Print calculated values

Report generated by:root, 18.02.2020 - 12:00:45

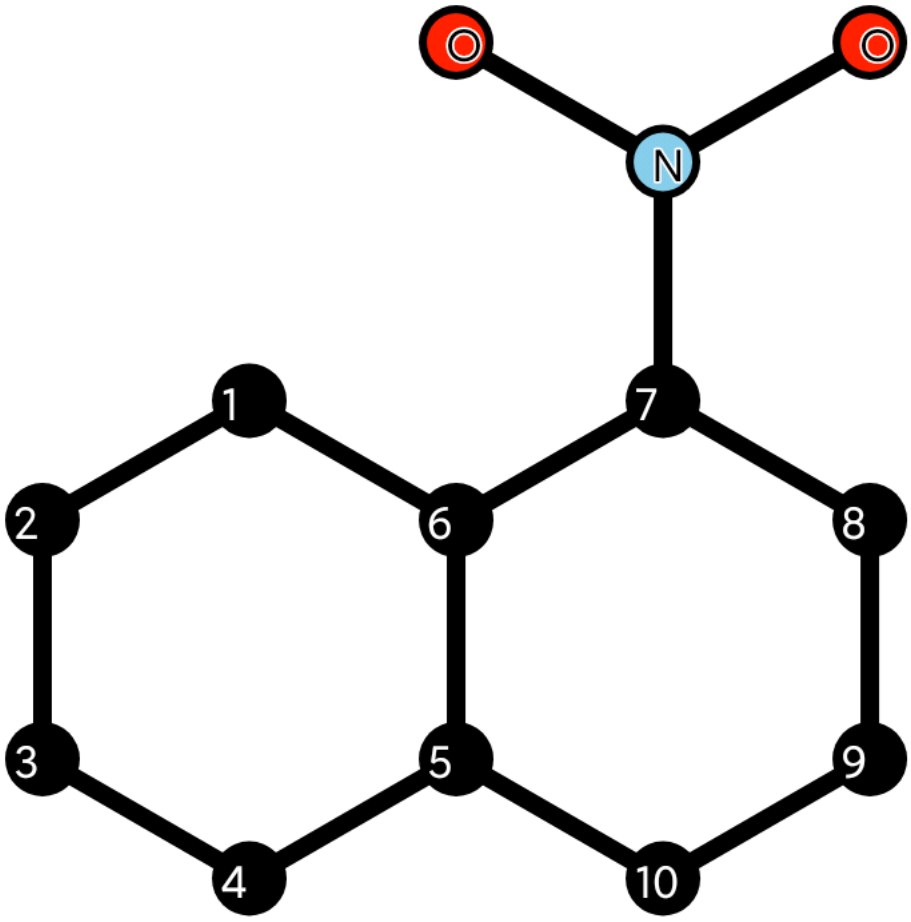
The following determinant is calculated:

-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	1.3	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	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	1.3	0.0	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 = 4.328; x2 = 2.281; x3 = 1.612; x4 = 1.299; x5 = 1.18; x6 = 1.0; x7 = 0.641; x8 = -0.499;
x9 = -1.0; x10 = -1.108; x11 = -1.535; x12 = -1.919; x13 = -2.449;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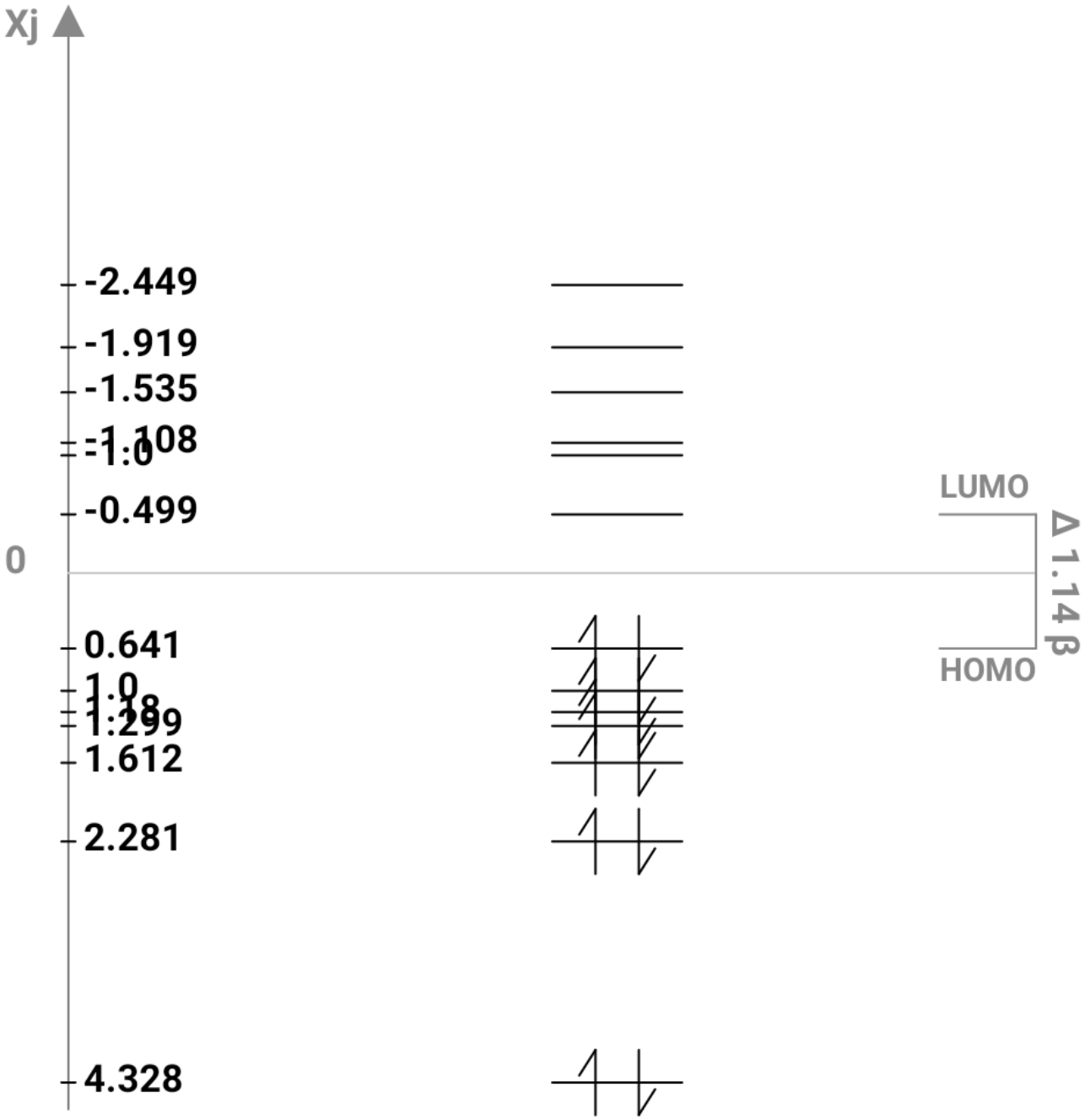
1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 13α + 24.682β -

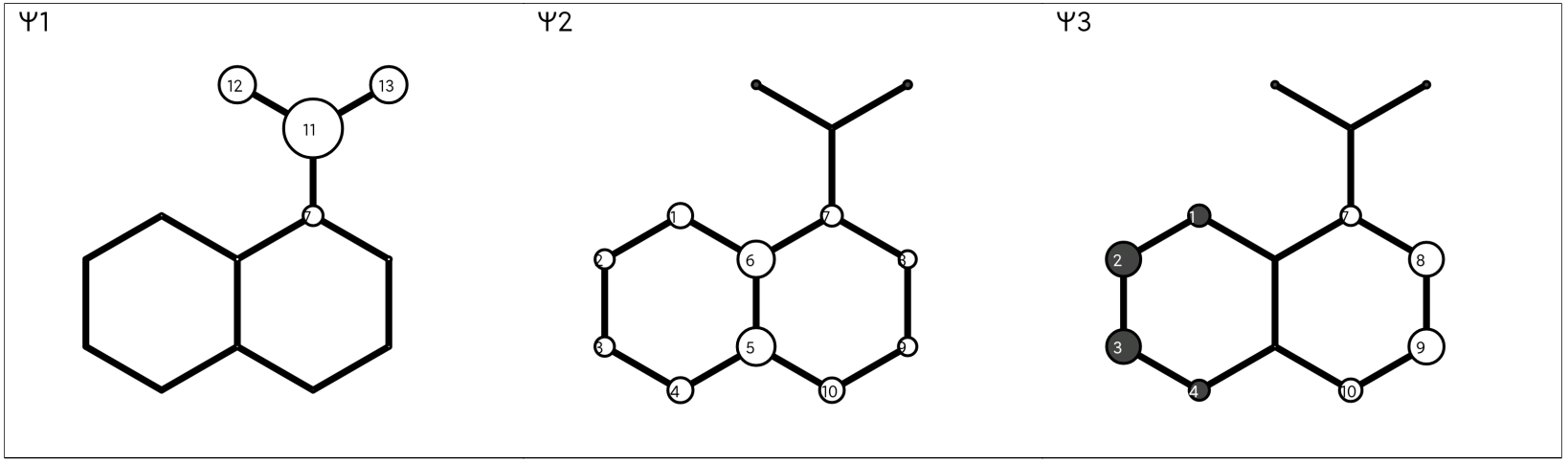
this corresponds to one πelectron: 1.763β

2. Hueckel-coefficient

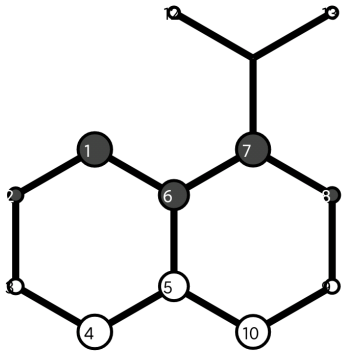
2.1. Calculated values:

	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= 4.328	**x2= 2.281**	**x3= 1.612**	**x4= 1.299**	**x5= 1.18**	**x6= 1.0**	**x7= 0.641**	**x8= -0.499**	**x9= -1.0**	**x10= -1.108**	**x11= -1.535**	**x12= -1.919**	**x13= -2.449**
1	0.016	0.302	-0.265	-0.394	0.0	0.0	0.43	0.32	0.0	-0.446	-0.308	0.21	0.24
2	0.004	0.237	-0.423	-0.169	0.0	0.408	0.254	-0.255	0.408	0.14	0.386	-0.281	-0.158
3	0.002	0.24	-0.417	0.175	0.0	0.408	-0.267	-0.192	-0.408	0.291	-0.285	0.329	0.148
4	0.005	0.31	-0.249	0.396	0.0	0.0	-0.426	0.351	0.0	-0.462	0.051	-0.35	-0.204
5	0.018	0.467	0.016	0.34	0.0	-0.408	-0.005	0.017	0.408	0.222	0.207	0.344	0.351
6	0.065	0.45	-0.004	-0.343	0.0	-0.408	0.022	0.095	-0.408	0.354	0.087	-0.122	-0.429
7	0.247	0.259	0.243	-0.391	0.0	0.0	-0.411	-0.385	0.0	-0.168	-0.032	-0.319	0.46
8	0.061	0.213	0.42	-0.175	0.0	0.408	-0.233	0.35	0.408	0.214	-0.3	0.158	-0.271
9	0.016	0.227	0.433	0.164	0.0	0.408	0.262	0.21	-0.408	-0.069	0.492	0.015	0.203
10	0.008	0.304	0.278	0.388	0.0	0.0	0.401	-0.455	0.0	-0.138	-0.455	-0.187	-0.226
11	0.725	-0.055	-0.018	0.008	0.0	0.0	-0.04	-0.195	0.0	-0.294	0.201	0.443	-0.328
12	0.449	-0.098	-0.082	0.13	-0.707	0.0	0.146	0.227	0.0	0.25	-0.144	-0.279	0.176
13	0.449	-0.098	-0.082	0.13	0.707	0.0	0.146	0.227	0.0	0.25	-0.144	-0.279	0.176

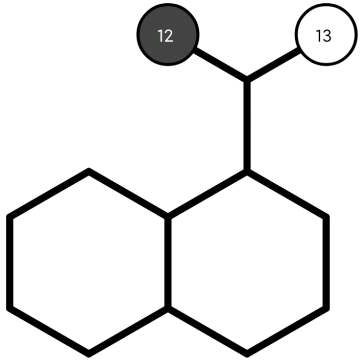
2.2. Molecule orbital presentation:



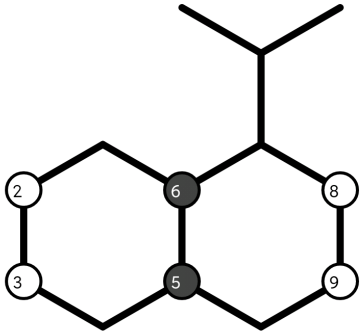
Ψ4



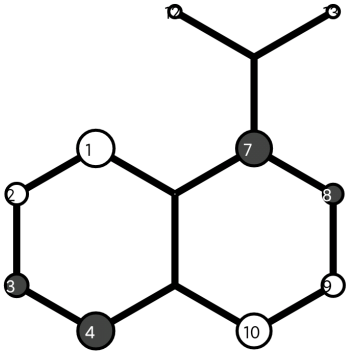
Ψ5



Ψ6



Ψ7



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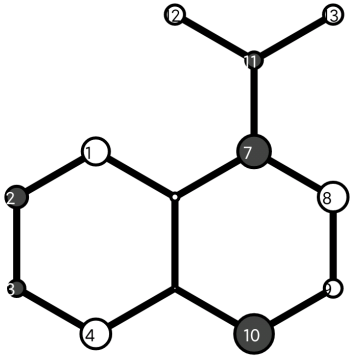

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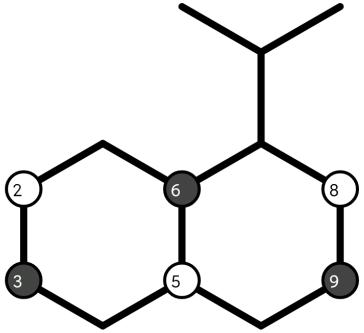
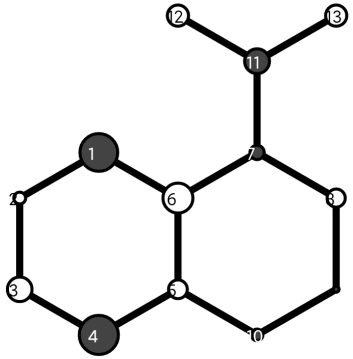
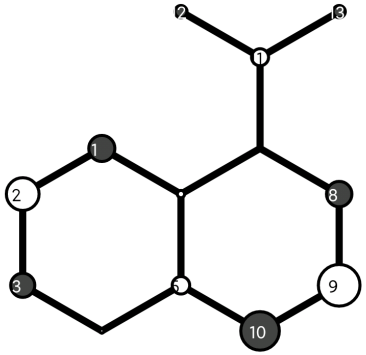


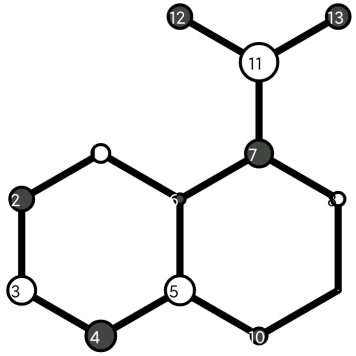
Ψ10



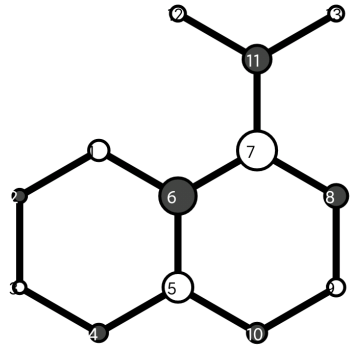
Ψ11



Ψ12



Ψ13

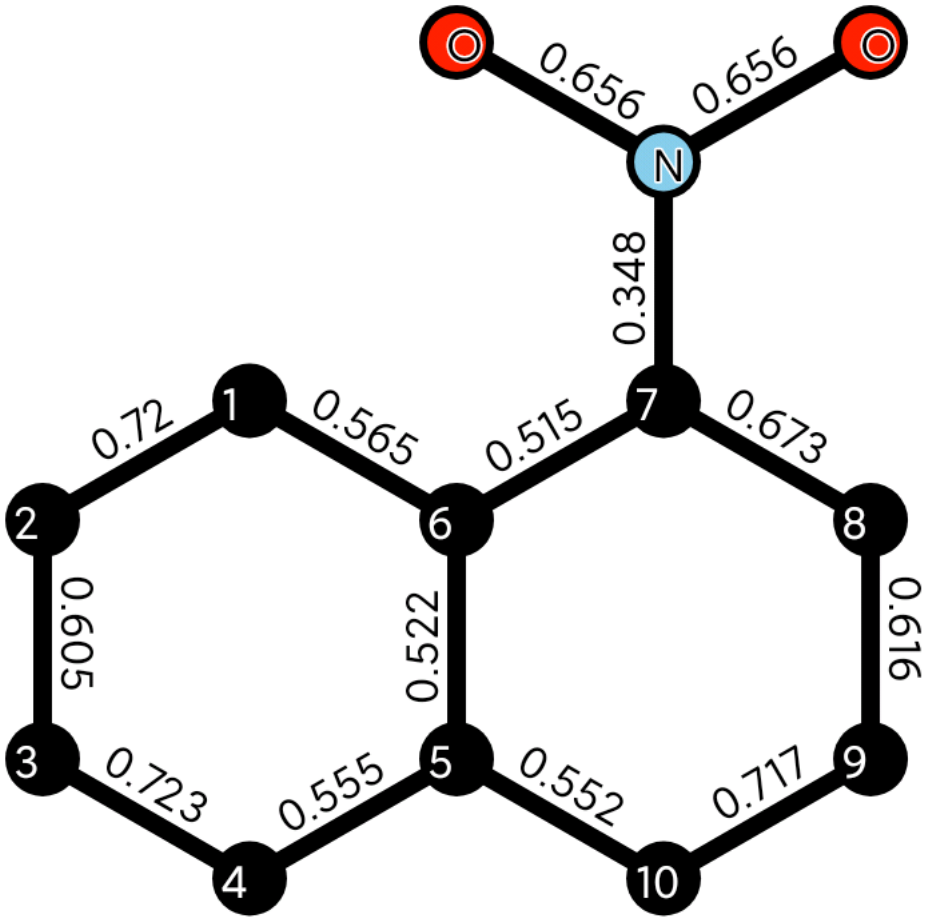


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13
1	1.005												
2	0.72	0.991											
3	-0.003	0.605	1.001										
4	-0.36	0.008	0.723	0.993									
5	0.001	-0.242	-0.001	0.555	1.0								
6	0.565	0.011	-0.246	-0.009	0.522	0.984							
7	-0.01	-0.158	0.005	0.082	-0.003	0.515	1.019						
8	-0.155	0.02	0.149	-0.017	-0.235	-0.027	0.673	0.953					
9	0.004	0.152	-0.002	-0.168	0.001	-0.232	-0.008	0.616	1.003				
10	0.075	-0.018	-0.165	0.016	0.552	0.023	-0.336	0.042	0.717	0.962			
11	-0.042	-0.028	0.016	0.022	-0.02	0.037	0.348	0.065	-0.036	-0.059	1.063		
12	0.021	0.057	-0.009	-0.037	0.009	-0.112	-0.09	-0.169	0.018	0.12	0.656	1.513	
13	0.021	0.057	-0.009	-0.037	0.009	-0.112	-0.09	-0.169	0.018	0.12	0.656	-0.487	1.513

3.2. Presentation of bond order:

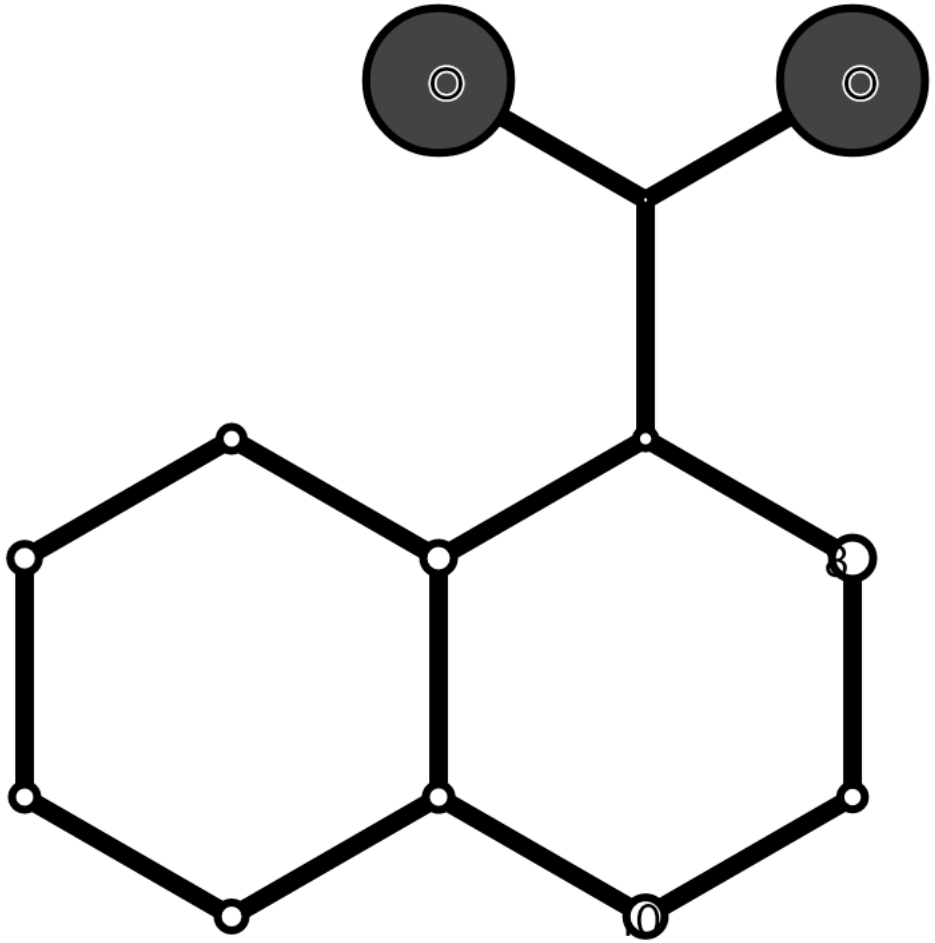

O
O
0.656
0.656
N
0.348
1
7
0.72
0.565
0.515
0.673
2
6
8
0.605
0.522
0.616
3
5
9
0.723
0.555
0.552
0.717
4
10

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13
1	0.072												
2		0.086											
3			0.076										
4				0.084									
5					0.077								
6						0.092							
7							0.058						
8								0.124					
9									0.074				
10										0.115			
11											0.014		
12												-0.436	
13													-0.436

4.2. Presentation of molecule:

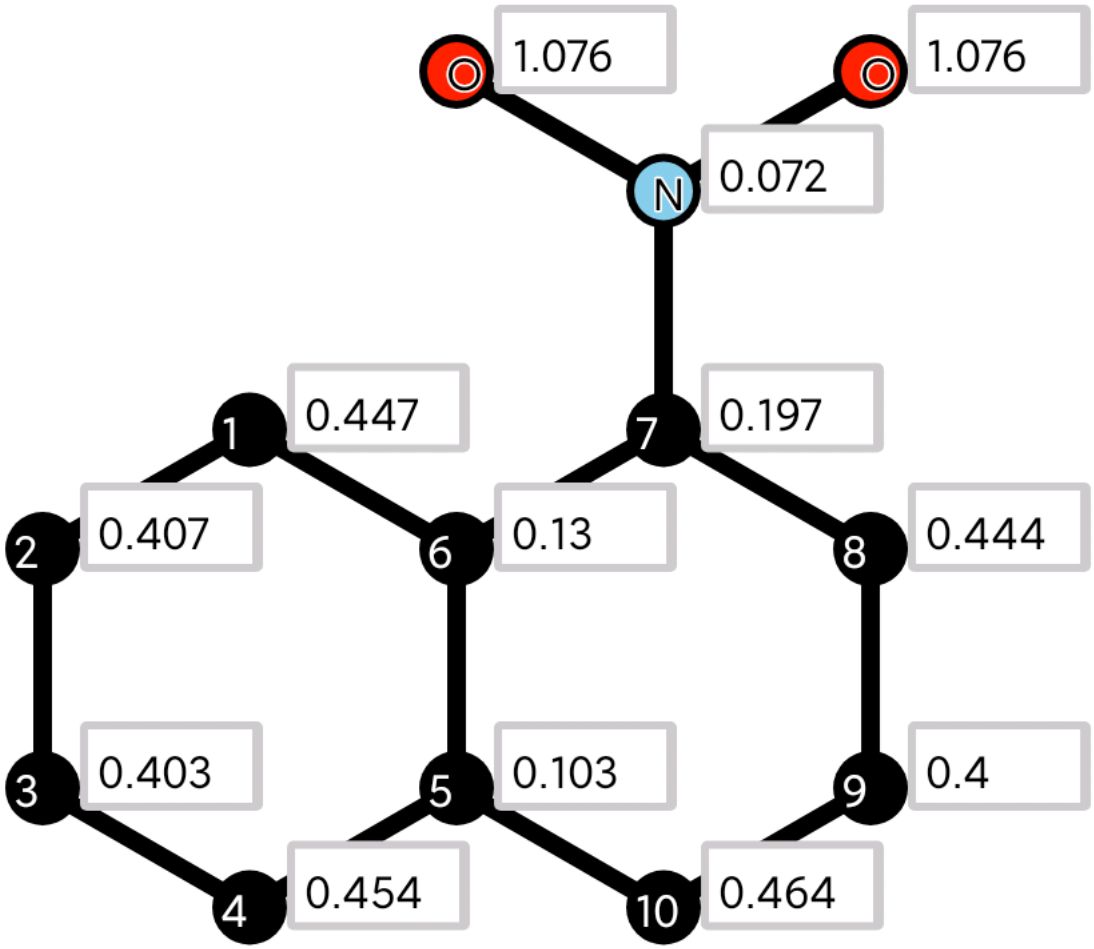


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11	12	13
0.447	0.407	0.403	0.454	0.103	0.13	0.197	0.444	0.4	0.464	0.072	1.076	1.076

5.2. Presentation of molecule:


1.076
1.076
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0.072
1
0.447
7
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5
0.103
9
0.4
4
0.454
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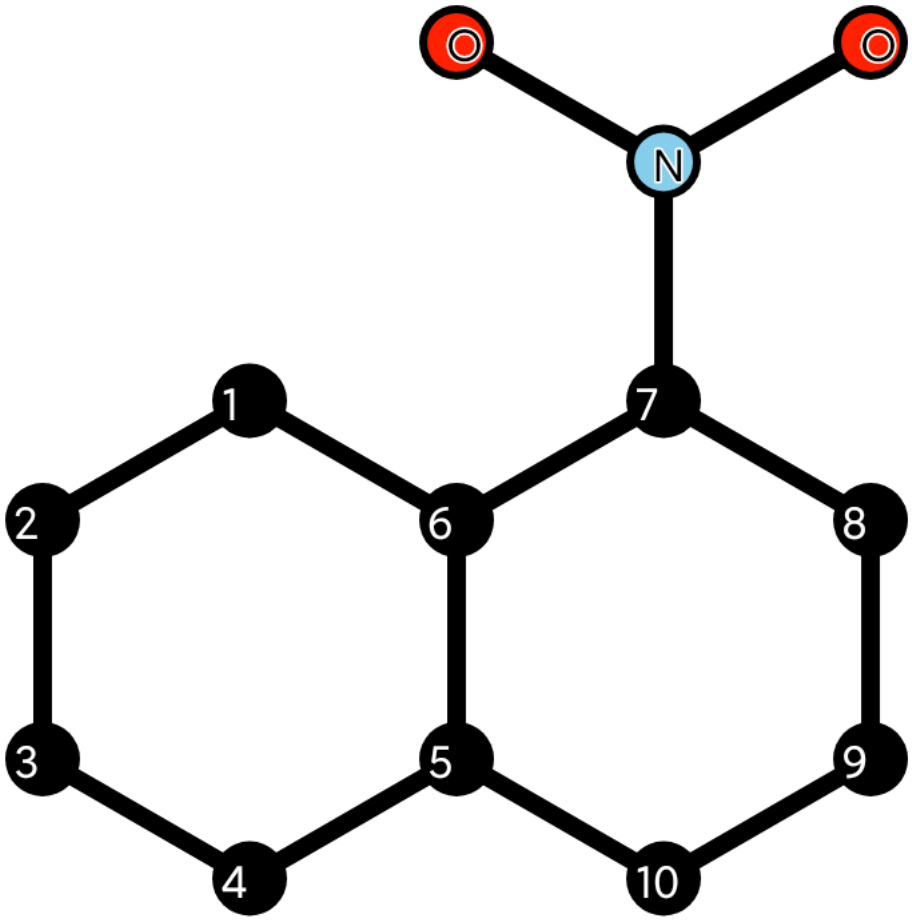
0.464

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13
1	0.438												
2	-0.209	0.407											
3	0.017	-0.111	0.404										
4	-0.137	0.018	-0.212	0.444									
5	0.004	-0.049	0.007	-0.089	0.329								
6	-0.094	0.008	-0.05	0.003	-0.078	0.34							
7	0.022	-0.029	0.005	-0.022	0.003	-0.075	0.378						
8	-0.028	0.0	-0.03	0.007	-0.047	0.003	-0.185	0.427					
9	0.006	-0.031	0.0	-0.032	0.008	-0.046	0.014	-0.116	0.402				
10	-0.021	0.007	-0.031	0.028	-0.087	0.004	-0.125	0.021	-0.207	0.454			
11	0.0	-0.001	0.0	-0.001	0.0	0.001	-0.014	-0.002	0.0	-0.004	0.167		
12	0.002	-0.005	0.001	-0.004	0.0	-0.008	0.014	-0.024	0.001	-0.019	-0.072	0.255	
13	0.002	-0.005	0.001	-0.004	0.0	-0.008	0.014	-0.024	0.001	-0.019	-0.072	-0.142	0.255

6.2. Presentation of molecule: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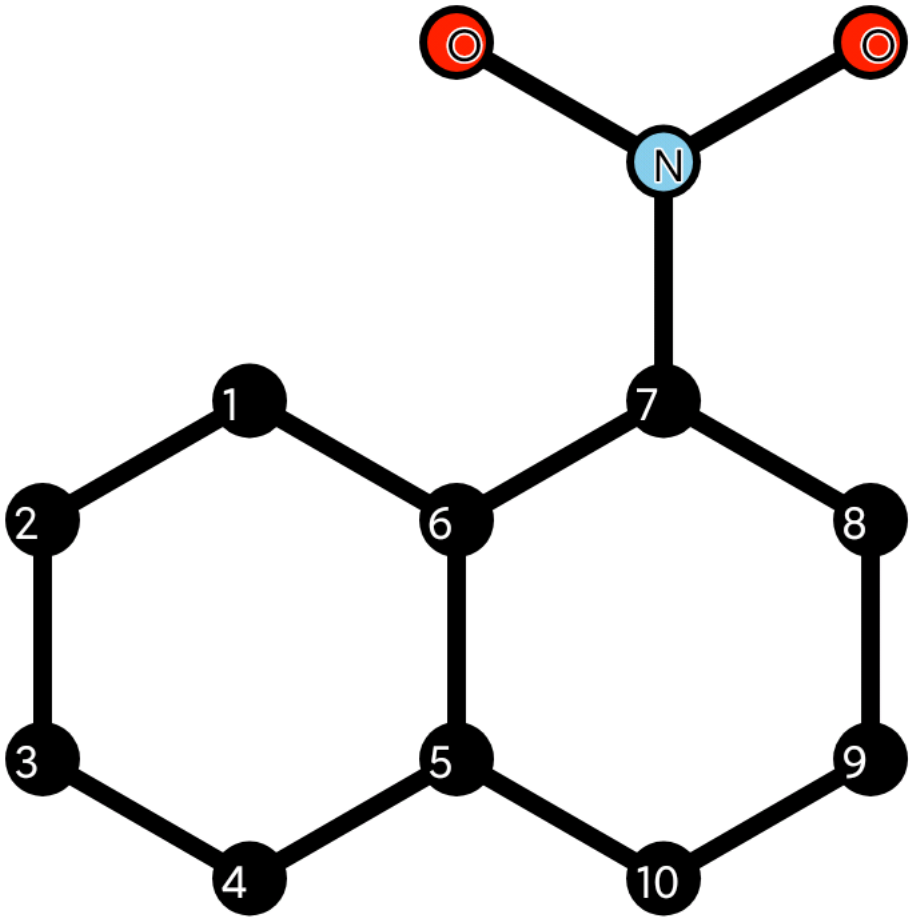
7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13
1 2	-0.004	0.004	0.0	0.004	0.0	-0.004	-0.003	0.005	-0.001	0.003	-0.001	-0.002	-0.002
1 6	0.001	-0.006	0.0	-0.005	0.0	0.007	0.005	-0.007	0.001	-0.004	0.002	0.003	0.003
2 3	0.002	0.004	0.0	-0.004	0.0	0.004	0.002	-0.005	0.0	-0.004	0.001	0.001	0.001
3 4	-0.001	-0.003	-0.001	0.004	0.0	-0.003	-0.001	0.004	0.0	0.003	0.0	-0.001	-0.001
4 5	0.0	0.003	0.0	0.003	0.0	0.003	0.0	-0.005	0.0	-0.005	0.0	0.0	0.0
5 6	-0.001	0.003	0.0	0.003	0.0	0.005	0.001	-0.007	0.0	-0.007	0.001	0.001	0.001
5 10	0.0	-0.006	0.0	-0.005	-0.001	-0.007	-0.002	0.012	0.0	0.011	-0.001	-0.001	-0.001
6 7	0.002	0.002	0.001	0.002	0.001	0.0	-0.011	0.015	-0.002	0.01	-0.004	-0.008	-0.008
7 8	-0.004	0.005	-0.001	0.004	-0.001	0.009	-0.018	0.016	0.001	0.018	-0.006	-0.011	-0.011
7 11	0.003	-0.006	0.001	-0.005	0.0	-0.01	0.011	-0.033	0.002	-0.027	0.007	0.029	0.029
8 9	0.002	-0.005	0.0	-0.004	0.0	-0.008	0.007	0.019	0.002	-0.022	0.002	0.004	0.004
9 10	-0.001	0.005	0.0	0.004	0.0	0.006	-0.005	-0.016	-0.004	0.019	-0.002	-0.003	-0.003
11 12	-0.001	0.002	0.0	0.002	0.0	0.003	0.001	0.011	0.0	0.01	-0.01	-0.134	0.116
11 13	-0.001	0.002	0.0	0.002	0.0	0.003	0.001	0.011	0.0	0.01	-0.01	0.116	-0.134

7.2. Presentation of molecule: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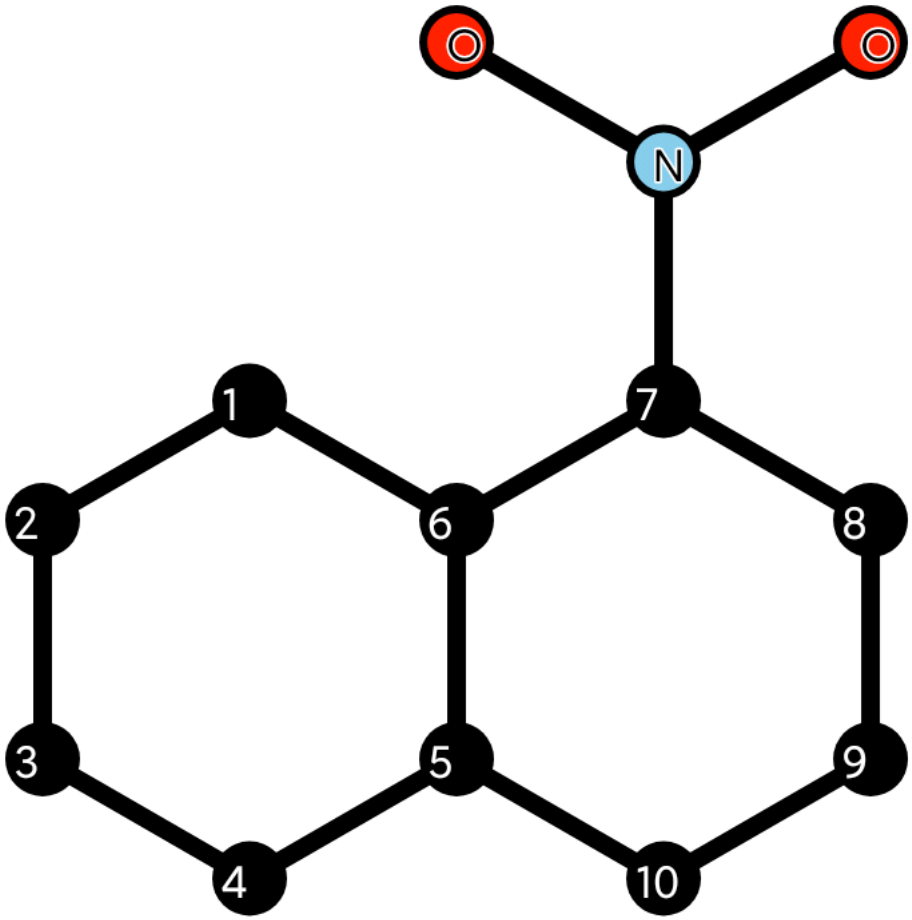
8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	2 3	3 4	4 5	5 6	5 10	6 7	7 8	7 11	8 9	9 10	11 12	11 13
1 2	0.212													
1 6	-0.186	0.289												
2 3	-0.208	0.113	0.295											
3 4	0.124	-0.075	-0.21	0.21										
4 5	-0.073	0.096	0.111	-0.181	0.288									
5 6	0.069	-0.113	-0.042	0.067	-0.109	0.257								
5 10	0.022	-0.022	-0.045	0.058	-0.145	-0.113	0.294							
6 7	0.058	-0.137	-0.044	0.025	-0.025	-0.101	0.091	0.282						
7 8	-0.026	0.048	0.028	-0.018	0.024	0.059	-0.068	-0.147	0.22					
7 11	-0.007	0.016	0.004	-0.002	0.001	0.006	-0.004	-0.057	-0.075	0.24				
8 9	0.028	-0.039	-0.031	0.031	-0.045	-0.041	0.11	0.097	-0.2	0.019	0.3			
9 10	-0.017	0.021	0.031	-0.031	0.059	0.065	-0.18	-0.066	0.122	-0.012	-0.219	0.22		
11 12	0.003	-0.006	-0.002	0.001	0.0	-0.002	0.002	0.017	0.024	-0.071	-0.007	0.005	0.192	
11 13	0.003	-0.006	-0.002	0.001	0.0	-0.002	0.002	0.017	0.024	-0.071	-0.007	0.005	-0.144	0.192

8.2. Presentation of molecule: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