Print calculated values

Report generated by:root, 17.02.2020 - 10:15:31

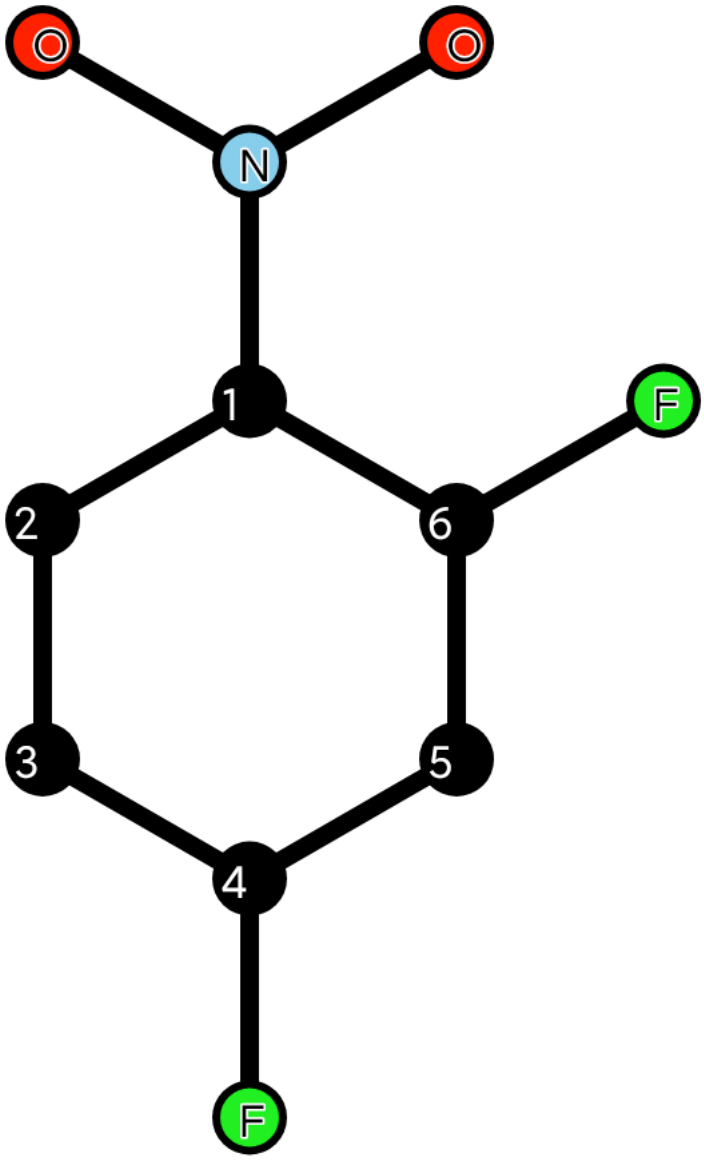
The following determinant is calculated:

-x	1.0	0.0	0.0	0.0	1.0	1.3	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	1.0	-x	1.0	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	0.68
0.0	0.0	0.0	1.0	-x	1.0	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	0.68	0.0
1.3	0.0	0.0	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	1.95	-x+1.18	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	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.68	0.0	0.0	0.0	-x+2.84	0.0
0.0	0.0	0.0	0.68	0.0	0.0	0.0	0.0	0.0	0.0	-x+2.84

It is about this molecule:

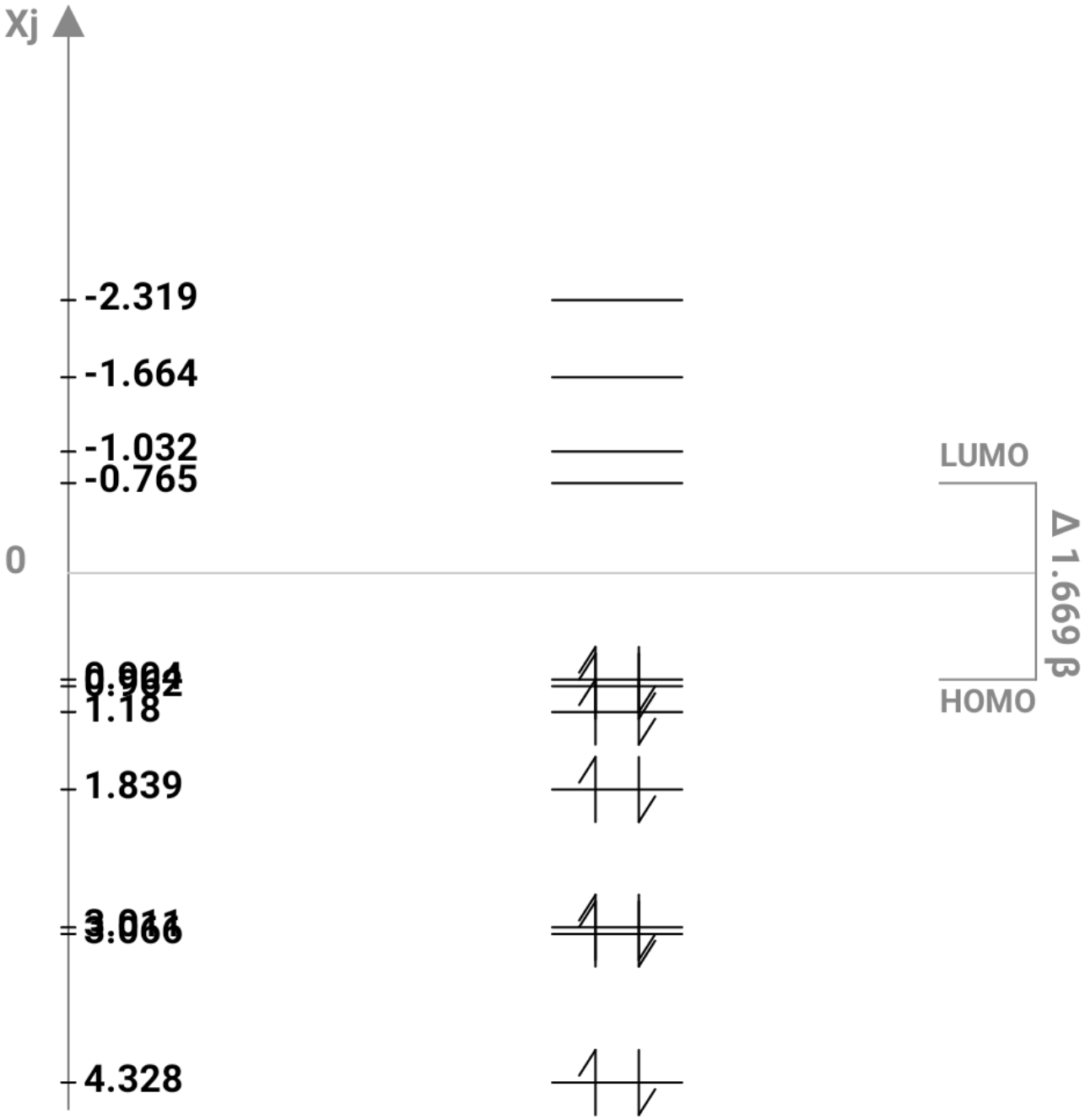
HMO-Energies

x1 = 4.328; x2 = 3.066; x3 = 3.011; x4 = 1.839; x5 = 1.18; x6 = 0.962; x7 = 0.904; x8 = -0.765;
x9 = -1.032; x10 = -1.664; x11 = -2.319;


O
O
N
1
F
2
6
3
5
4
F

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 11α + 30.58β -

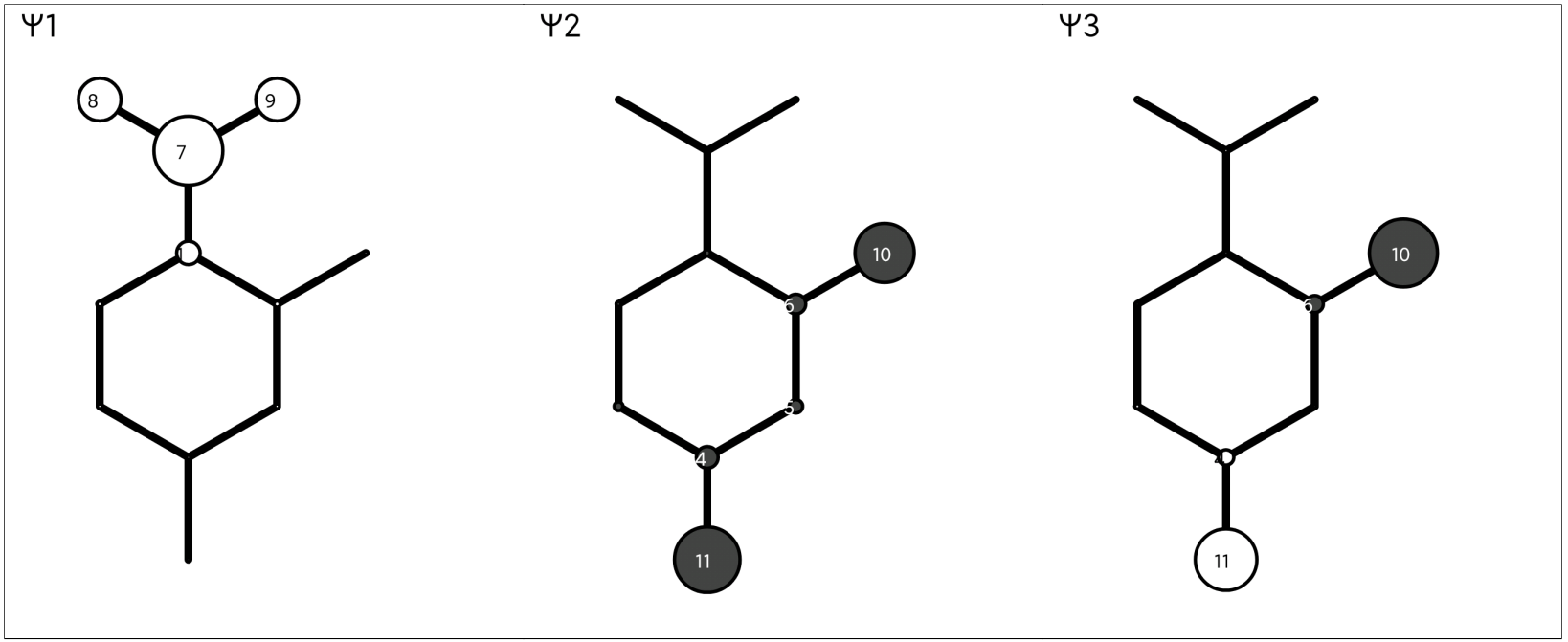
this corresponds to one πelectron: 2.184β

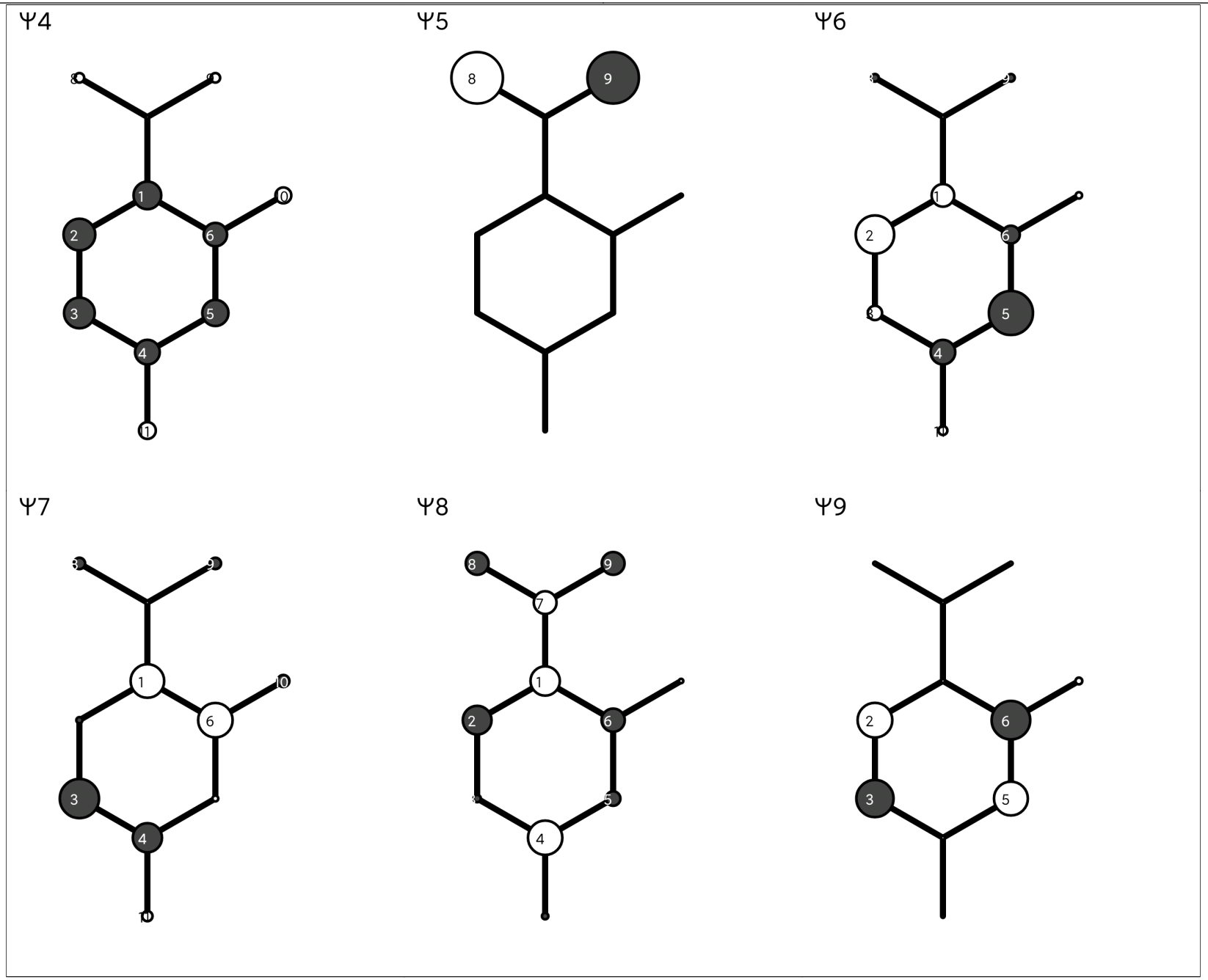
2. Hueckel-coefficient

2.1. Calculated values:

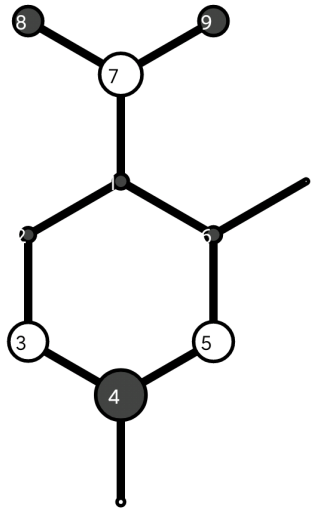
	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11
	x1= 4.328	x2= 3.066	x3= 3.011	x4= 1.839	x5= 1.18	x6= 0.962	x7= 0.904	x8= -0.765	x9= -1.032	x10= -1.664	x11= -2.319
1	0.247	-0.069	-0.049	-0.381	0.0	0.311	0.461	0.403	0.019	-0.151	0.54
2	0.061	-0.053	0.002	-0.437	0.0	0.528	-0.086	-0.395	0.477	-0.144	-0.335
3	0.016	-0.092	0.055	-0.422	0.0	0.197	-0.539	-0.101	-0.511	0.391	0.238
4	0.008	-0.229	0.163	-0.34	0.0	-0.339	-0.401	0.472	0.05	-0.507	-0.217
5	0.017	-0.142	-0.006	-0.36	0.0	-0.606	0.08	-0.2	0.465	0.4	0.245
6	0.066	-0.207	-0.18	-0.322	0.0	-0.244	0.474	-0.32	-0.53	-0.159	-0.352
7	0.725	0.037	0.024	0.044	0.0	0.012	0.022	0.313	0.026	0.427	-0.434
8	0.449	0.038	0.026	0.131	0.707	-0.105	-0.157	-0.314	-0.023	-0.293	0.242
9	0.449	0.038	0.026	0.131	-0.707	-0.105	-0.157	-0.314	-0.023	-0.293	0.242
10	0.03	-0.623	-0.716	0.219	0.0	0.088	-0.166	0.06	0.093	0.024	0.046
11	0.004	-0.69	0.649	0.231	0.0	0.123	0.141	-0.089	-0.009	0.077	0.029

2.2. Molecule orbital presentation:

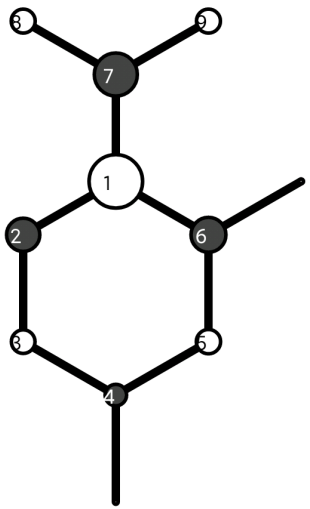

Ψ1
8
9
7
1
Ψ2
10
6
5
4
11
Ψ3
10
6
1
11


Ψ4
Ψ5
Ψ6
Ψ7
Ψ8
Ψ9

Ψ10



Ψ11

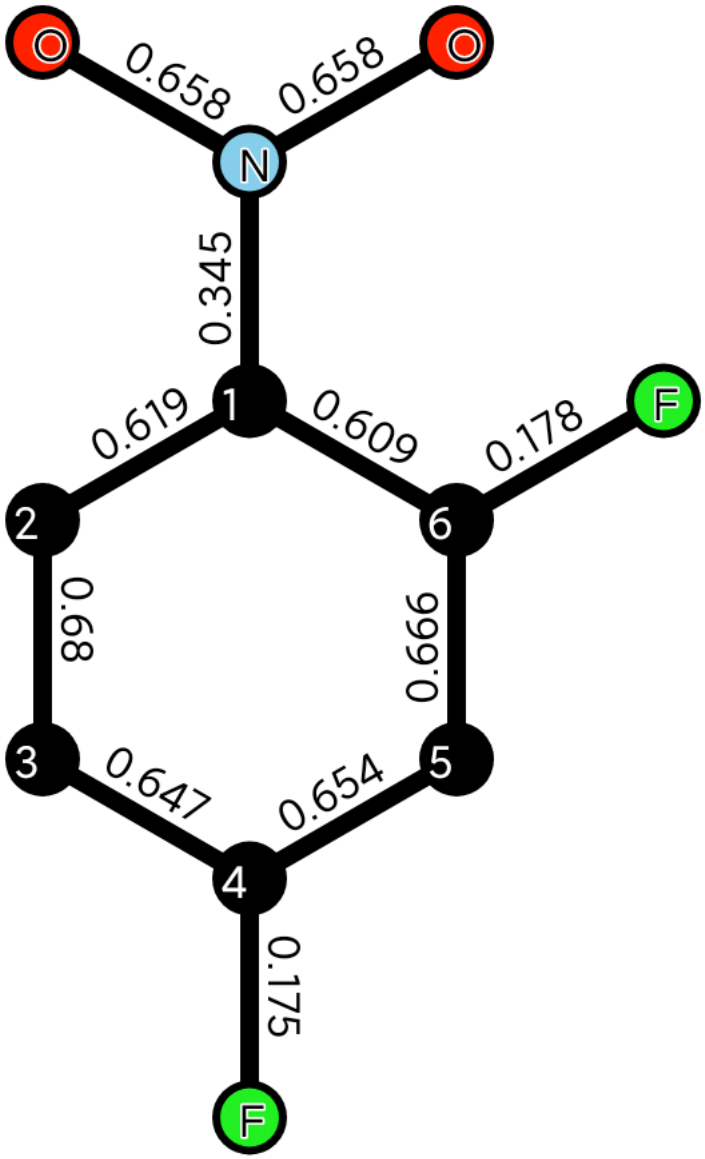


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	1.046										
2	0.619	0.966									
3	-0.038	0.68	1.038								
4	-0.302	0.034	0.647	0.941							
5	0.0	-0.322	0.005	0.654	1.046						
6	0.609	-0.029	-0.314	0.041	0.666	0.934					
7	0.345	0.054	-0.038	-0.053	-0.029	0.058	1.061				
8	-0.096	-0.148	0.027	0.106	0.012	-0.148	0.658	1.514			
9	-0.096	-0.148	0.027	0.106	0.012	-0.148	0.658	-0.486	1.514		
10	-0.095	-0.003	0.066	-0.022	-0.105	0.178	-0.023	0.034	0.034	1.97	
11	0.064	-0.021	-0.1	0.175	-0.103	-0.022	0.016	-0.025	-0.025	0.006	1.971

3.2. Presentation of bond order:

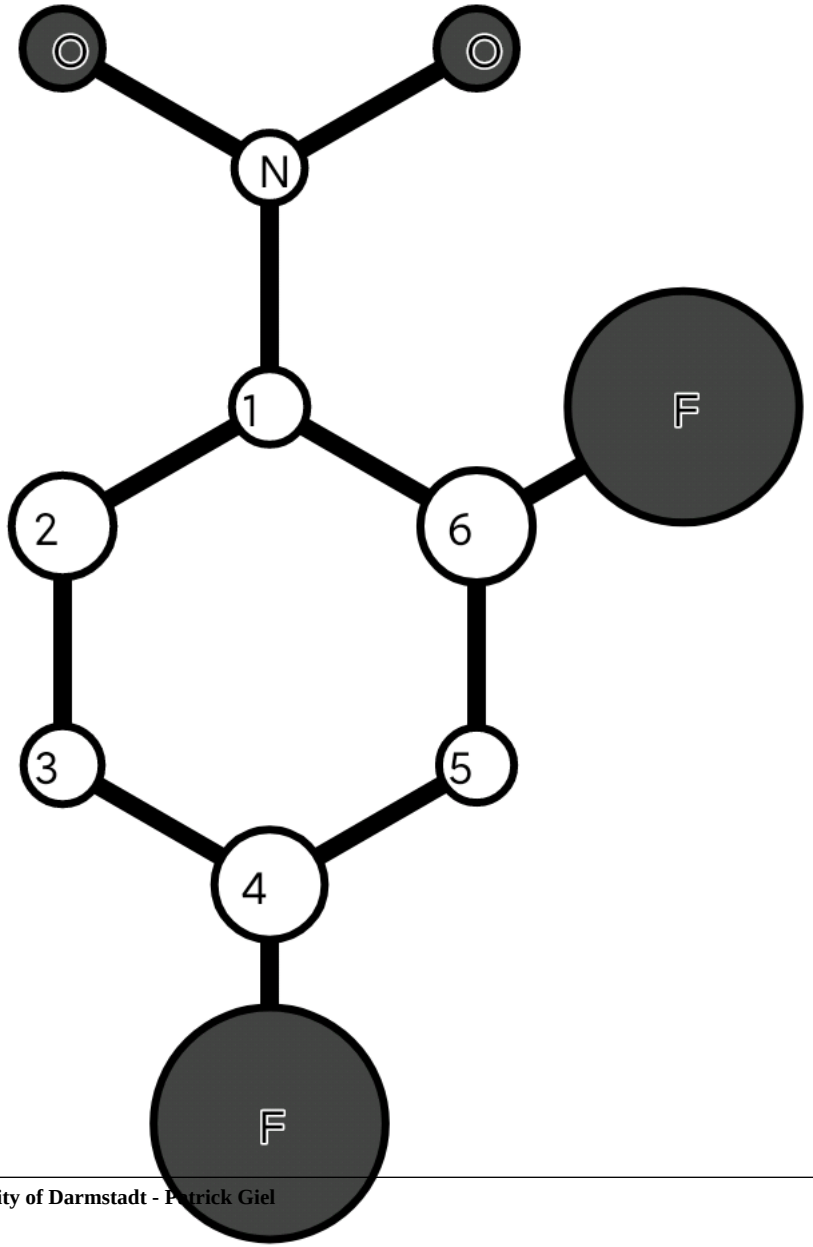

O
O
0.658
0.658
N
0.345
1
0.619
0.609
F
0.178
2
6
0.68
0.666
3
5
0.647
0.654
4
0.175
F

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.227										
2		0.307									
3			0.235								
4				0.332							
5					0.226						
6						0.338					
7							0.212				
8								-0.241			
9									-0.241		
10										-0.697	
11											-0.698

4.2. Presentation of molecule:

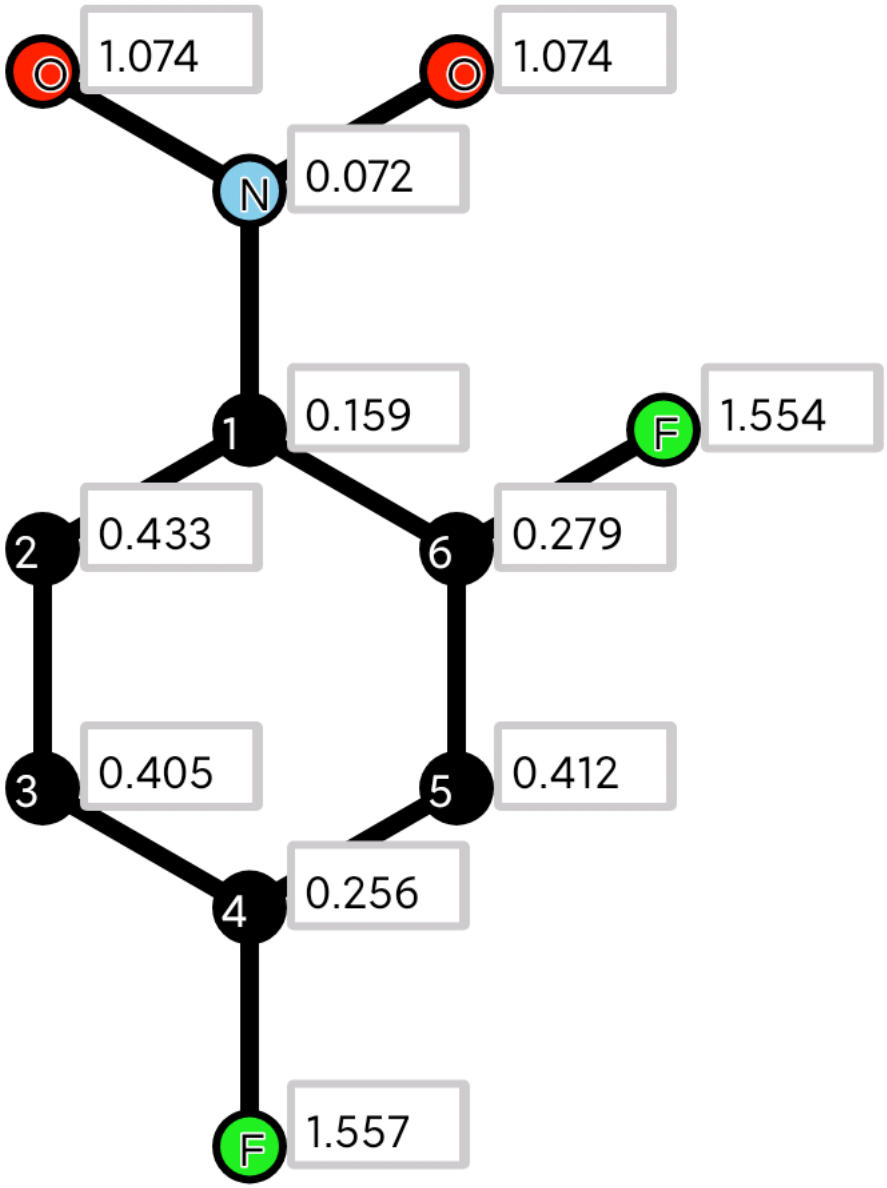

O
O
N
1
F
2
6
3
5
4
F

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11
0.159	0.433	0.405	0.256	0.412	0.279	0.072	1.074	1.074	1.554	1.557

5.2. Presentation of molecule:

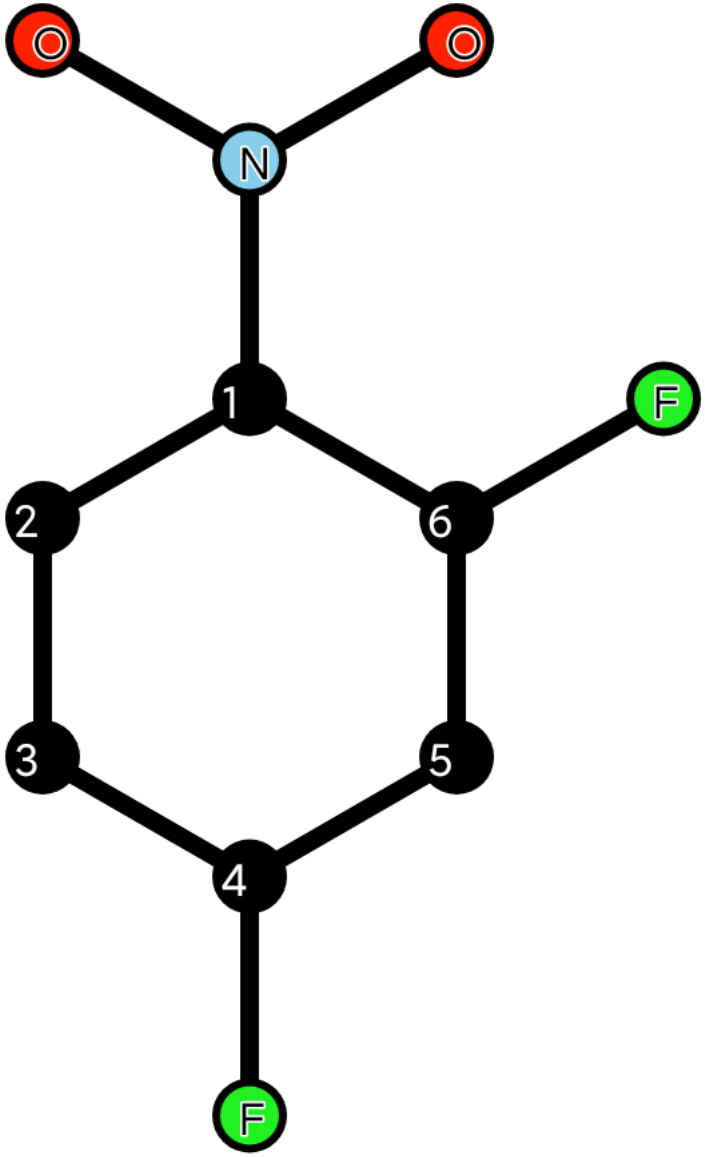

O
1.074
O
1.074
N
0.072
1
0.159
F
1.554
2
0.433
6
0.279
3
0.405
5
0.412
4
0.256
F
1.557

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.345										
2	-0.134	0.416									
3	0.006	-0.167	0.4								
4	-0.088	0.011	-0.145	0.39							
5	0.007	-0.097	0.009	-0.151	0.402						
6	-0.131	0.003	-0.092	0.01	-0.158	0.399					
7	-0.014	0.0	-0.001	-0.003	0.0	-0.001	0.167				
8	0.009	-0.016	0.0	-0.014	0.001	-0.017	-0.073	0.251			
9	0.009	-0.016	0.0	-0.014	0.001	-0.017	-0.073	-0.14	0.251		
10	-0.006	0.0	-0.005	0.0	-0.007	0.004	0.0	-0.001	-0.001	0.015	
11	-0.005	0.0	-0.006	0.004	-0.006	0.0	0.0	-0.001	-0.001	0.0	0.015

6.2. Presentation of molecule:

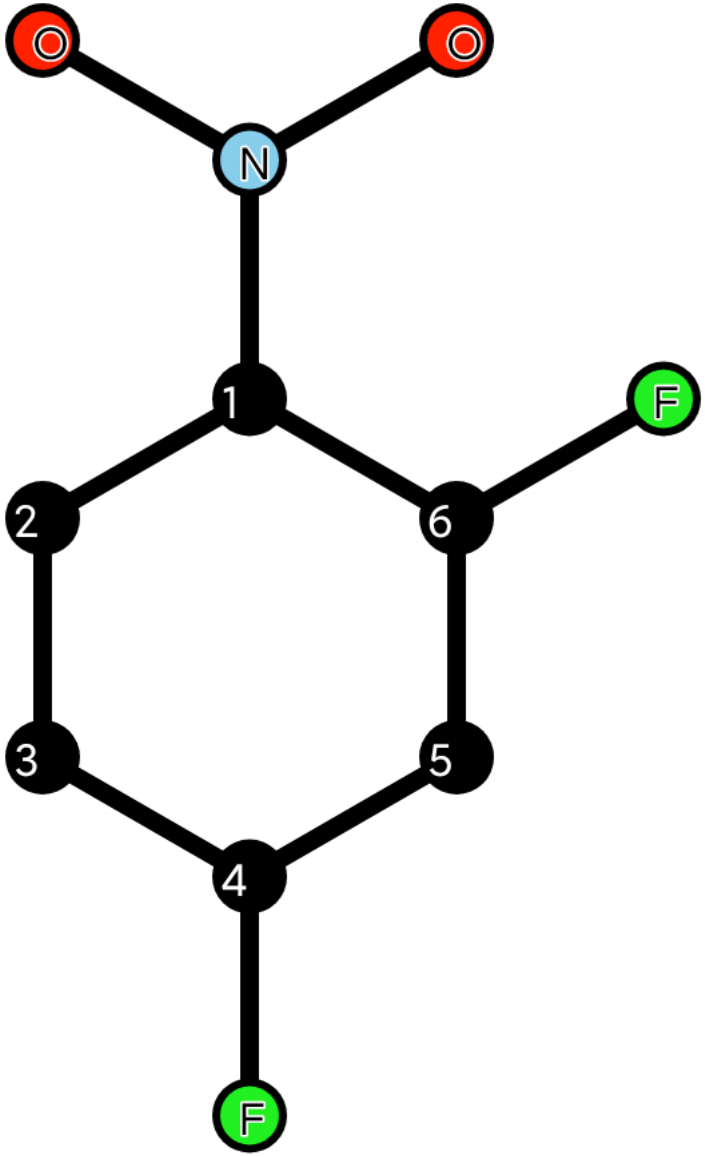

O
O
N
1
F
2
6
3
5
4
F

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1 2	-0.023	0.008	0.016	0.012	0.0	0.012	-0.005	-0.01	-0.01	0.0	0.001
1 6	-0.017	0.013	-0.012	0.013	-0.001	0.021	-0.005	-0.01	-0.01	0.005	0.001
1 7	0.004	-0.022	0.0	-0.019	0.001	-0.024	0.005	0.029	0.029	-0.002	-0.001
2 3	0.016	0.016	-0.015	-0.015	0.001	-0.011	0.002	0.004	0.004	0.0	-0.002
3 4	-0.013	-0.015	-0.008	0.025	-0.002	0.015	-0.002	-0.003	-0.003	0.001	0.005
4 5	0.0	0.013	-0.003	0.022	-0.014	-0.018	-0.001	-0.001	-0.001	-0.002	0.005
4 11	0.02	-0.002	0.03	-0.044	0.032	-0.002	0.001	0.003	0.003	0.0	-0.043
5 6	0.0	-0.012	0.002	-0.017	-0.011	0.029	0.001	0.002	0.002	0.006	-0.002
6 10	0.028	-0.001	0.021	-0.002	0.033	-0.045	0.001	0.004	0.004	-0.044	0.0
7 8	0.003	0.007	0.0	0.007	0.0	0.007	-0.009	-0.133	0.116	0.001	0.0
7 9	0.003	0.007	0.0	0.007	0.0	0.007	-0.009	0.116	-0.133	0.001	0.0

7.2. Presentation of molecule:

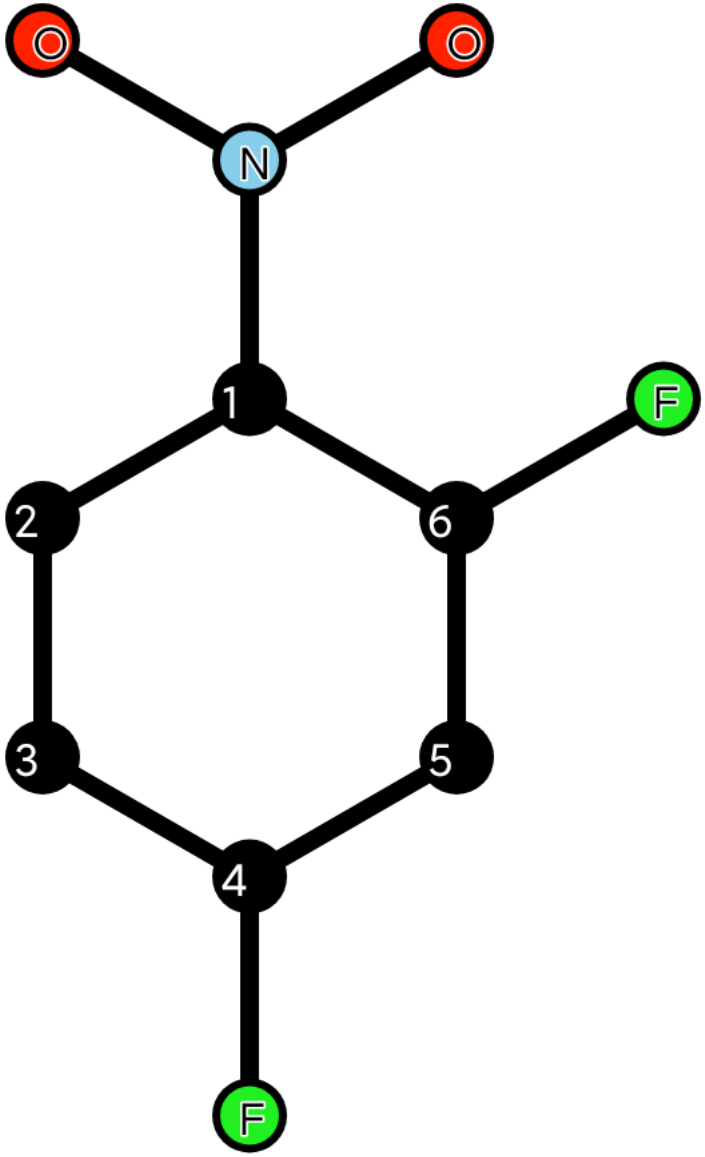

O
O
N
1
F
2
6
3
5
4
F

8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	1 7	2 3	3 4	4 5	4 11	5 6	6 10	7 8	7 9
1 2	0.249										
1 6	-0.163	0.246									
1 7	-0.069	-0.066	0.237								
2 3	-0.197	0.111	0.019	0.245							
3 4	0.126	-0.078	-0.013	-0.21	0.254						
4 5	-0.083	0.12	-0.007	0.123	-0.195	0.25					
4 11	-0.008	-0.009	0.01	0.012	-0.037	-0.036	0.265				
5 6	0.114	-0.186	0.011	-0.088	0.123	-0.208	0.013	0.248			
6 10	-0.003	-0.033	0.014	0.003	-0.01	0.013	0.0	-0.04	0.269		
7 8	0.021	0.02	-0.068	-0.007	0.005	0.003	-0.004	-0.004	-0.004	0.191	
7 9	0.021	0.02	-0.068	-0.007	0.005	0.003	-0.004	-0.004	-0.004	-0.147	0.191

8.2. Presentation of molecule:


O
O
N
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F