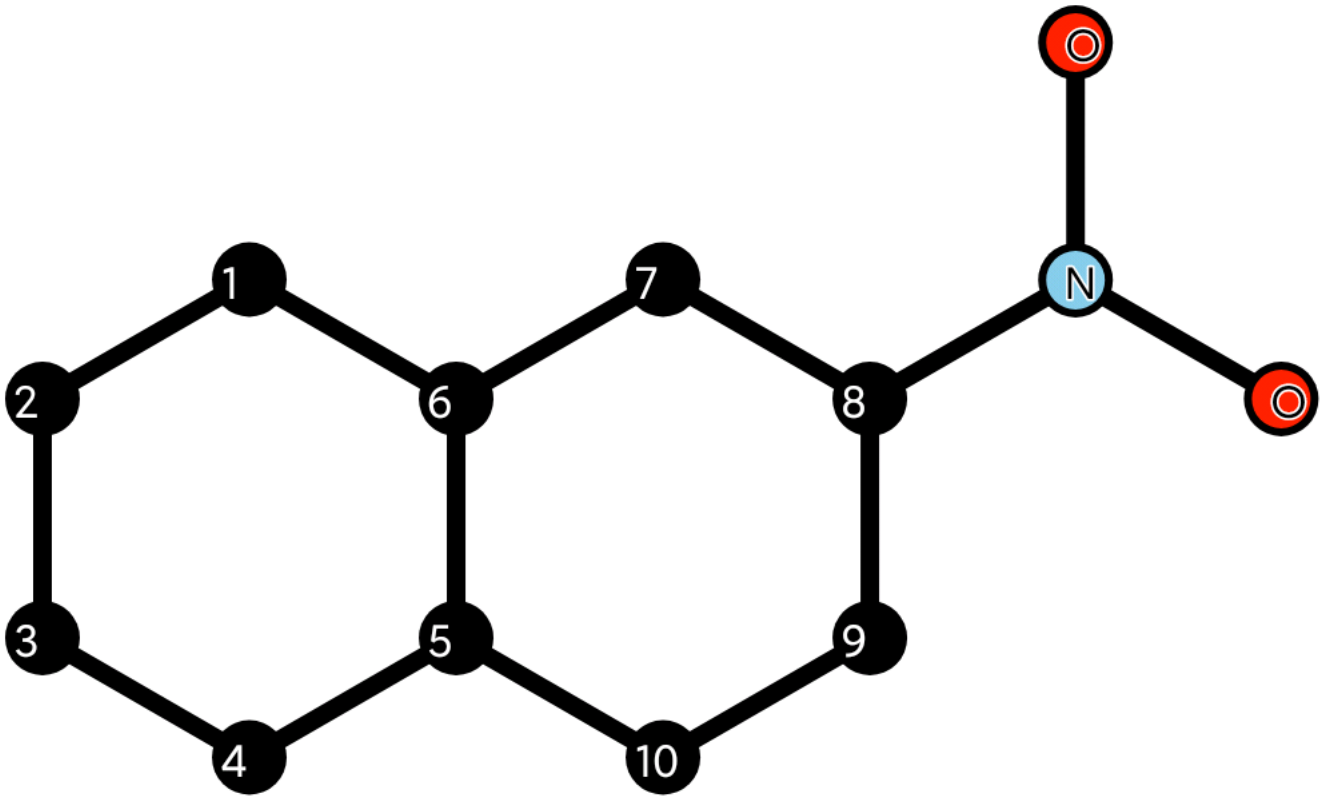

O
1
7
N
2
6
8
O
3
5
9
4
10

8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	2 3	3 4	4 5	5 6	5 10	6 7	7 8	8 9	8 11	9 10	11 12	11 13
1 2	0.21													
1 6	-0.181	0.289												
2 3	-0.21	0.11	0.296											
3 4	0.124	-0.073	-0.209	0.212										
4 5	-0.074	0.094	0.111	-0.184	0.289									
5 6	0.065	-0.106	-0.041	0.066	-0.109	0.256								
5 10	0.025	-0.025	-0.045	0.06	-0.145	-0.108	0.293							
6 7	0.06	-0.149	-0.045	0.023	-0.023	-0.114	0.093	0.294						
7 8	-0.03	0.058	0.031	-0.018	0.022	0.064	-0.066	-0.173	0.216					
8 9	0.031	-0.041	-0.031	0.032	-0.045	-0.038	0.108	0.1	-0.174	0.291				
8 11	0.0	-0.003	0.0	-0.003	0.005	-0.005	-0.008	0.012	-0.068	-0.06	0.234			
9 10	-0.02	0.024	0.032	-0.033	0.062	0.064	-0.186	-0.071	0.11	-0.198	0.015	0.21		
11 12	0.0	0.001	0.0	0.002	-0.002	0.002	0.003	-0.004	0.021	0.017	-0.066	-0.005	0.19	
11 13	0.0	0.001	0.0	0.002	-0.002	0.002	0.003	-0.004	0.021	0.017	-0.066	-0.005	-0.148	0.19

8.2. Presentation of molecule:


O
1
7
N
2
6
8
O
3
5
9
4
10