Print calculated values

Report generated by:root, 20.01.2020 - 20:41:43

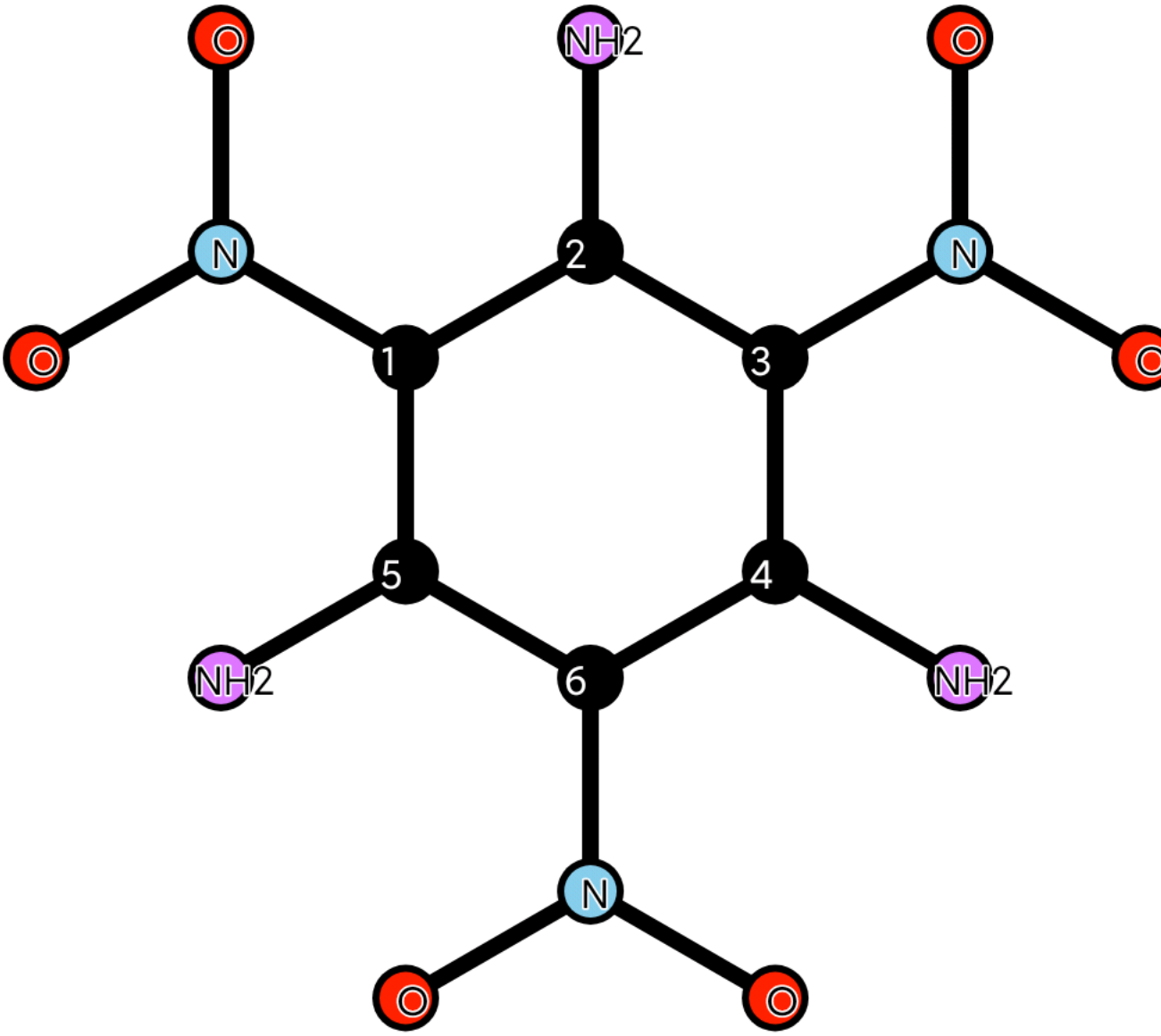
The following determinant is calculated:

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

It is about this molecule:

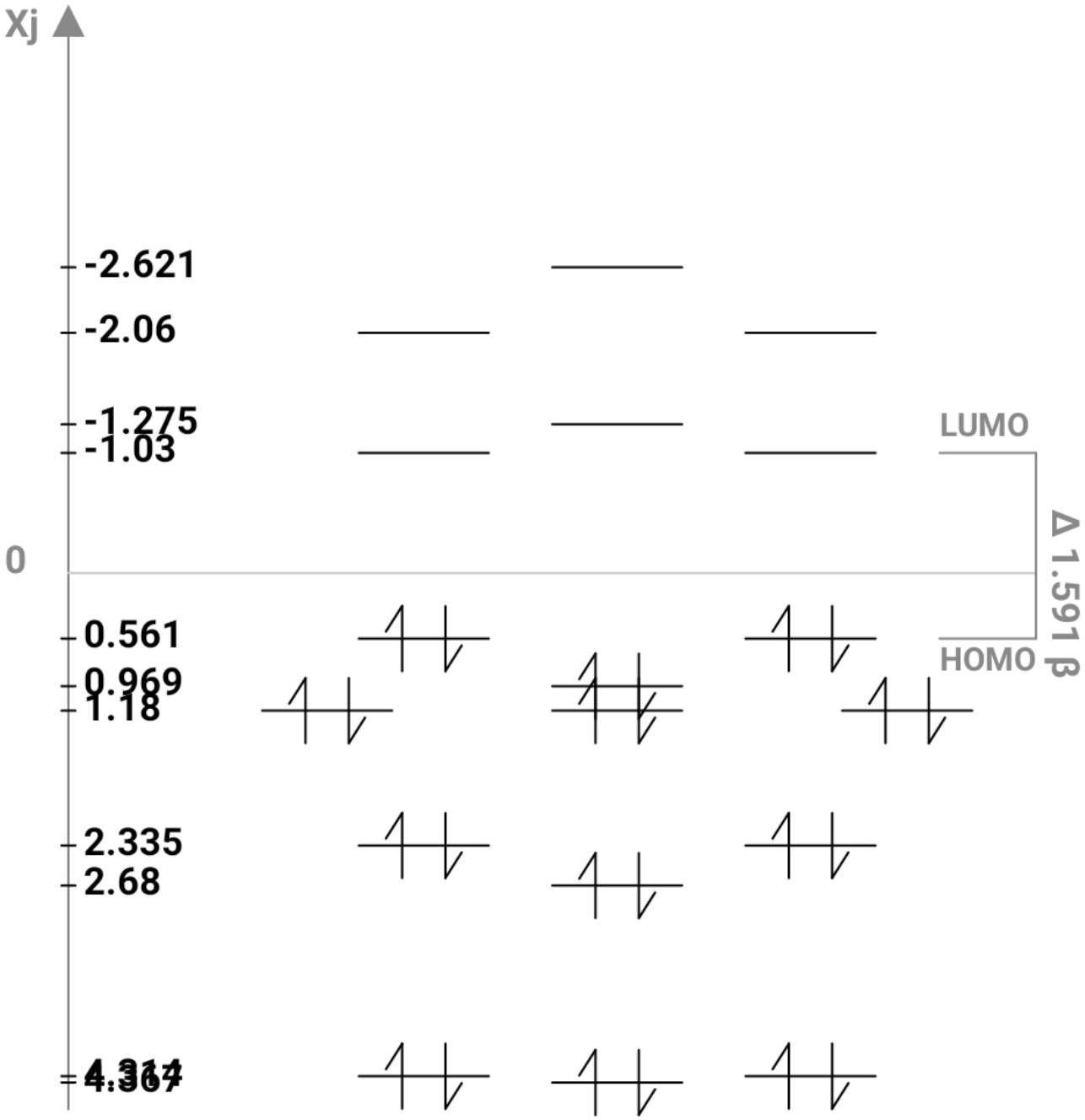
HMO-Energies

x1 = 4.367; x2 = 4.314; x3 = 4.314; x4 = 2.68; x5 = 2.335; x6 = 2.335; x7 = 1.18; x8 = 1.18; x9 = 1.18; x10 = 0.969; x11 = 0.561; x12 = 0.561; x13 = -1.03; x14 = -1.03; x15 = -1.275; x16 = -2.06; x17 = -2.06; x18 = -2.621;


O
NH2
O
N
2
N
O
1
3
O
5
4
NH2
6
NH2
N
O
O

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 18α + 51.952β -

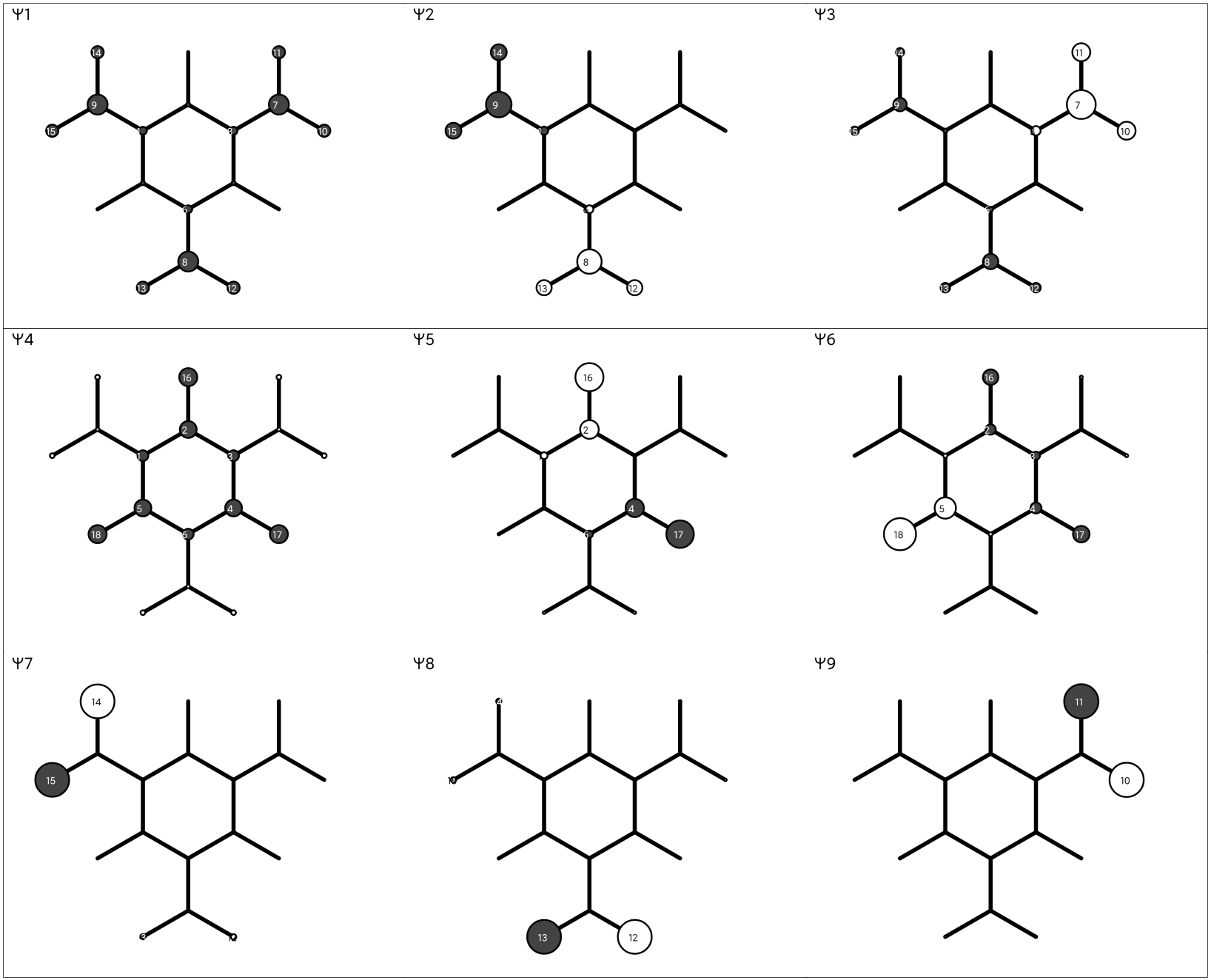
this corresponds to one πelectron: 2.165β

2. Hueckel-coefficient

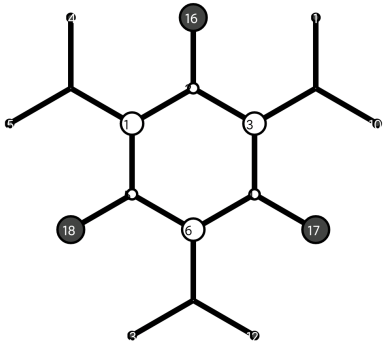
2.1. Calculated values:

	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	Psi 18
	x1= 4.367	x2= 4.314	x3= 4.314	x4= 2.68	x5= 2.335	x6= 2.335	x7= 1.18	x8= 1.18	x9= 1.18	x10= 0.969	x11= 0.561	x12= 0.561	x13= -1.03	x14= -1.03	x15= -1.275	x16= -2.06	x17= -2.06	x18= -2.621
1	-0.162	-0.169	-0.089	-0.223	0.143	0.086	0.0	0.0	0.0	0.341	0.538	0.288	-0.11	0.172	0.088	0.402	0.164	-0.366
2	-0.086	-0.043	0.027	-0.347	0.384	-0.213	0.0	0.0	0.0	0.157	0.214	-0.133	-0.266	-0.511	-0.267	-0.217	0.168	0.331
3	-0.162	0.007	0.191	-0.223	0.003	-0.167	0.0	0.0	0.0	0.341	-0.019	-0.61	0.204	0.009	0.088	-0.059	-0.43	-0.366
4	-0.086	0.045	0.024	-0.347	-0.376	-0.226	0.0	0.0	0.0	0.157	-0.222	-0.119	-0.31	0.486	-0.267	0.254	0.104	0.331
5	-0.086	-0.002	-0.051	-0.347	-0.008	0.439	0.0	0.0	0.0	0.157	0.008	0.252	0.576	0.025	-0.267	-0.037	-0.272	0.331
6	-0.162	0.162	-0.102	-0.223	-0.146	0.081	0.0	0.0	0.0	0.341	-0.518	0.321	-0.094	-0.181	0.088	-0.343	0.266	-0.366
7	-0.413	0.022	0.594	0.075	-0.001	0.038	0.0	0.0	0.0	0.012	-0.002	-0.07	0.281	0.012	0.325	0.064	0.473	0.227
8	-0.413	0.503	-0.316	0.075	0.033	-0.018	0.0	0.0	0.0	0.012	-0.059	0.037	-0.13	-0.25	0.325	0.377	-0.292	0.227
9	-0.413	-0.526	-0.278	0.075	-0.033	-0.02	0.0	0.0	0.0	0.012	0.061	0.033	-0.152	0.238	0.325	-0.442	-0.181	0.227
10	-0.253	0.014	0.37	0.097	-0.001	0.064	-0.034	0.055	0.704	-0.115	0.007	0.219	-0.248	-0.011	-0.258	-0.039	-0.284	-0.117
11	-0.253	0.014	0.37	0.097	-0.001	0.064	0.034	-0.055	-0.704	-0.115	0.007	0.219	-0.248	-0.011	-0.258	-0.039	-0.284	-0.117
12	-0.253	0.313	-0.197	0.097	0.056	-0.031	0.113	0.696	-0.049	-0.115	0.187	-0.116	0.115	0.221	-0.258	-0.227	0.176	-0.117
13	-0.253	0.313	-0.197	0.097	0.056	-0.031	-0.113	-0.696	0.049	-0.115	0.187	-0.116	0.115	0.221	-0.258	-0.227	0.176	-0.117
14	-0.253	-0.327	-0.173	0.097	-0.055	-0.033	0.697	-0.11	0.042	-0.115	-0.193	-0.104	0.134	-0.21	-0.258	0.266	0.109	-0.117
15	-0.253	-0.327	-0.173	0.097	-0.055	-0.033	-0.697	0.11	-0.042	-0.115	-0.193	-0.104	0.134	-0.21	-0.258	0.266	0.109	-0.117
16	-0.038	-0.02	0.012	-0.373	0.578	-0.32	0.0	0.0	0.0	-0.407	-0.306	0.19	0.138	0.266	0.126	0.08	-0.062	-0.105
17	-0.038	0.021	0.011	-0.373	-0.566	-0.34	0.0	0.0	0.0	-0.407	0.318	0.17	0.161	-0.253	0.126	-0.094	-0.038	-0.105
18	-0.038	-0.001	-0.023	-0.373	-0.012	0.66	0.0	0.0	0.0	-0.407	-0.011	-0.36	-0.299	-0.013	0.126	0.014	0.1	-0.105

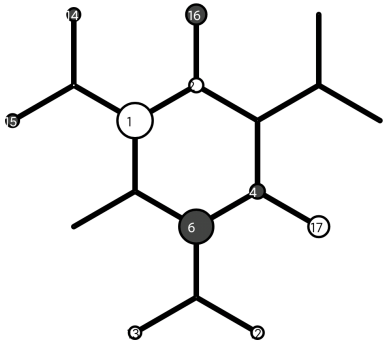
2.2. Molecule orbital presentation:


Ψ1
Ψ2
Ψ3
Ψ4
Ψ5
Ψ6
Ψ7
Ψ8
Ψ9

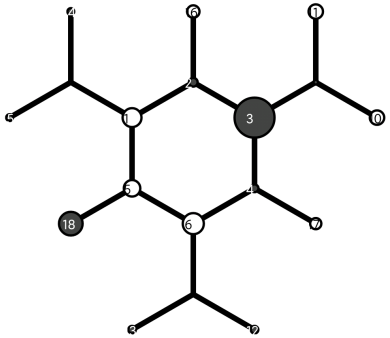
Ψ10



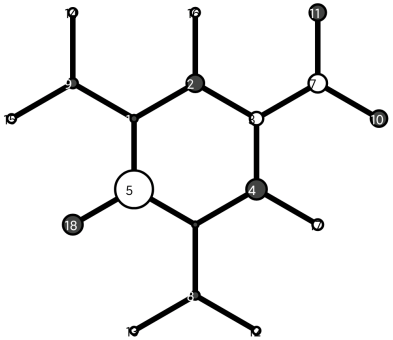
Ψ11



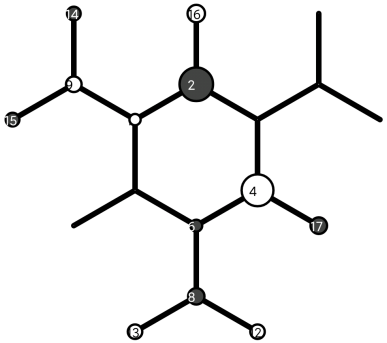
Ψ12



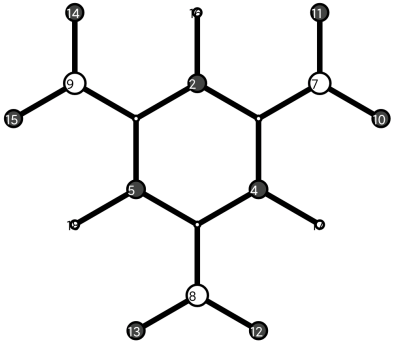
Ψ13



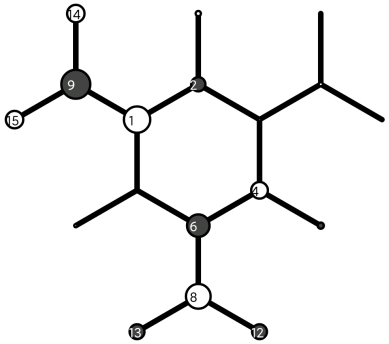
Ψ14



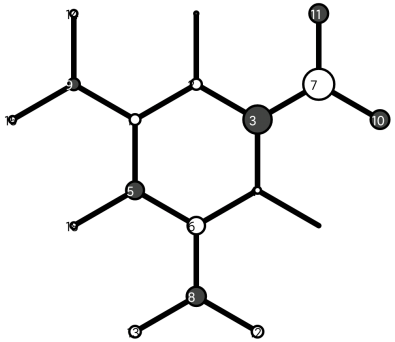
Ψ15



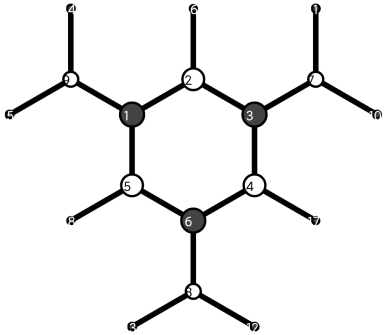
Ψ16



Ψ17



Ψ18

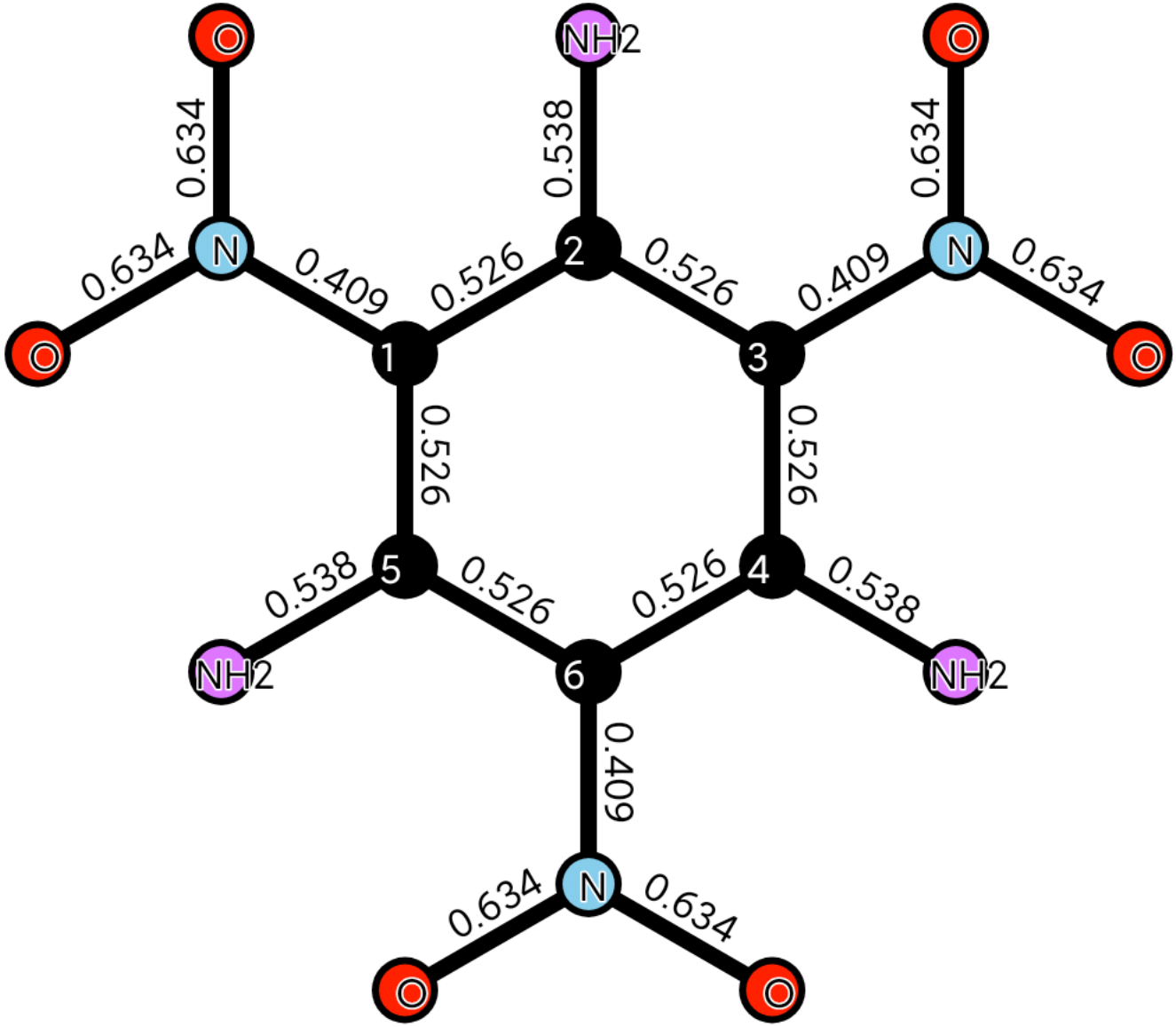


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1.257																	
2	0.526	0.823																
3	-0.053	0.526	1.257															
4	-0.184	0.046	0.526	0.823														
5	0.526	0.046	-0.184	0.046	0.823													
6	-0.053	-0.184	-0.053	0.526	0.526	1.257												
7	-0.041	0.054	0.409	0.054	-0.04	-0.041	1.072											
8	-0.041	-0.04	-0.041	0.054	0.054	0.409	-0.007	1.072										
9	0.409	0.054	-0.041	-0.04	0.054	-0.041	-0.007	-0.007	1.072									
10	0.034	-0.125	-0.188	-0.125	0.069	0.034	0.634	0.013	0.013	1.551								
11	0.034	-0.125	-0.188	-0.125	0.069	0.034	0.634	0.013	0.013	-0.449	1.551							
12	0.034	0.069	0.034	-0.125	-0.125	-0.188	0.013	0.634	0.013	-0.016	-0.016	1.551						
13	0.034	0.069	0.034	-0.125	-0.125	-0.188	0.013	0.634	0.013	-0.016	-0.016	-0.449	1.551					
14	-0.188	-0.125	0.034	0.069	-0.125	0.034	0.013	0.013	0.634	-0.016	-0.016	-0.016	-0.016	1.551				
15	-0.188	-0.125	0.034	0.069	-0.125	0.034	0.013	0.013	0.634	-0.016	-0.016	-0.016	-0.016	-0.449	1.551			
16	-0.204	0.538	-0.204	-0.063	-0.063	0.111	-0.07	0.038	-0.07	0.086	0.086	-0.05	-0.05	0.086	0.086	1.746		
17	0.111	-0.063	-0.204	0.538	-0.063	-0.204	-0.07	-0.07	0.038	0.086	0.086	0.086	0.086	-0.05	-0.05	0.046	1.746	
18	-0.204	-0.063	0.111	-0.063	0.538	-0.204	0.038	-0.07	-0.07	-0.05	-0.05	0.086	0.086	0.086	0.086	0.046	0.046	1.746

3.2. Presentation of bond order:

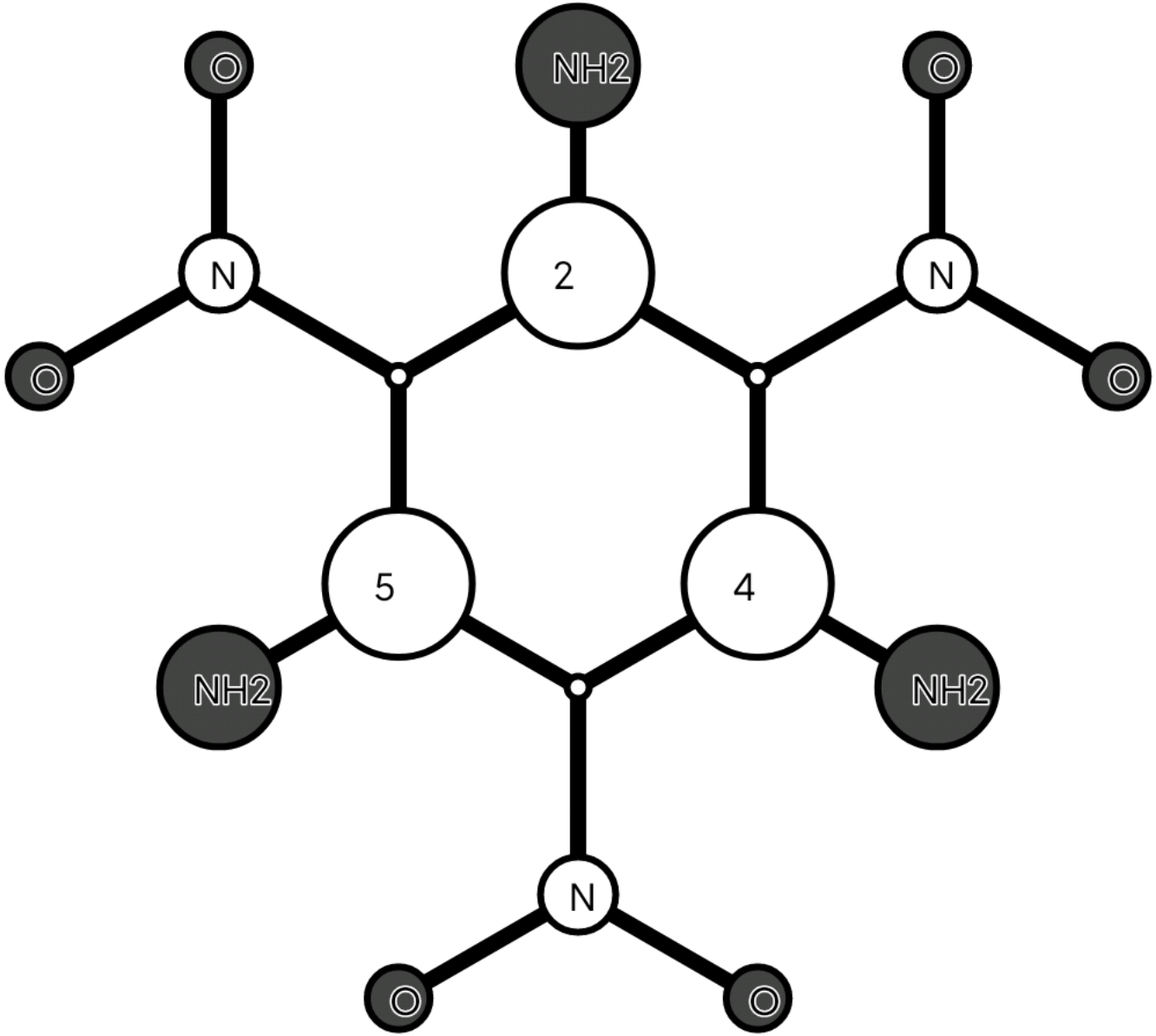

O
NH2
O
0.634
0.538
0.634
0.634
N
2
N
0.634
O
0.409
0.526
0.526
0.409
1
3
O
0.526
0.526
0.538
5
0.526
0.526
4
0.538
NH2
6
NH2
0.409
0.634
N
0.634
O
O

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.077																	
2		0.511																
3			0.077															
4				0.511														
5					0.511													
6						0.077												
7							0.261											
8								0.261										
9									0.261									
10										-0.218								
11											-0.218							
12												-0.218						
13													-0.218					
14														-0.218				
15															-0.218			
16																-0.412		
17																	-0.412	
18																		-0.412

4.2. Presentation of molecule:

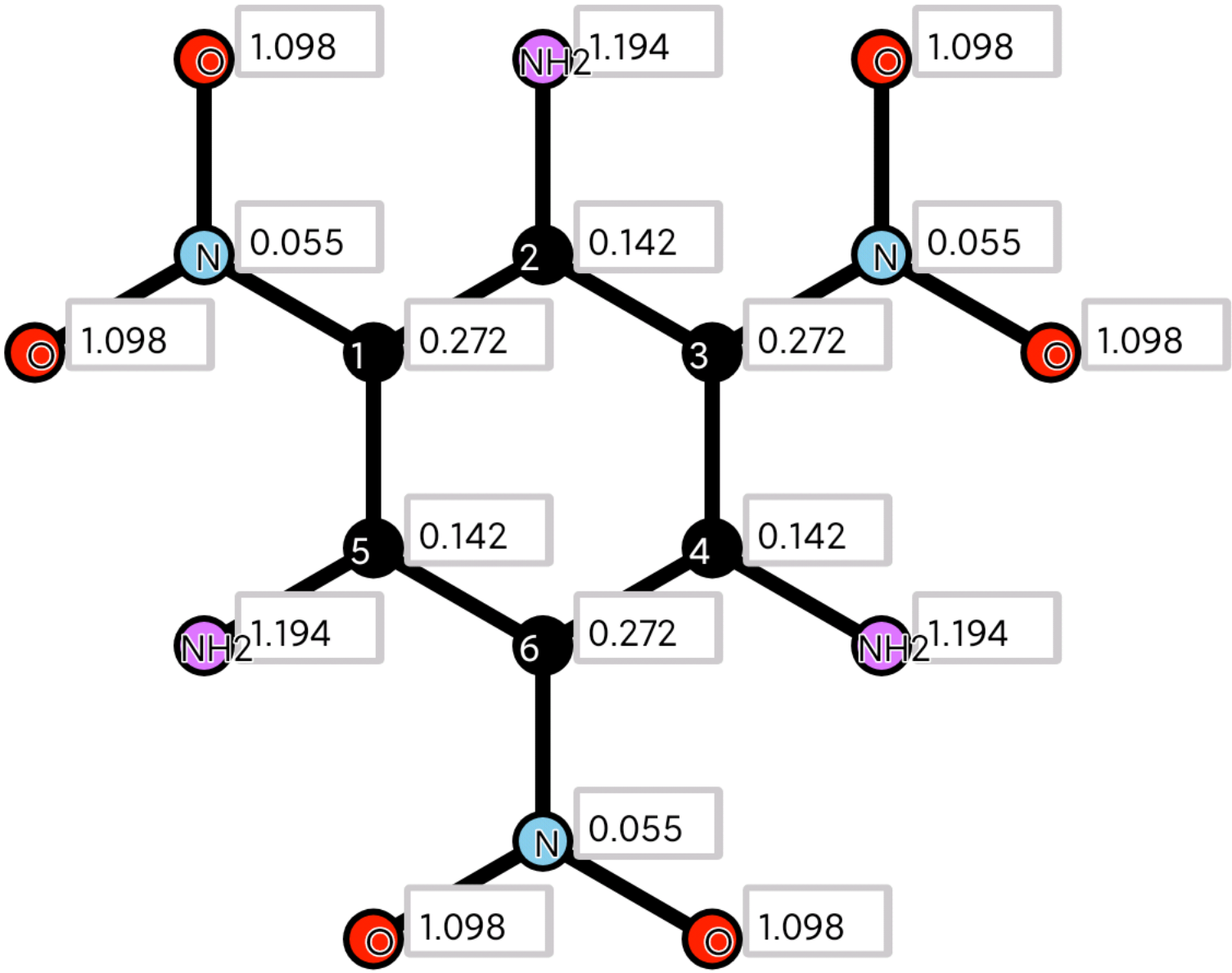

O
NH2
O
N
2
N
O
O
5
4
NH2
NH2
N
O
O

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
0.272	0.142	0.272	0.142	0.142	0.272	0.055	0.055	0.055	1.098	1.098	1.098	1.098	1.098	1.098	1.194	1.194	1.194

5.2. Presentation of molecule:

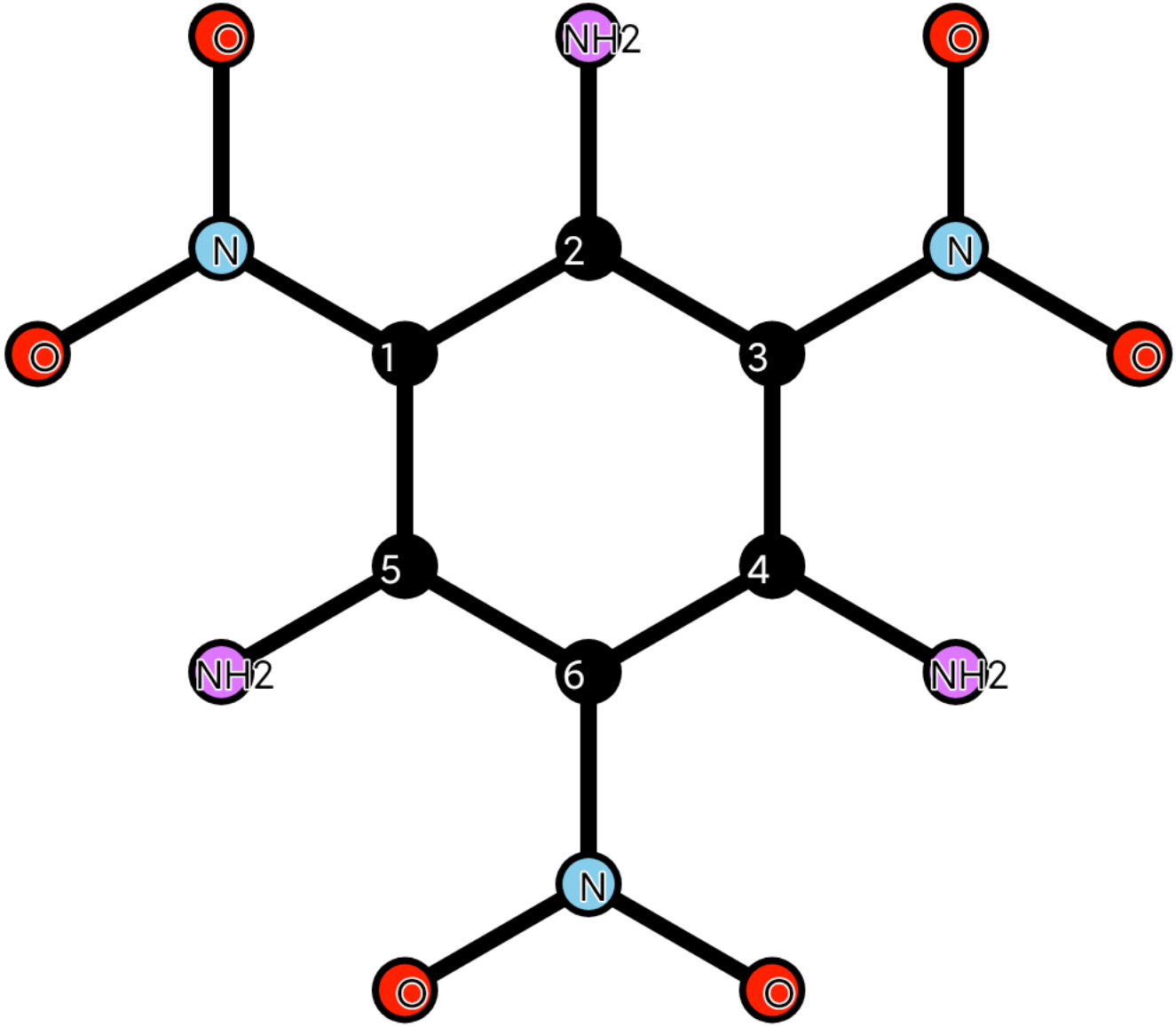

O
1.098
NH2
1.194
O
1.098
N
0.055
2
0.142
N
0.055
O
1.098
1
0.272
3
0.272
O
1.098
5
0.142
4
0.142
NH2
1.194
6
0.272
NH2
1.194
N
0.055
O
1.098
O
1.098

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	18
1	0.312																	
2	-0.084	0.299																
3	0.002	-0.084	0.312															
4	-0.031	0.002	-0.084	0.299														
5	-0.084	0.002	-0.031	0.002	0.299													
6	0.002	-0.031	0.002	-0.084	-0.084	0.312												
7	-0.001	-0.002	-0.027	-0.002	-0.002	-0.001	0.168											
8	-0.001	-0.002	-0.001	-0.002	-0.002	-0.027	0.0	0.168										
9	-0.027	-0.002	-0.001	-0.002	-0.002	-0.001	0.0	0.0	0.168									
10	-0.001	-0.012	-0.008	-0.012	-0.006	-0.001	-0.062	0.0	0.0	0.228								
11	-0.001	-0.012	-0.008	-0.012	-0.006	-0.001	-0.062	0.0	0.0	-0.108	0.228							
12	-0.001	-0.006	-0.001	-0.012	-0.012	-0.008	0.0	-0.062	0.0	0.0	0.0	0.228						
13	-0.001	-0.006	-0.001	-0.012	-0.012	-0.008	0.0	-0.062	0.0	0.0	0.0	-0.108	0.228					
14	-0.008	-0.012	-0.001	-0.006	-0.012	-0.001	0.0	0.0	-0.062	0.0	0.0	0.0	0.0	0.228				
15	-0.008	-0.012	-0.001	-0.006	-0.012	-0.001	0.0	0.0	-0.062	0.0	0.0	0.0	0.0	-0.108	0.228			
16	-0.028	-0.037	-0.028	-0.002	-0.002	-0.014	-0.003	-0.002	-0.003	-0.007	-0.007	-0.003	-0.003	-0.007	-0.007	0.157		
17	-0.014	-0.002	-0.028	-0.037	-0.002	-0.028	-0.003	-0.003	-0.002	-0.007	-0.007	-0.007	-0.007	-0.003	-0.003	-0.002	0.157	
18	-0.028	-0.002	-0.014	-0.002	-0.037	-0.028	-0.002	-0.003	-0.003	-0.003	-0.003	-0.007	-0.007	-0.007	-0.007	-0.002	-0.002	0.157

6.2. Presentation of molecule:

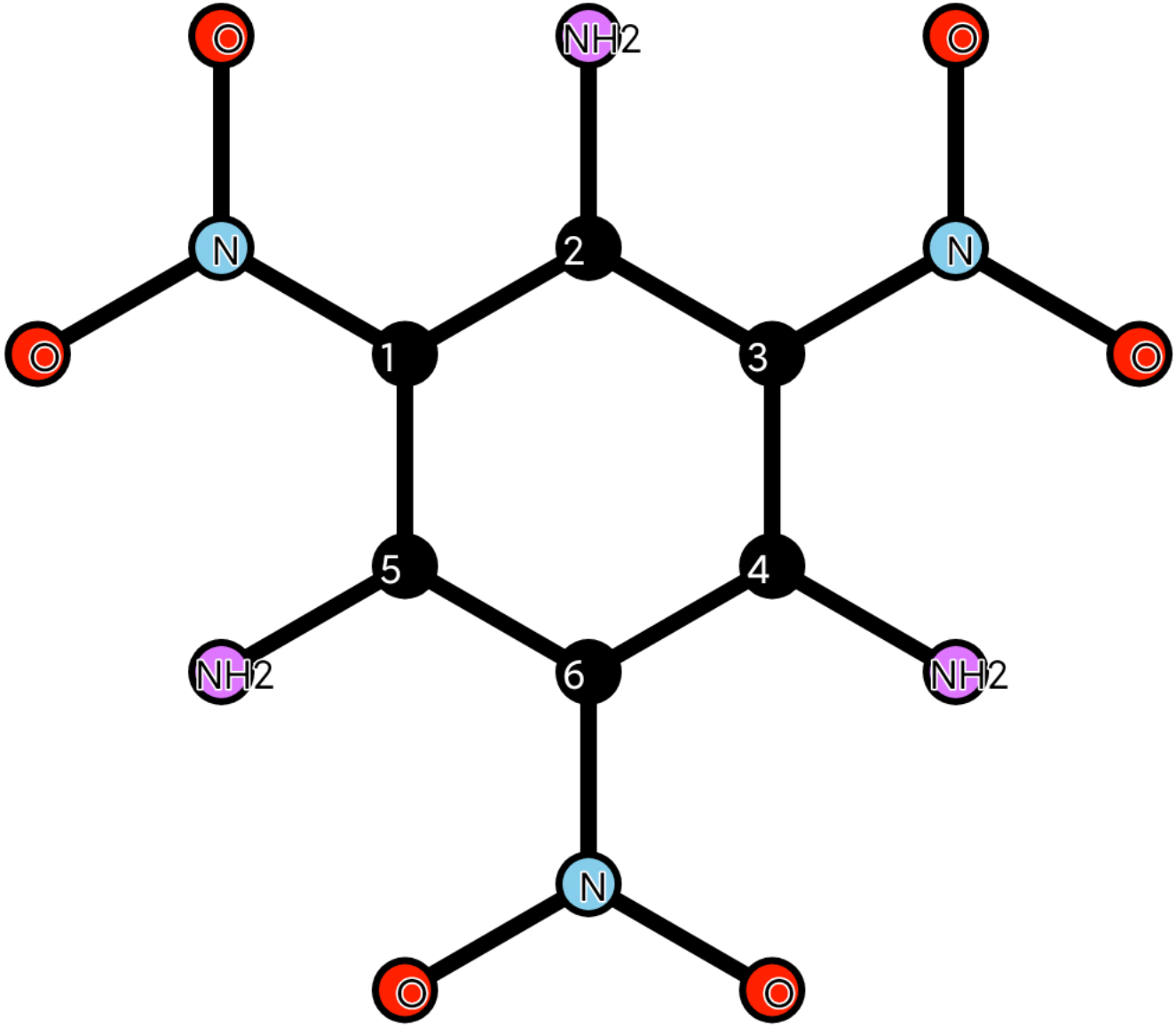

O
NH2
O
N
2
N
O
1
3
O
5
4
NH2
6
NH2
N
O
O

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	18
1 2	-0.062	0.055	0.015	0.01	-0.014	-0.01	0.002	-0.002	-0.009	0.004	0.004	-0.003	-0.003	-0.019	-0.019	0.053	0.007	-0.012
1 5	-0.062	-0.014	-0.01	0.01	0.055	0.015	-0.002	0.002	-0.009	-0.003	-0.003	0.004	0.004	-0.019	-0.019	-0.012	0.007	0.053
1 9	-0.03	-0.018	-0.001	-0.009	-0.018	-0.001	0.0	0.0	0.011	0.0	0.0	0.0	0.0	0.051	0.051	-0.013	-0.006	-0.013
2 3	0.015	0.055	-0.062	-0.014	0.01	-0.01	-0.009	-0.002	0.002	-0.019	-0.019	-0.003	-0.003	0.004	0.004	0.053	-0.012	0.007
2 16	0.05	-0.03	0.05	0.001	0.001	0.021	0.003	0.002	0.003	0.01	0.01	0.005	0.005	0.01	0.01	-0.153	0.002	0.002
3 4	-0.01	-0.014	-0.062	0.055	0.01	0.015	-0.009	0.002	-0.002	-0.019	-0.019	0.004	0.004	-0.003	-0.003	-0.012	0.053	0.007
3 7	-0.001	-0.018	-0.03	-0.018	-0.009	-0.001	0.011	0.0	0.0	0.051	0.051	0.0	0.0	0.0	0.0	-0.013	-0.013	-0.006
4 6	-0.01	0.01	0.015	0.055	-0.014	-0.062	0.002	-0.009	-0.002	0.004	0.004	-0.019	-0.019	-0.003	-0.003	0.007	0.053	-0.012
4 17	0.021	0.001	0.05	-0.03	0.001	0.05	0.003	0.003	0.002	0.01	0.01	0.01	0.01	0.005	0.005	0.002	-0.153	0.002
5 6	0.015	0.01	-0.01	-0.014	0.055	-0.062	-0.002	-0.009	0.002	-0.003	-0.003	-0.019	-0.019	0.004	0.004	0.007	-0.012	0.053
5 18	0.05	0.001	0.021	0.001	-0.03	0.05	0.002	0.003	0.003	0.005	0.005	0.01	0.01	0.01	0.01	0.002	0.002	-0.153
6 8	-0.001	-0.009	-0.001	-0.018	-0.018	-0.03	0.0	0.011	0.0	0.0	0.0	0.051	0.051	0.0	0.0	-0.006	-0.013	-0.013
7 10	0.001	0.006	0.02	0.006	0.004	0.001	-0.013	0.0	0.0	-0.134	0.096	0.0	0.0	0.0	0.0	0.005	0.005	0.003
7 11	0.001	0.006	0.02	0.006	0.004	0.001	-0.013	0.0	0.0	0.096	-0.134	0.0	0.0	0.0	0.0	0.005	0.005	0.003
8 12	0.001	0.004	0.001	0.006	0.006	0.02	0.0	-0.013	0.0	0.0	0.0	-0.134	0.096	0.0	0.0	0.003	0.005	0.005
8 13	0.001	0.004	0.001	0.006	0.006	0.02	0.0	-0.013	0.0	0.0	0.0	0.096	-0.134	0.0	0.0	0.003	0.005	0.005
9 14	0.02	0.006	0.001	0.004	0.006	0.001	0.0	0.0	-0.013	0.0	0.0	0.0	0.0	-0.134	0.096	0.005	0.003	0.005
9 15	0.02	0.006	0.001	0.004	0.006	0.001	0.0	0.0	-0.013	0.0	0.0	0.0	0.0	0.096	-0.134	0.005	0.003	0.005

7.2. Presentation of molecule:

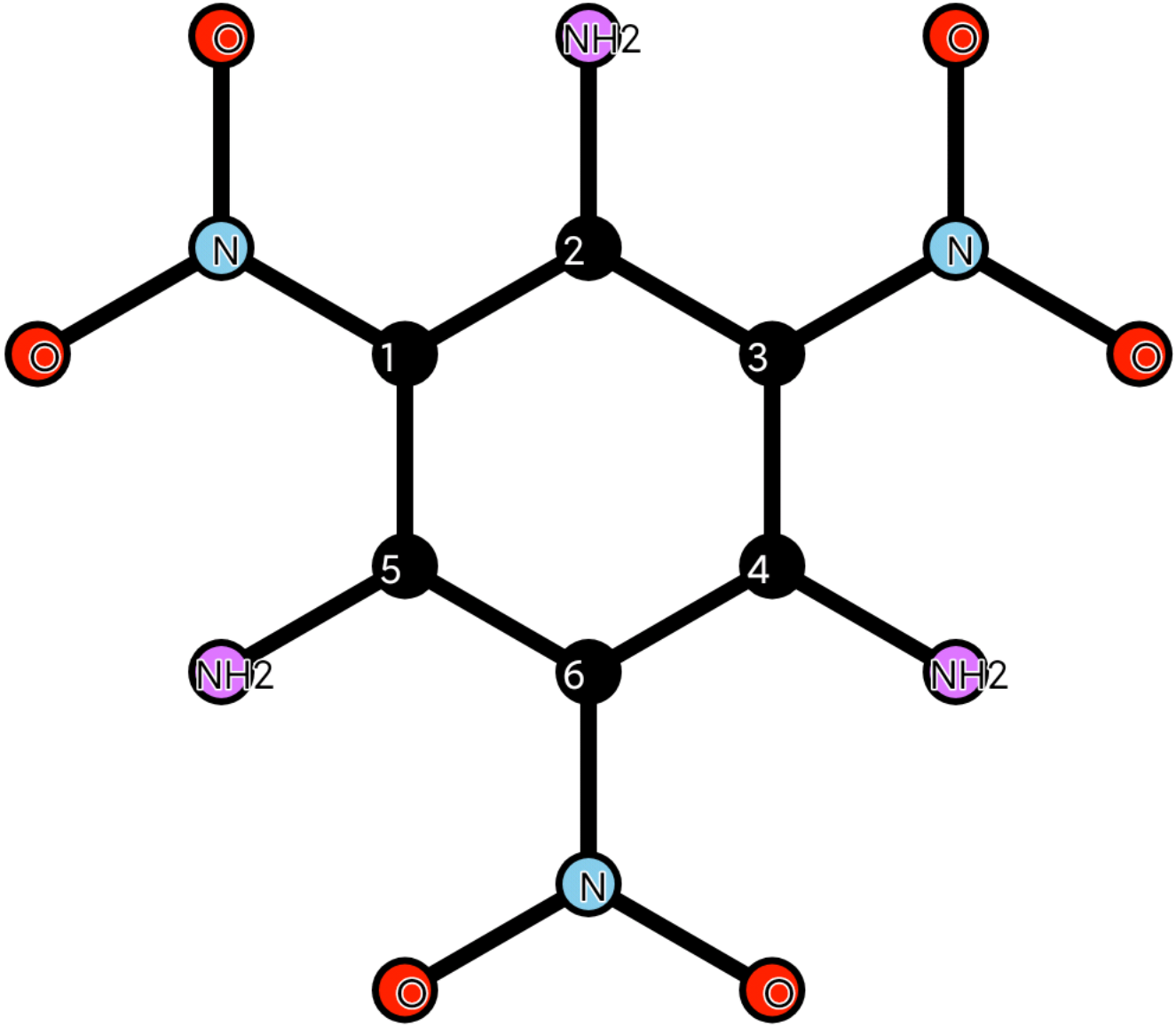

O
NH2
O
N
2
N
O
1
3
O
5
4
NH2
6
NH2
N
O
O

8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 5	1 9	2 3	2 16	3 4	3 7	4 6	4 17	5 6	5 18	6 8	7 10	7 11	8 12	8 13	9 14	9 15
1 2	0.319																	
1 5	-0.129	0.319																
1 9	-0.092	-0.092	0.26															
2 3	-0.129	0.056	0.018	0.319														
2 16	-0.145	0.03	0.035	-0.145	0.34													
3 4	0.056	-0.022	-0.01	-0.129	0.03	0.319												
3 7	0.018	-0.01	-0.002	-0.092	0.035	-0.092	0.26											
4 6	-0.022	0.056	-0.01	0.056	-0.018	-0.129	0.018	0.319										
4 17	-0.018	-0.018	0.015	0.03	-0.004	-0.145	0.035	-0.145	0.34									
5 6	0.056	-0.129	0.018	-0.022	-0.018	0.056	-0.01	-0.129	0.03	0.319								
5 18	0.03	-0.145	0.035	-0.018	-0.004	-0.018	0.015	0.03	-0.004	-0.145	0.34							
6 8	-0.01	0.018	-0.002	-0.01	0.015	0.018	-0.002	-0.092	0.035	-0.092	0.035	0.26						
7 10	-0.007	0.005	0.001	0.031	-0.013	0.031	-0.094	-0.007	-0.013	0.005	-0.006	0.001	0.201					
7 11	-0.007	0.005	0.001	0.031	-0.013	0.031	-0.094	-0.007	-0.013	0.005	-0.006	0.001	-0.124	0.201				
8 12	0.005	-0.007	0.001	0.005	-0.006	-0.007	0.001	0.031	-0.013	0.031	-0.013	-0.094	0.0	0.0	0.201			
8 13	0.005	-0.007	0.001	0.005	-0.006	-0.007	0.001	0.031	-0.013	0.031	-0.013	-0.094	0.0	0.0	-0.124	0.201		
9 14	0.031	0.031	-0.094	-0.007	-0.013	0.005	0.001	0.005	-0.006	-0.007	-0.013	0.001	0.0	0.0	0.0	0.0	0.201	
9 15	0.031	0.031	-0.094	-0.007	-0.013	0.005	0.001	0.005	-0.006	-0.007	-0.013	0.001	0.0	0.0	0.0	0.0	-0.124	0.201

8.2. Presentation of molecule:


O
NH2
O
N
2
N
O
1
3
O
5
4
NH2
6
NH2
N
O
O