Print calculated values

Report generated by:root, 17.02.2020 - 09:33:40

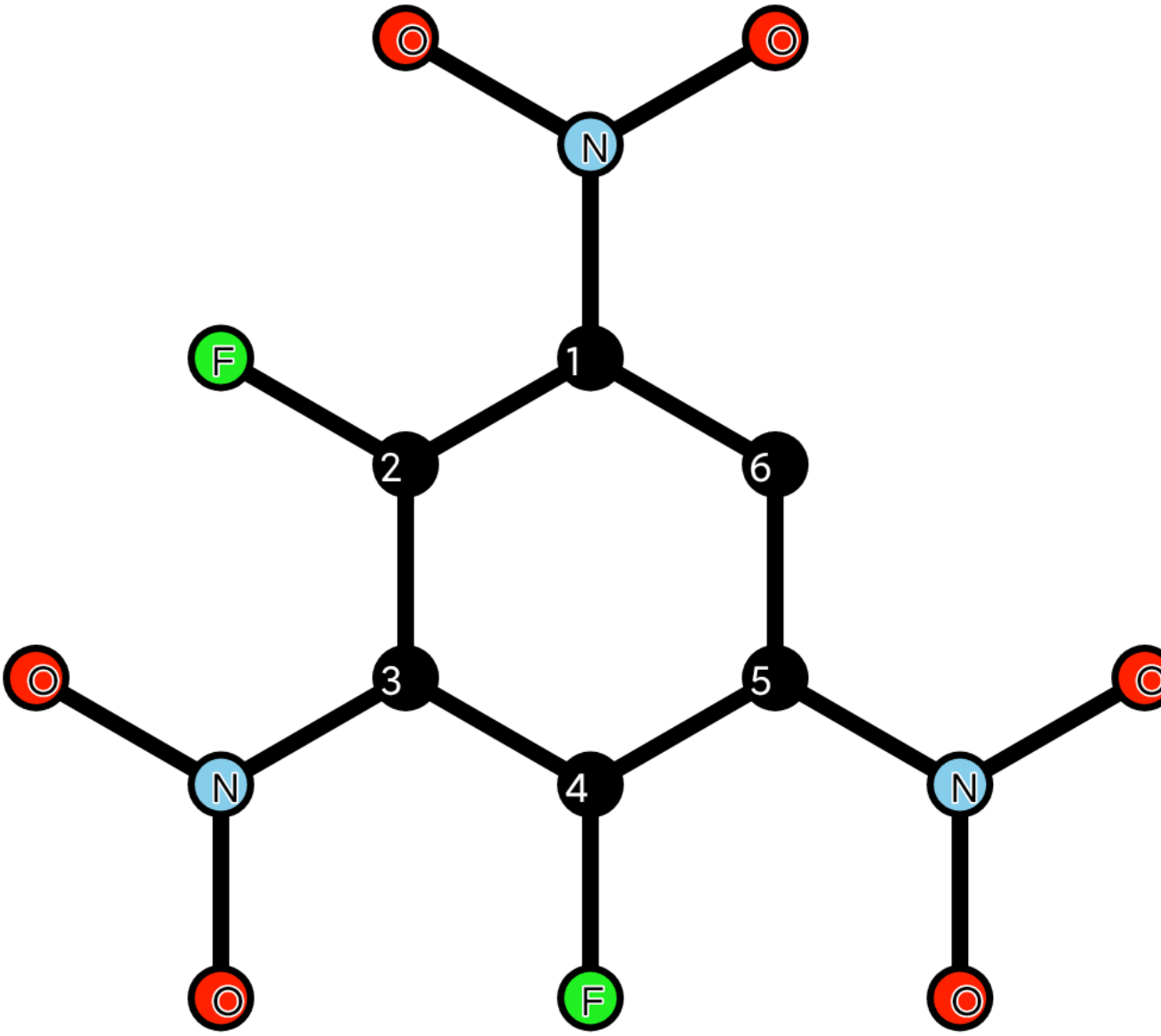
The following determinant is calculated:

-x	1.0	0.0	0.0	0.0	1.0	1.3	0.0	0.0	0.0	0.0	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	0.0	0.0	0.68
0.0	1.0	-x	1.0	0.0	0.0	0.0	1.3	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	0.68	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	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	0.0
1.3	0.0	0.0	0.0	0.0	0.0	-x+1.47	0.0	0.0	1.95	1.95	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	1.3	0.0	0.0	0.0	0.0	-x+1.47	0.0	0.0	0.0	1.95	1.95	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	0.0	0.0	0.0	0.0	1.95	1.95	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	1.95	0.0	0.0	-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	0.0	0.0	1.95	0.0	0.0	0.0	-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	0.0	0.0	1.95	0.0	0.0	0.0	-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	0.0	1.95	0.0	0.0	0.0	0.0	-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	0.0	1.95	0.0	0.0	0.0	0.0	-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	0.0	0.0	0.0	0.0	-x+1.18	0.0	0.0
0.0	0.0	0.0	0.68	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-x+2.84	0.0
0.0	0.68	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-x+2.84

It is about this molecule:

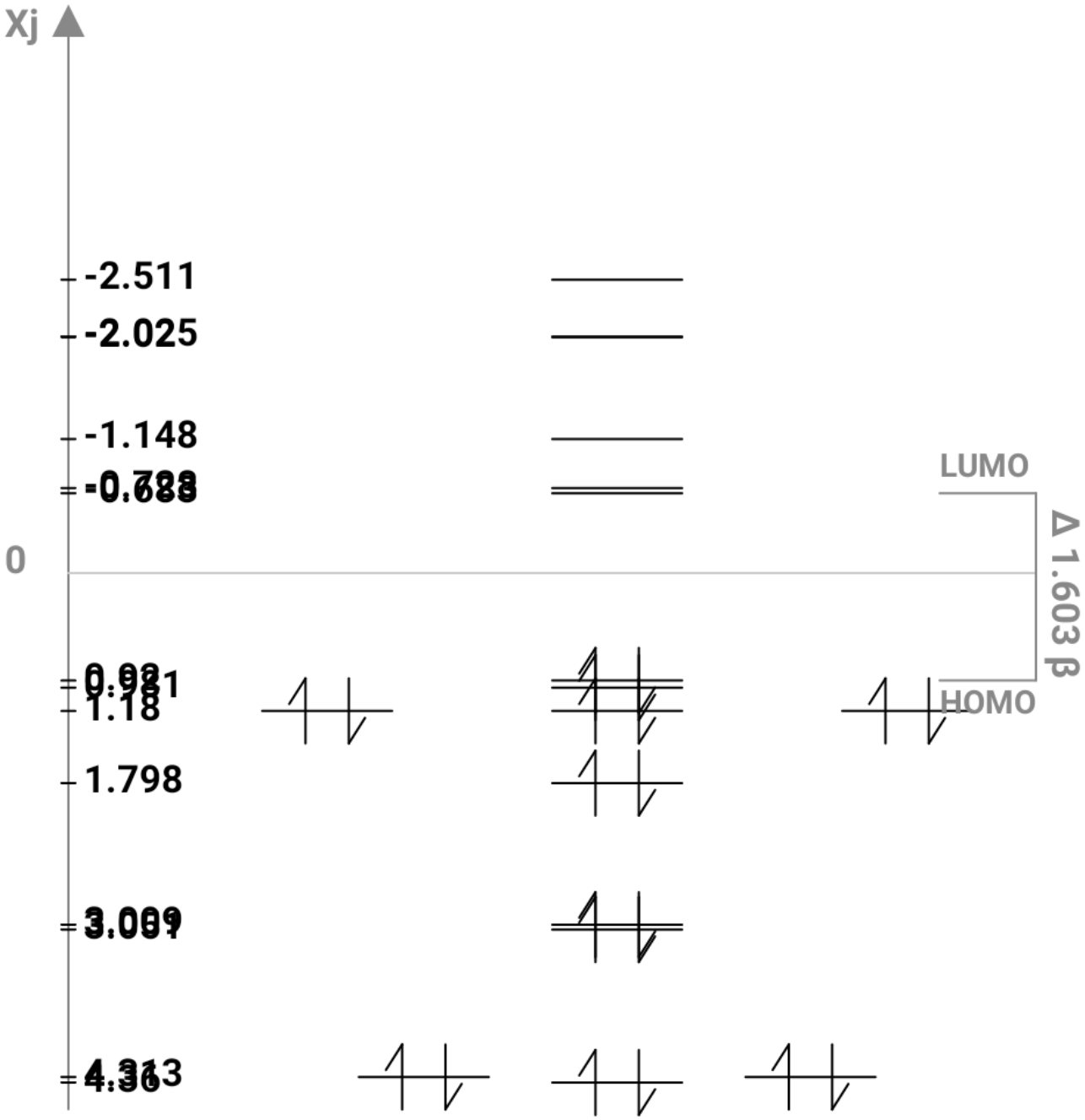
HMO-Energies

x1 = 4.36; x2 = 4.313; x3 = 4.313; x4 = 3.051; x5 = 3.009; x6 = 1.798; x7 = 1.18; x8 = 1.18; x9 = 1.18; x10 = 0.981; x11 = 0.92; x12 = -0.683; x13 = -0.728; x14 = -1.148; x15 = -2.02; x16 = -2.025; x17 = -2.511;


O
O
N
F
1
2
6
O
3
5
O
N
4
N
O
F
O

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 17α + 52.57β -

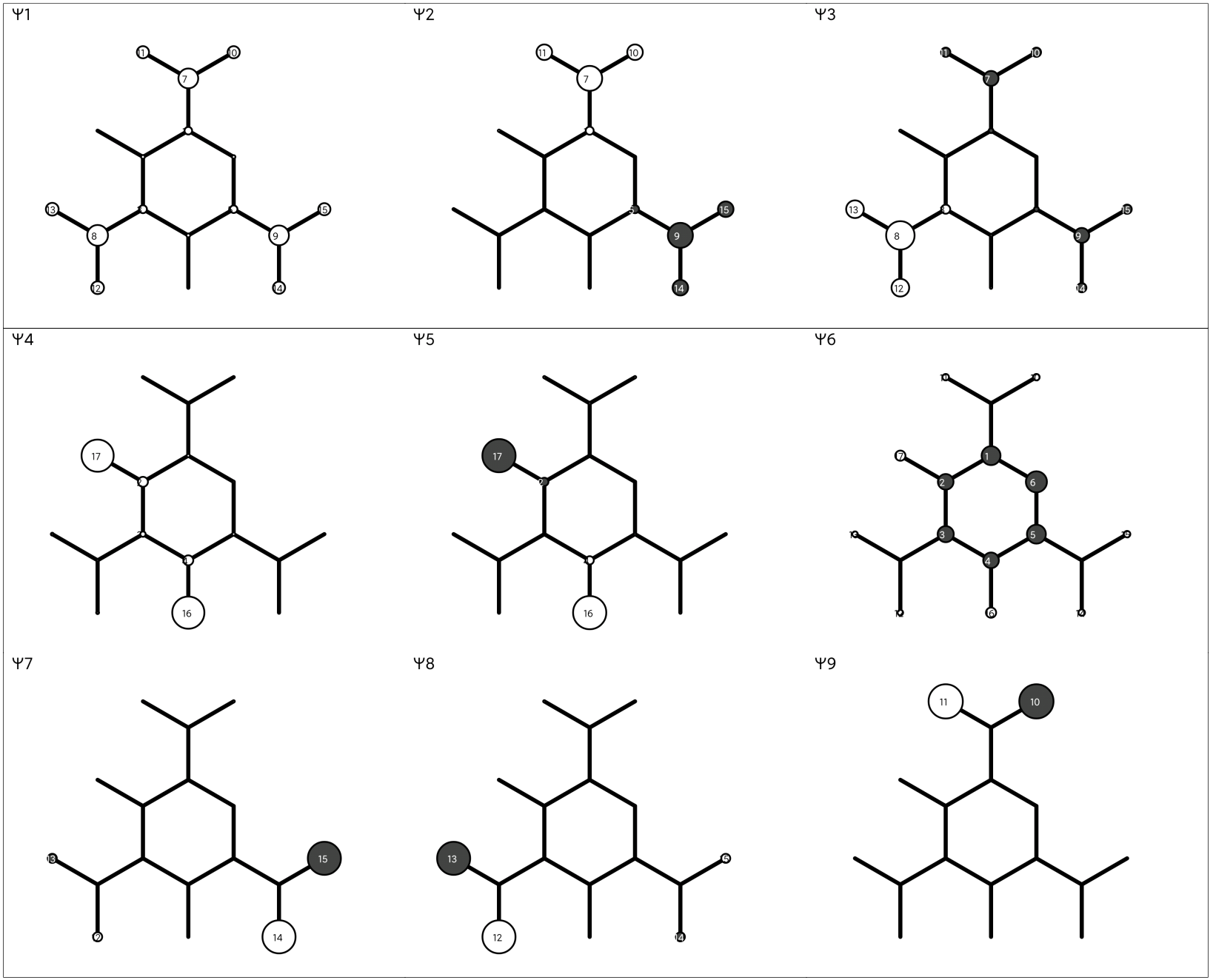
this corresponds to one πelectron: 2.39β

2. Hueckel-coefficient

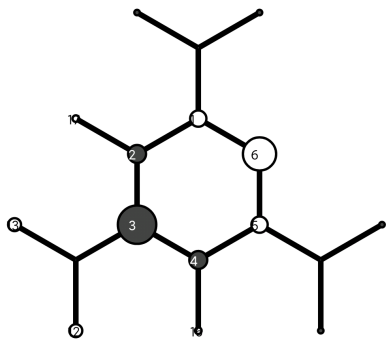
2.1. Calculated values:

	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	Psi 14	Psi 15	Psi 16	Psi 17
	x1= 4.36	x2= 4.313	x3= 4.313	x4= 3.051	x5= 3.009	x6= 1.798	x7= 1.18	x8= 1.18	x9= 1.18	x10= 0.981	x11= 0.92	x12= -0.683	x13= -0.728	x14= -1.148	x15= -2.02	x16= -2.025	x17= -2.511
1	0.156	0.165	-0.098	0.067	-0.046	-0.39	0.0	0.0	0.0	0.248	-0.492	0.2	-0.301	0.149	-0.219	-0.372	-0.371
2	0.079	0.041	0.022	0.205	-0.17	-0.322	0.0	0.0	0.0	-0.274	-0.424	0.274	0.503	-0.3	-0.107	0.193	0.309
3	0.164	0.0	0.187	0.11	0.0	-0.332	0.0	0.0	0.0	-0.585	0.0	-0.352	0.0	0.16	0.424	0.0	-0.379
4	0.079	-0.041	0.022	0.205	0.17	-0.322	0.0	0.0	0.0	-0.274	0.424	0.274	-0.503	-0.3	-0.107	-0.193	0.309
5	0.156	-0.165	-0.098	0.067	0.046	-0.39	0.0	0.0	0.0	0.248	0.492	0.2	0.301	0.149	-0.219	0.372	-0.371
6	0.072	0.0	-0.045	0.044	0.0	-0.434	0.0	0.0	0.0	0.507	0.0	-0.587	0.0	-0.26	0.217	0.0	0.295
7	0.408	0.515	-0.307	-0.035	0.023	0.042	0.0	0.0	0.0	0.009	-0.022	0.135	-0.219	0.299	0.255	0.431	0.251
8	0.428	0.0	0.585	-0.058	0.0	0.036	0.0	0.0	0.0	-0.02	0.0	-0.237	0.0	0.32	-0.495	0.0	0.257
9	0.408	-0.515	-0.307	-0.035	-0.023	0.042	0.0	0.0	0.0	0.009	0.022	0.135	0.219	0.299	0.255	-0.431	0.251
10	0.25	0.321	-0.191	-0.036	0.025	0.133	0.028	-0.045	-0.705	-0.084	0.167	-0.141	0.223	-0.251	-0.156	-0.262	-0.133
11	0.25	0.321	-0.191	-0.036	0.025	0.133	-0.028	0.045	0.705	-0.084	0.167	-0.141	0.223	-0.251	-0.156	-0.262	-0.133
12	0.262	0.0	0.364	-0.06	0.0	0.114	0.188	0.681	-0.036	0.198	0.0	0.248	0.0	-0.268	0.302	0.0	-0.136
13	0.262	0.0	0.364	-0.06	0.0	0.114	-0.188	-0.681	0.036	0.198	0.0	0.248	0.0	-0.268	0.302	0.0	-0.136
14	0.25	-0.321	-0.191	-0.036	-0.025	0.133	0.681	-0.186	0.039	-0.084	-0.167	-0.141	-0.223	-0.251	-0.156	0.262	-0.133
15	0.25	-0.321	-0.191	-0.036	-0.025	0.133	-0.681	0.186	-0.039	-0.084	-0.167	-0.141	-0.223	-0.251	-0.156	0.262	-0.133
16	0.035	-0.019	0.01	0.661	0.684	0.21	0.0	0.0	0.0	0.1	-0.15	-0.053	0.096	0.051	0.015	0.027	-0.039
17	0.035	0.019	0.01	0.661	-0.684	0.21	0.0	0.0	0.0	0.1	0.15	-0.053	-0.096	0.051	0.015	-0.027	-0.039

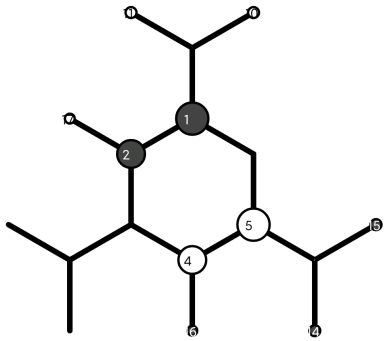
2.2. Molecule orbital presentation:


Ψ1
Ψ2
Ψ3
Ψ4
Ψ5
Ψ6
Ψ7
Ψ8
Ψ9

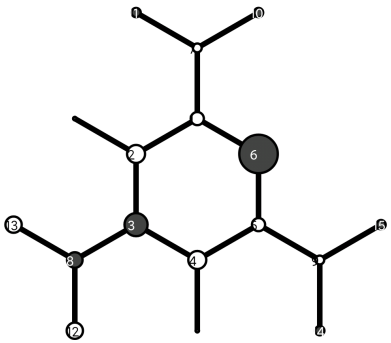
Ψ10



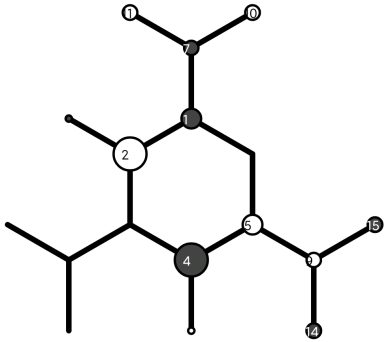
Ψ11



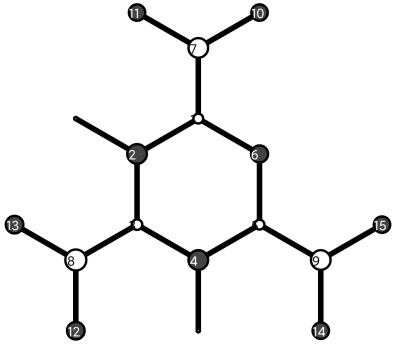
Ψ12



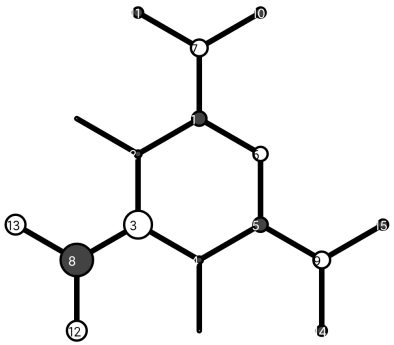
Ψ13



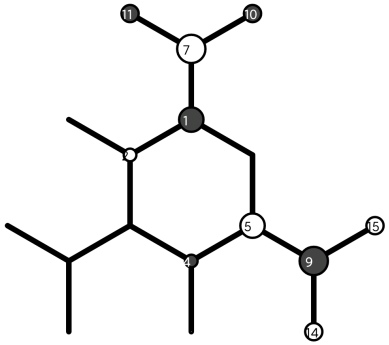
Ψ14



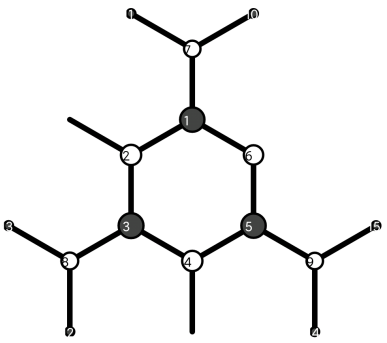
Ψ15



Ψ16



Ψ17

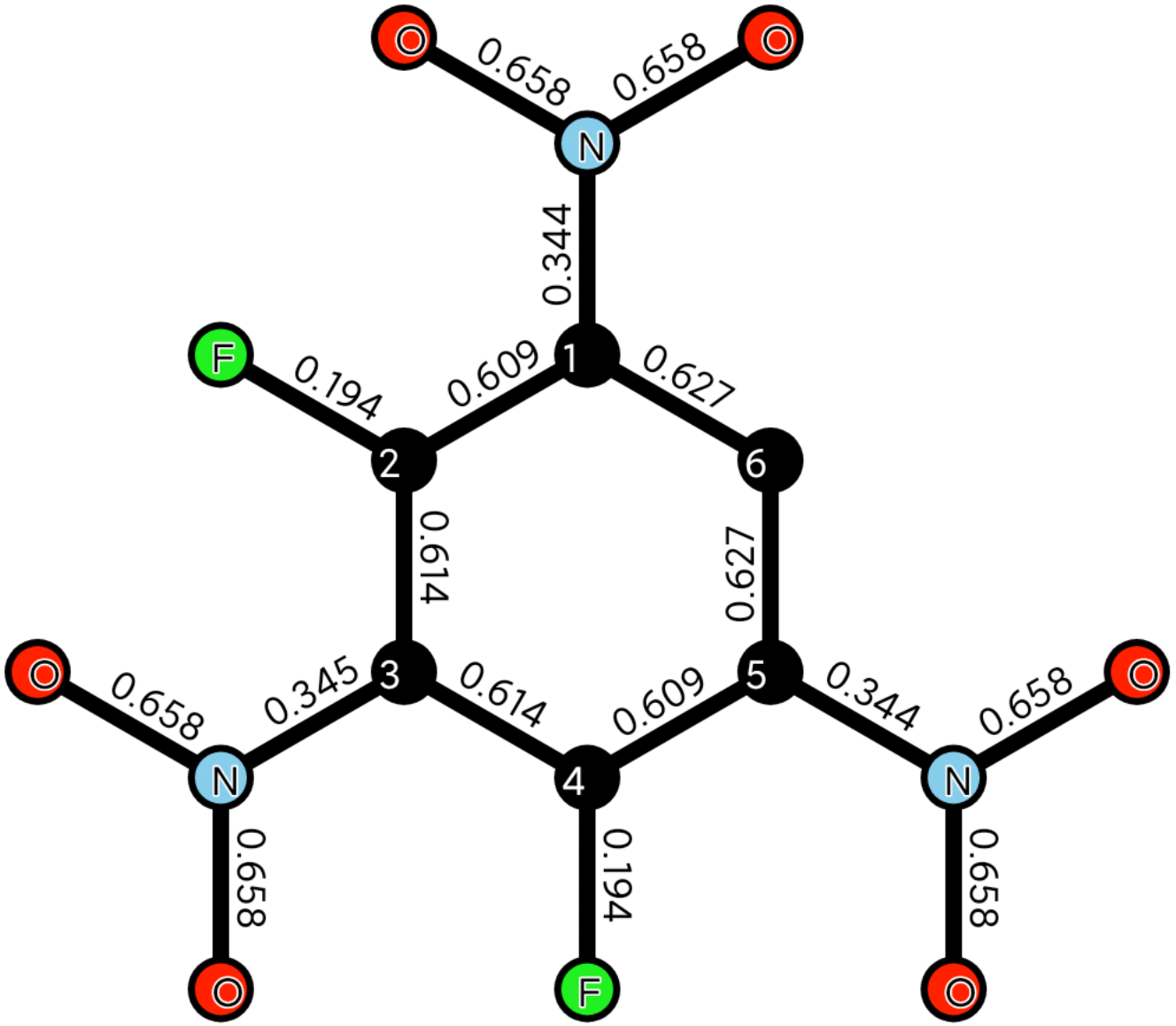


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	1.046																
2	0.609	0.875															
3	-0.003	0.614	1.054														
4	-0.283	0.035	0.614	0.875													
5	-0.038	-0.283	-0.003	0.609	1.046												
6	0.627	0.029	-0.289	0.029	0.627	0.908											
7	0.344	0.058	-0.027	-0.049	-0.035	0.055	1.061										
8	-0.027	0.058	0.345	0.058	-0.027	-0.049	-0.004	1.061									
9	-0.035	-0.049	-0.027	0.058	0.344	0.055	-0.005	-0.004	1.061								
10	-0.096	-0.147	0.012	0.1	0.026	-0.151	0.658	0.008	0.01	1.513							
11	-0.096	-0.147	0.012	0.1	0.026	-0.151	0.658	0.008	0.01	-0.487	1.513						
12	0.012	-0.149	-0.098	-0.149	0.012	0.101	0.008	0.658	0.008	-0.006	-0.006	1.514					
13	0.012	-0.149	-0.098	-0.149	0.012	0.101	0.008	0.658	0.008	-0.006	-0.006	-0.486	1.514				
14	0.026	0.1	0.012	-0.147	-0.096	-0.151	0.01	0.008	0.658	-0.012	-0.012	-0.006	-0.006	1.513			
15	0.026	0.1	0.012	-0.147	-0.096	-0.151	0.01	0.008	0.658	-0.012	-0.012	-0.006	-0.006	-0.487	1.513		
16	0.061	-0.02	-0.096	0.194	-0.094	-0.019	0.014	-0.023	-0.023	-0.024	-0.024	0.034	0.034	0.034	0.034	1.966	
17	-0.094	0.194	-0.096	-0.02	0.061	-0.019	-0.023	-0.023	0.014	0.034	0.034	0.034	0.034	-0.024	-0.024	0.005	1.966

3.2. Presentation of bond order:

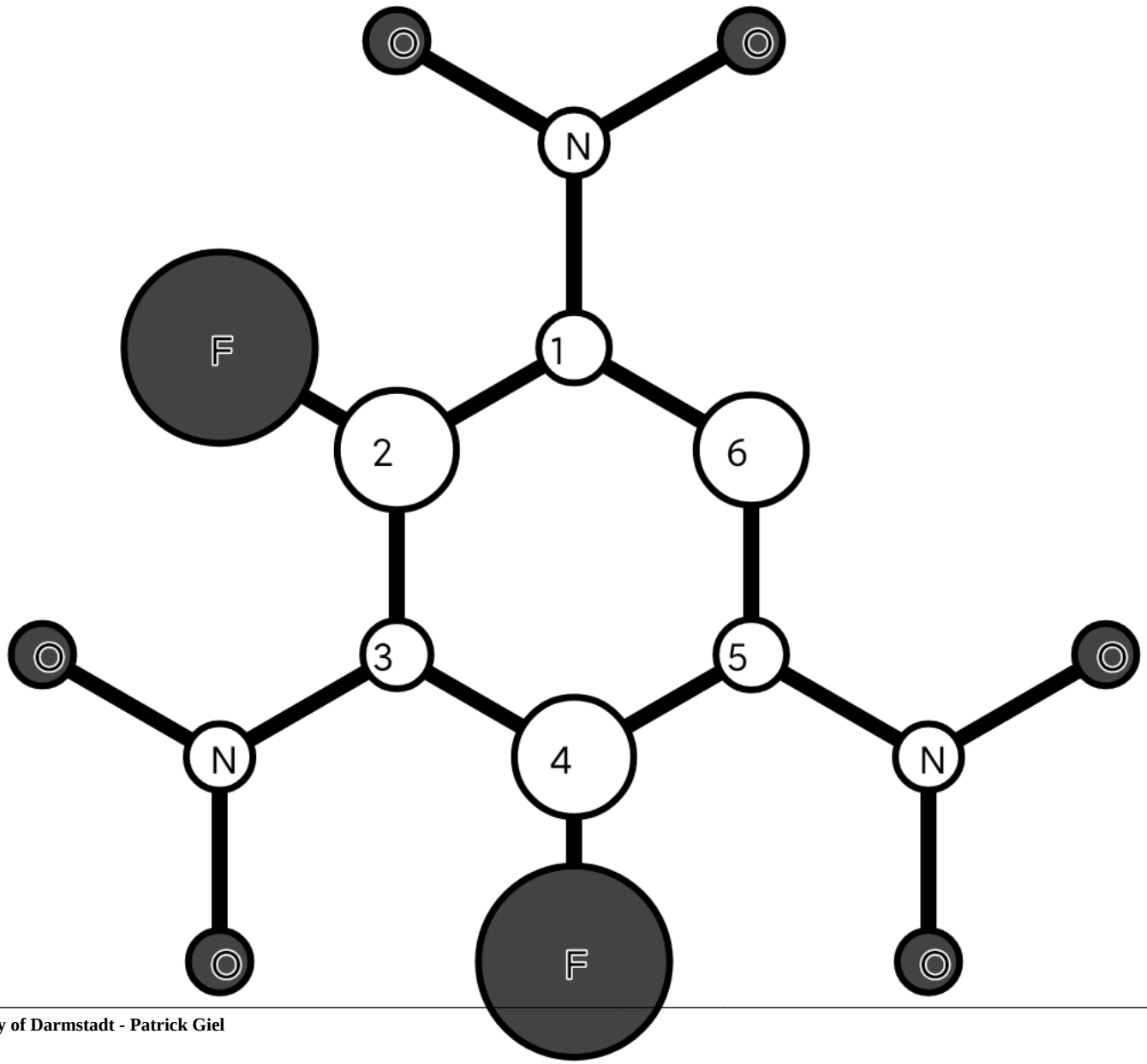

O
0.658
0.658
O
N
0.344
F
0.194
0.609
1
0.627
2
6
0.614
0.627
O
0.658
0.345
3
0.614
0.609
5
0.344
0.658
O
N
4
N
0.658
0.194
0.658
O
F
O

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	0.248																
2		0.419															
3			0.24														
4				0.419													
5					0.248												
6						0.387											
7							0.233										
8								0.234									
9									0.233								
10										-0.219							
11											-0.219						
12												-0.22					
13													-0.22				
14														-0.219			
15															-0.219		
16																-0.672	
17																	-0.672

4.2. Presentation of molecule:

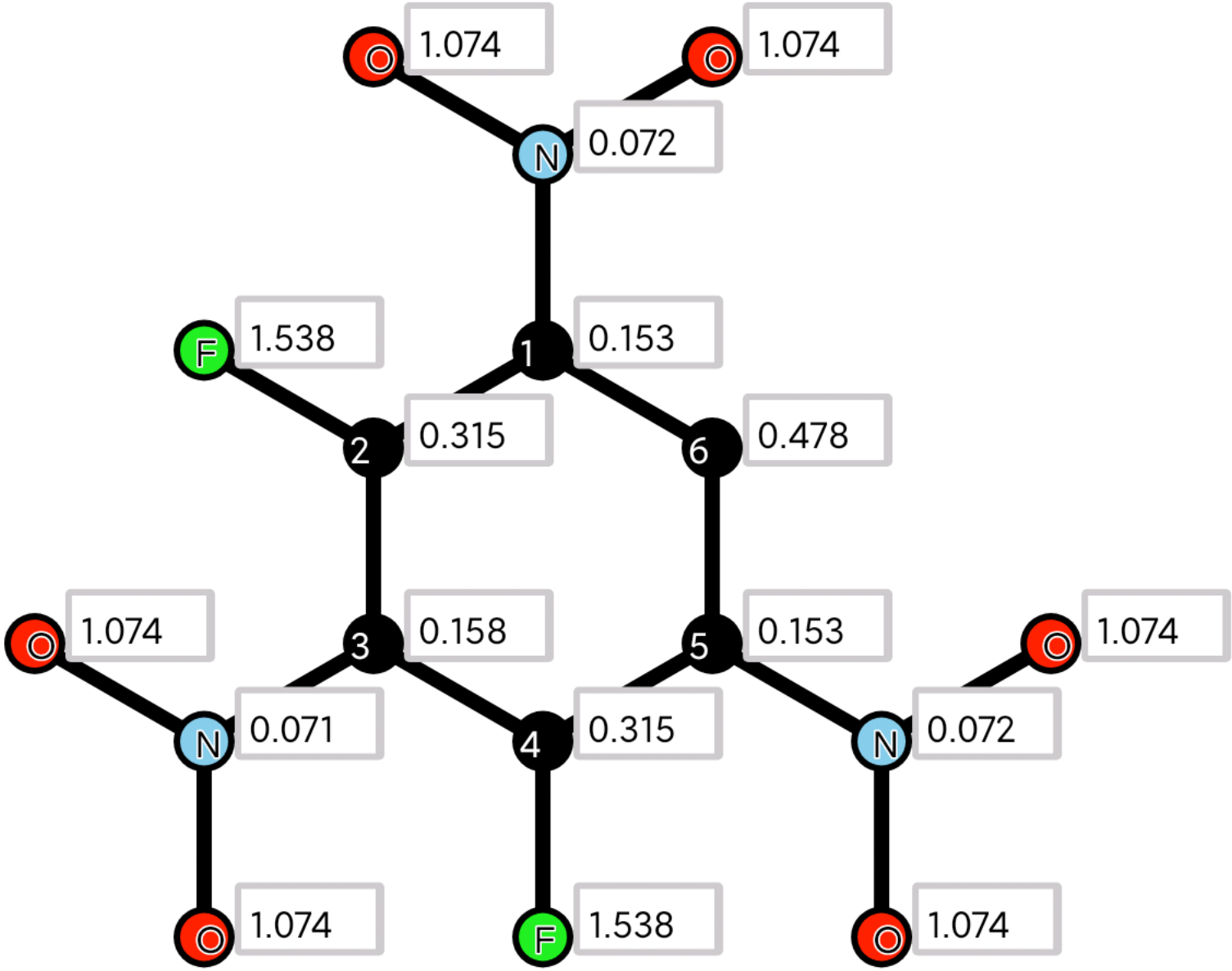

O
O
N
F
1
2
6
3
5
O
O
N
4
N
O
F
O

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
0.153	0.315	0.158	0.315	0.153	0.478	0.072	0.071	0.072	1.074	1.074	1.074	1.074	1.074	1.074	1.538	1.538

5.2. Presentation of molecule:

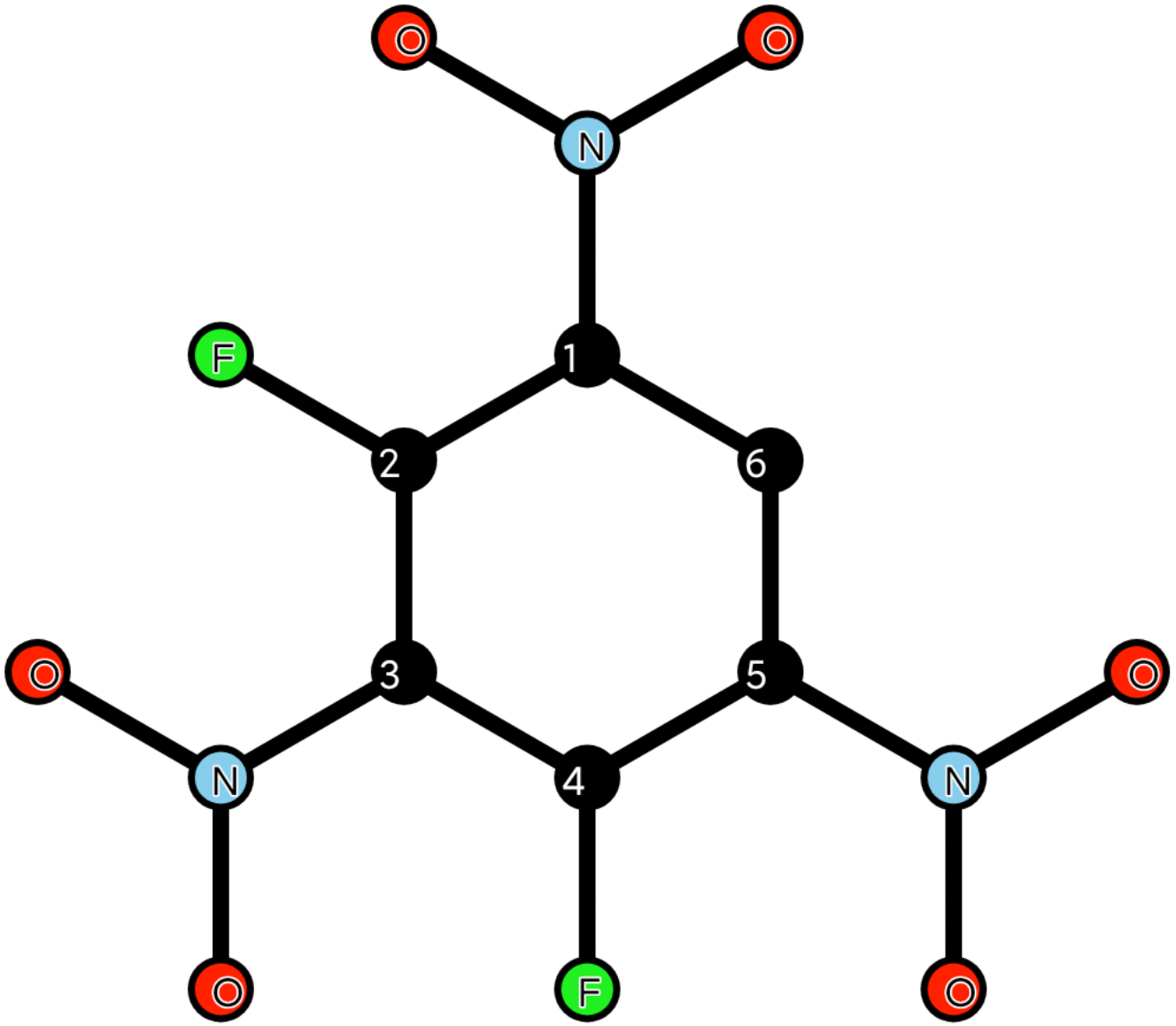

O
1.074
O
1.074
N
0.072
F
1.538
1
0.153
2
0.315
6
0.478
O
1.074
3
0.158
5
0.153
O
1.074
N
0.071
4
0.315
N
0.072
O
1.074
F
1.538
O
1.074

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	0.342																
2	-0.129	0.414															
3	0.006	-0.133	0.343														
4	-0.079	0.008	-0.133	0.414													
5	0.005	-0.079	0.006	-0.129	0.342												
6	-0.139	0.01	-0.082	0.01	-0.139	0.437											
7	-0.014	-0.001	0.0	-0.002	-0.001	-0.001	0.167										
8	0.0	-0.001	-0.015	-0.001	0.0	-0.002	0.0	0.167									
9	-0.001	-0.002	0.0	-0.001	-0.014	-0.001	0.0	0.0	0.167								
10	0.009	-0.016	0.001	-0.012	0.0	-0.017	-0.073	0.0	0.0	0.251							
11	0.009	-0.016	0.001	-0.012	0.0	-0.017	-0.073	0.0	0.0	-0.14	0.251						
12	0.001	-0.017	0.009	-0.017	0.001	-0.012	0.0	-0.073	0.0	0.0	0.0	0.25					
13	0.001	-0.017	0.009	-0.017	0.001	-0.012	0.0	-0.073	0.0	0.0	0.0	-0.139	0.25				
14	0.0	-0.012	0.001	-0.016	0.009	-0.017	0.0	0.0	-0.073	0.0	0.0	0.0	0.0	0.251			
15	0.0	-0.012	0.001	-0.016	0.009	-0.017	0.0	0.0	-0.073	0.0	0.0	0.0	0.0	-0.14	0.251		
16	-0.004	0.0	-0.006	0.004	-0.006	0.0	0.0	0.0	0.0	-0.001	-0.001	-0.001	-0.001	-0.001	-0.001	0.018	
17	-0.006	0.004	-0.006	0.0	-0.004	0.0	0.0	0.0	0.0	-0.001	-0.001	-0.001	-0.001	-0.001	-0.001	0.0	0.018

6.2. Presentation of molecule:

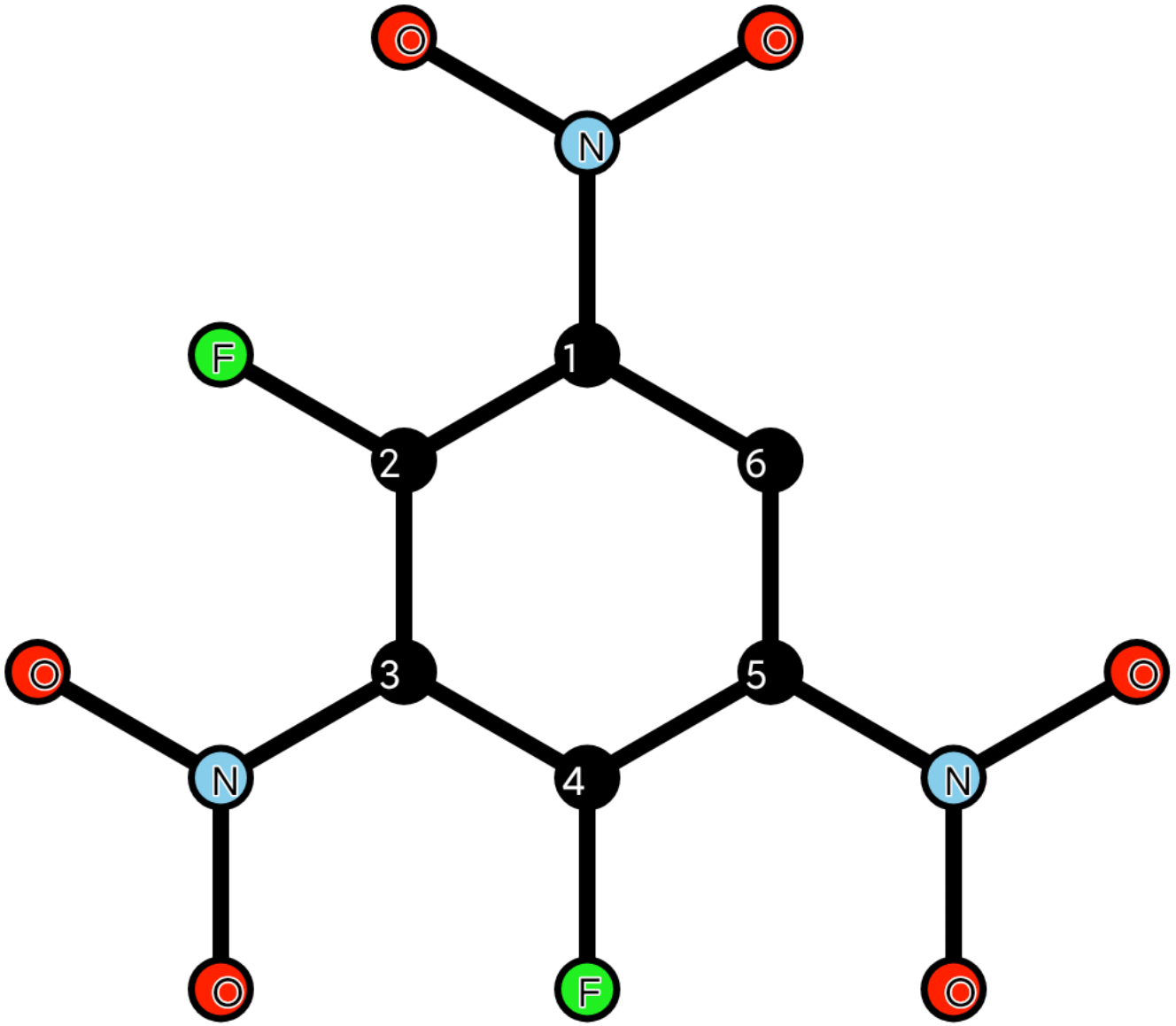

O
O
N
F
1
2
6
O
3
5
O
N
4
N
O
F
O

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1 2	-0.016	0.046	0.002	0.011	-0.013	-0.01	-0.005	0.001	-0.001	-0.01	-0.01	0.002	0.002	-0.003	-0.003	0.001	0.006
1 6	-0.024	-0.012	-0.002	0.01	0.017	0.032	-0.005	-0.001	0.002	-0.011	-0.011	-0.001	-0.001	0.004	0.004	0.001	-0.001
1 7	0.004	-0.023	0.001	-0.017	0.0	-0.023	0.005	0.0	0.0	0.029	0.029	0.0	0.0	0.0	0.0	-0.001	-0.002
2 3	0.001	0.044	-0.02	-0.013	-0.002	0.009	0.001	-0.005	-0.001	0.002	0.002	-0.01	-0.01	-0.001	-0.001	-0.001	0.006
2 17	0.027	-0.046	0.029	-0.001	0.018	-0.002	0.001	0.001	0.001	0.004	0.004	0.004	0.004	0.003	0.003	0.0	-0.05
3 4	-0.002	-0.013	-0.02	0.044	0.001	0.009	-0.001	-0.005	0.001	-0.001	-0.001	-0.01	-0.01	0.002	0.002	0.006	-0.001
3 8	0.001	-0.023	0.003	-0.023	0.001	-0.017	0.0	0.005	0.0	0.0	0.0	0.029	0.029	0.0	0.0	-0.002	-0.002
4 5	-0.013	0.011	0.002	0.046	-0.016	-0.01	-0.001	0.001	-0.005	-0.003	-0.003	0.002	0.002	-0.01	-0.01	0.006	0.001
4 16	0.018	-0.001	0.029	-0.046	0.027	-0.002	0.001	0.001	0.001	0.003	0.003	0.004	0.004	0.004	0.004	-0.05	0.0
5 6	0.017	0.01	-0.002	-0.012	-0.024	0.032	0.002	-0.001	-0.005	0.004	0.004	-0.001	-0.001	-0.011	-0.011	-0.001	0.001
5 9	0.0	-0.017	0.001	-0.023	0.004	-0.023	0.0	0.0	0.005	0.0	0.0	0.0	0.0	0.029	0.029	-0.002	-0.001
7 10	0.003	0.007	0.0	0.006	0.0	0.007	-0.009	0.0	0.0	-0.133	0.116	0.0	0.0	0.0	0.0	0.0	0.001
7 11	0.003	0.007	0.0	0.006	0.0	0.007	-0.009	0.0	0.0	0.116	-0.133	0.0	0.0	0.0	0.0	0.0	0.001
8 12	0.0	0.007	0.004	0.007	0.0	0.006	0.0	-0.008	0.0	0.0	0.0	-0.133	0.116	0.0	0.0	0.001	0.001
8 13	0.0	0.007	0.004	0.007	0.0	0.006	0.0	-0.008	0.0	0.0	0.0	0.116	-0.133	0.0	0.0	0.001	0.001
9 14	0.0	0.006	0.0	0.007	0.003	0.007	0.0	0.0	-0.009	0.0	0.0	0.0	0.0	-0.133	0.116	0.001	0.0
9 15	0.0	0.006	0.0	0.007	0.003	0.007	0.0	0.0	-0.009	0.0	0.0	0.0	0.0	0.116	-0.133	0.001	0.0

7.2. Presentation of molecule:

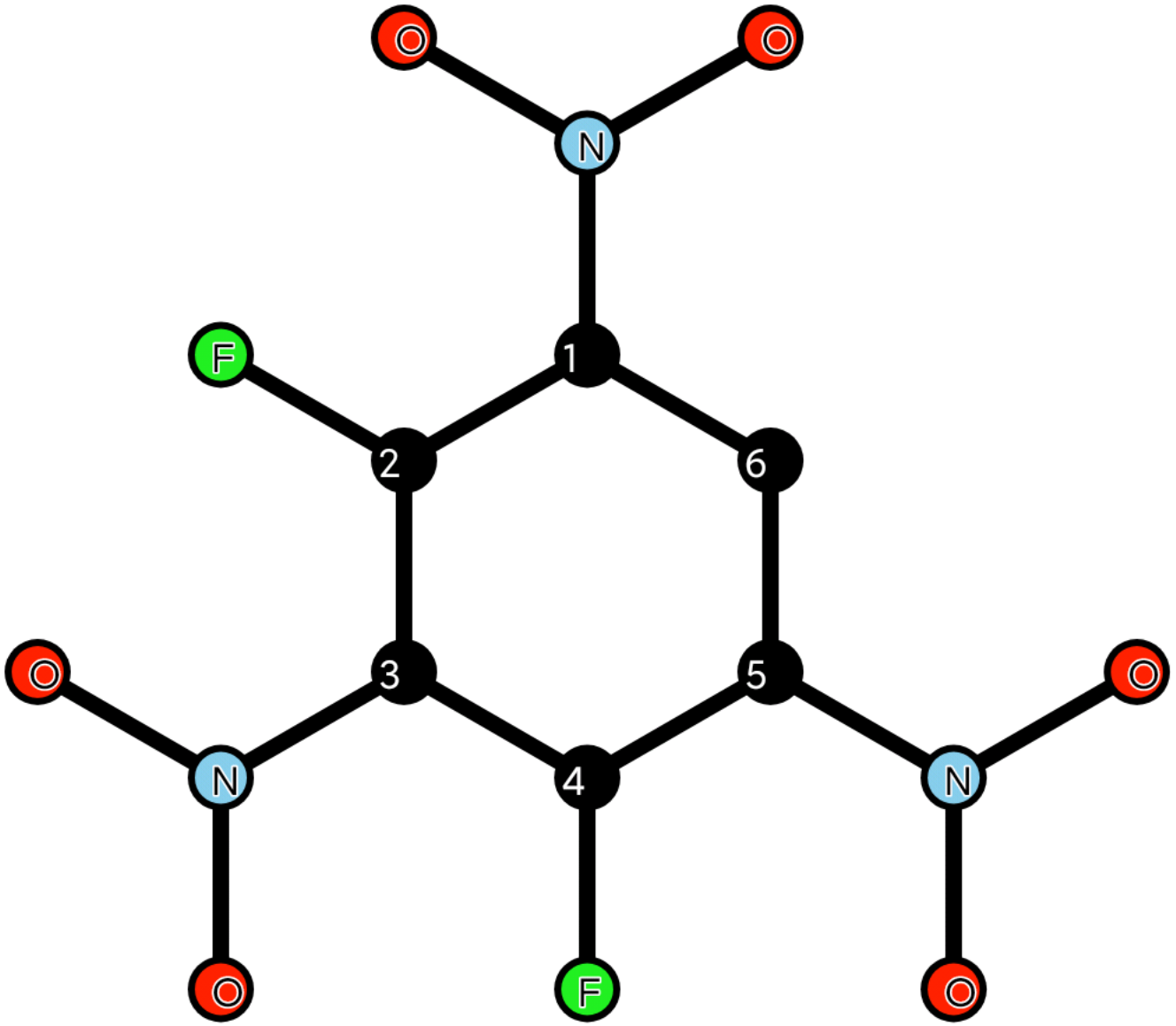

O
O
N
F
1
2
6
O
3
5
O
N
4
N
O
F
O

8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	1 7	2 3	2 17	3 4	3 8	4 5	4 16	5 6	5 9	7 10	7 11	8 12	8 13	9 14	9 15
1 2	0.262																
1 6	-0.179	0.259															
1 7	-0.065	-0.069	0.236														
2 3	-0.173	0.106	0.01	0.259													
2 17	-0.046	0.01	0.013	-0.046	0.293												
3 4	0.105	-0.072	-0.006	-0.177	0.01	0.259											
3 8	0.011	-0.007	0.0	-0.068	0.014	-0.068	0.237										
4 5	-0.069	0.11	-0.012	0.105	-0.007	-0.173	0.011	0.262									
4 16	-0.007	-0.007	0.009	0.01	0.0	-0.046	0.014	-0.046	0.293								
5 6	0.11	-0.19	0.018	-0.072	-0.007	0.106	-0.007	-0.179	0.01	0.259							
5 9	-0.012	0.018	-0.001	-0.006	0.009	0.01	0.0	-0.065	0.013	-0.069	0.236						
7 10	0.02	0.021	-0.068	-0.004	-0.004	0.003	0.0	0.005	-0.003	-0.006	0.0	0.191					
7 11	0.02	0.021	-0.068	-0.004	-0.004	0.003	0.0	0.005	-0.003	-0.006	0.0	-0.147	0.191				
8 12	-0.004	0.003	0.0	0.02	-0.004	0.02	-0.068	-0.004	-0.004	0.003	0.0	0.0	0.0	0.191			
8 13	-0.004	0.003	0.0	0.02	-0.004	0.02	-0.068	-0.004	-0.004	0.003	0.0	0.0	0.0	-0.147	0.191		
9 14	0.005	-0.006	0.0	0.003	-0.003	-0.004	0.0	0.02	-0.004	0.021	-0.068	0.0	0.0	0.0	0.0	0.191	
9 15	0.005	-0.006	0.0	0.003	-0.003	-0.004	0.0	0.02	-0.004	0.021	-0.068	0.0	0.0	0.0	0.0	-0.147	0.191

8.2. Presentation of molecule:


O
O
N
F
1
2
6
O
3
5
O
N
4
N
O
F
O