Print calculated values

Report generated by:root, 16.05.2020 - 18:54:02

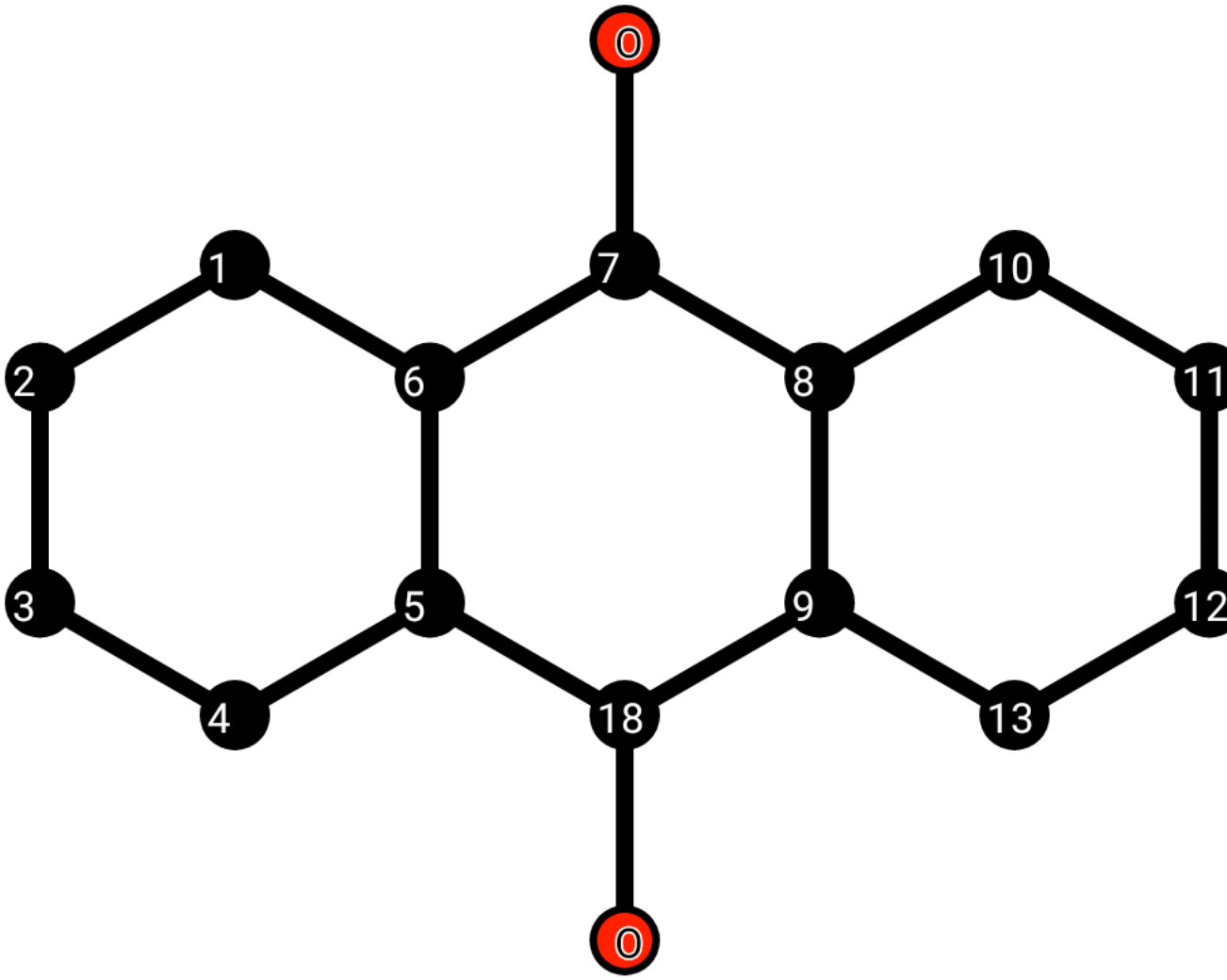
The following determinant is calculated:

-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	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	0.0	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	0.0	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	0.0
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	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	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	1.93	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	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	0.0	0.0	0.0	1.0	-x	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	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	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	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	0.0	1.0	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	0.0	1.93	0.0	0.0	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	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	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	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	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-x	1.93
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	0.0	0.0	0.0	1.93	-x+1.18

It is about this molecule:

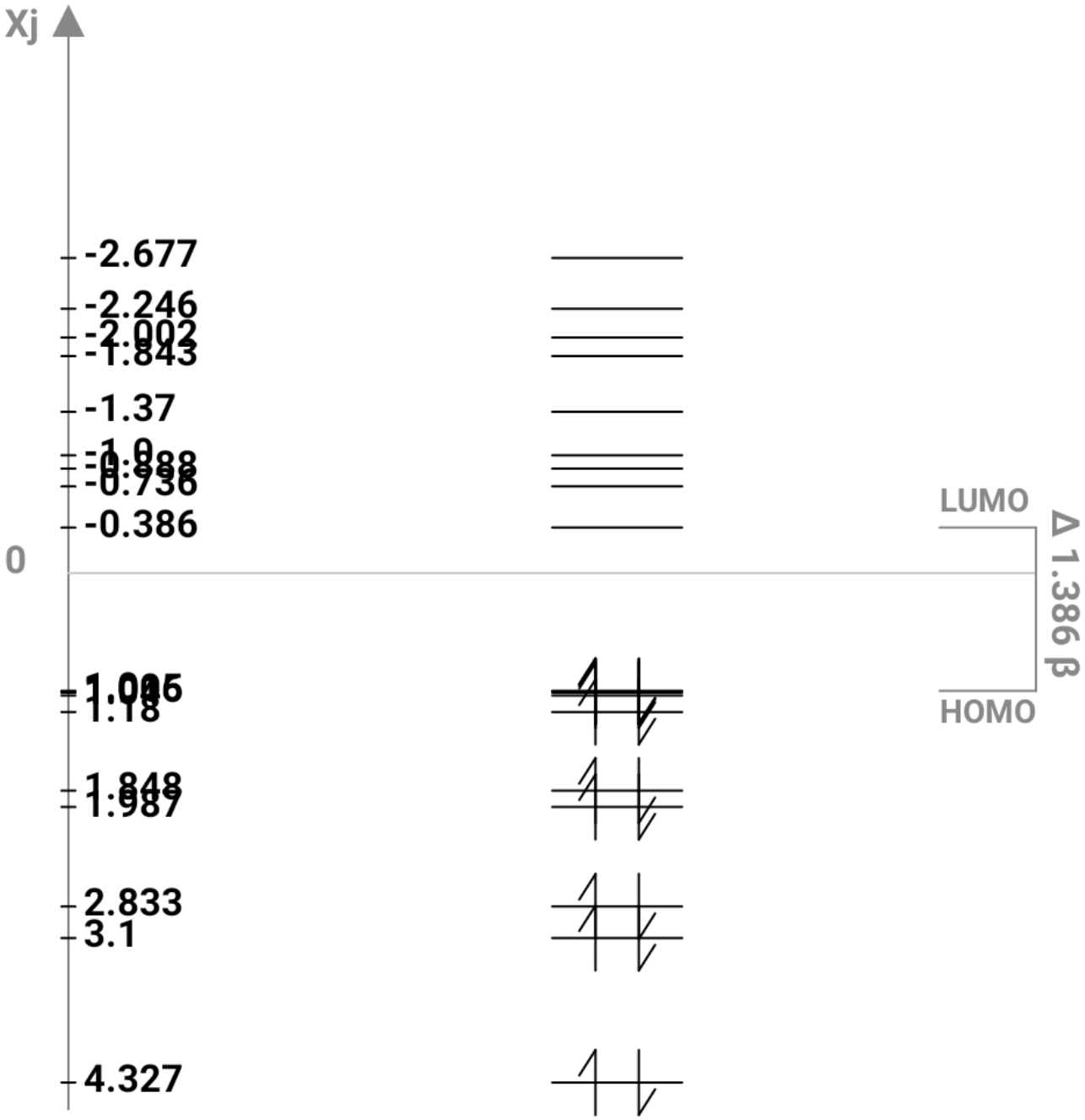
HMO-Energies

x1 = 4.327; x2 = 3.1; x3 = 2.833; x4 = 1.987; x5 = 1.848; x6 = 1.18; x7 = 1.04; x8 = 1.016; x9 = 1.005; x10 = 1.0; x11 = -0.386; x12 = -0.736; x13 = -0.888; x14 = -1.0; x15 = -1.37; x16 = -1.843; x17 = -2.002; x18 = -2.246; x19 = -2.677;


0
1
7
10
2
6
8
11
3
5
9
12
4
18
13
0

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 19α + 38.672β -

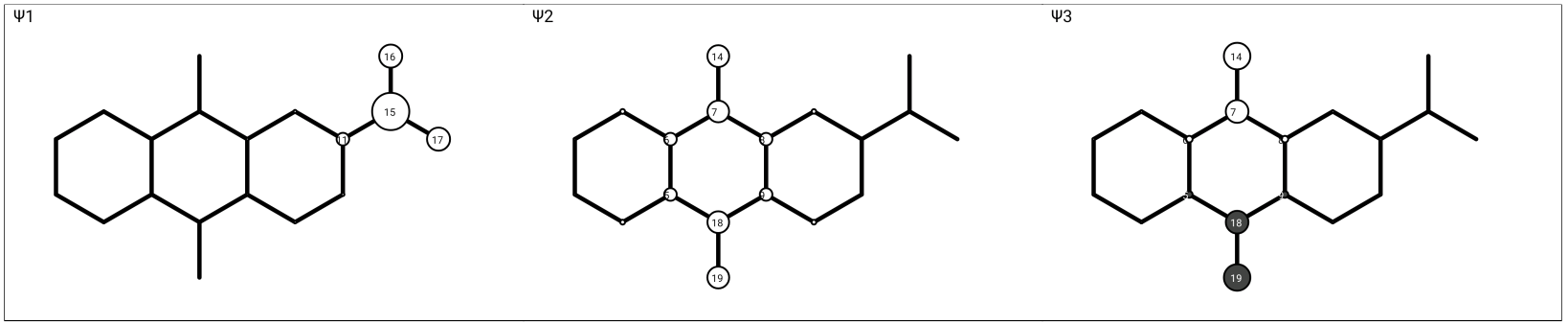
this corresponds to one πelectron: 1.934β

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	Psi 19
	x1= 4.327	x2= 3.1	x3= 2.833	x4= 1.987	x5= 1.848	x6= 1.18	x7= 1.04	x8= 1.016	x9= 1.005	x10= 1.0	x11= -0.386	x12= -0.736	x13= -0.888	x14= -1.0	x15= -1.37	x16= -1.843	x17= -2.002	x18= -2.246	x19= -2.677
1	0.0	0.094	0.05	-0.313	0.236	0.0	-0.022	-0.33	-0.29	-0.354	-0.112	0.247	0.364	0.354	0.162	-0.292	0.17	-0.141	0.155
2	0.0	0.045	0.013	-0.318	0.279	0.0	-0.282	-0.056	-0.475	0.0	-0.206	0.028	-0.418	0.0	-0.362	0.364	-0.085	0.117	-0.093
3	0.0	0.045	-0.013	-0.318	0.278	0.0	-0.272	0.273	-0.188	0.354	0.192	-0.268	0.007	-0.354	0.333	-0.378	0.0	-0.122	0.092
4	0.0	0.094	-0.05	-0.314	0.236	0.0	-0.001	0.334	0.287	0.354	0.132	0.169	0.412	0.354	-0.095	0.333	0.086	0.156	-0.155
5	0.001	0.246	-0.128	-0.306	0.158	0.0	0.271	0.066	0.476	0.0	-0.243	0.143	-0.373	0.0	-0.203	-0.235	-0.171	-0.229	0.322
6	0.002	0.246	0.129	-0.305	0.158	0.0	0.26	-0.279	0.184	-0.354	0.249	-0.21	0.095	-0.354	0.139	0.175	-0.256	0.2	-0.323
7	0.006	0.422	0.443	0.013	-0.102	0.0	0.021	-0.02	-0.001	0.0	0.259	-0.236	-0.076	0.0	-0.15	0.205	0.514	-0.079	0.388
8	0.017	0.244	0.128	0.272	0.22	0.0	0.311	-0.192	-0.207	0.354	0.266	-0.076	-0.164	0.354	-0.153	-0.3	-0.172	-0.108	-0.341
9	0.008	0.245	-0.128	0.276	0.224	0.0	0.37	0.238	-0.302	0.0	-0.33	-0.221	0.212	0.0	0.224	0.28	-0.256	0.046	0.335
10	0.061	0.09	0.049	0.253	0.283	0.0	-0.067	-0.413	0.095	0.354	-0.031	0.513	0.01	-0.354	0.136	0.067	0.085	0.277	0.19
11	0.246	0.034	0.01	0.231	0.304	0.0	-0.381	-0.228	0.302	0.0	-0.254	-0.302	0.156	0.0	-0.033	0.176	0.001	-0.514	-0.166
12	0.061	0.041	-0.014	0.249	0.325	0.0	-0.318	0.19	0.197	-0.354	0.273	-0.002	-0.347	0.354	0.307	-0.018	-0.086	0.296	0.127
13	0.016	0.092	-0.05	0.264	0.297	0.0	0.051	0.421	-0.104	-0.354	0.149	0.303	0.153	-0.354	-0.388	-0.142	0.171	-0.152	-0.173
14	0.004	0.424	0.517	0.03	-0.293	0.0	-0.285	0.234	0.012	0.0	-0.319	0.238	0.071	0.0	0.114	-0.131	-0.312	0.045	-0.194
15	0.726	-0.019	-0.004	-0.034	-0.036	0.0	-0.009	-0.006	0.009	0.0	-0.11	-0.223	0.153	0.0	-0.306	-0.287	-0.001	0.446	0.099
16	0.45	-0.019	-0.005	-0.081	-0.105	0.707	0.128	0.077	-0.102	0.0	0.137	0.226	-0.145	0.0	0.234	0.185	0.001	-0.254	-0.05
17	0.45	-0.019	-0.005	-0.081	-0.105	-0.707	0.128	0.077	-0.102	0.0	0.137	0.226	-0.145	0.0	0.234	0.185	0.001	-0.254	-0.05
18	0.003	0.423	-0.442	0.011	-0.103	0.0	0.023	0.013	0.008	0.0	-0.288	-0.065	-0.176	0.0	0.234	-0.074	0.514	0.158	-0.384
19	0.002	0.425	-0.515	0.027	-0.296	0.0	-0.32	-0.151	-0.086	0.0	0.355	0.065	0.164	0.0	-0.177	0.048	-0.312	-0.089	0.192

2.2. Molecule orbital presentation:



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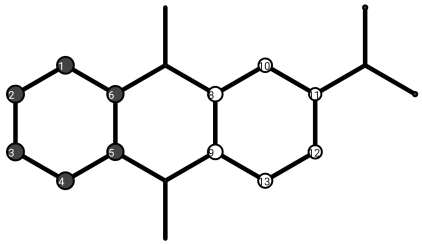

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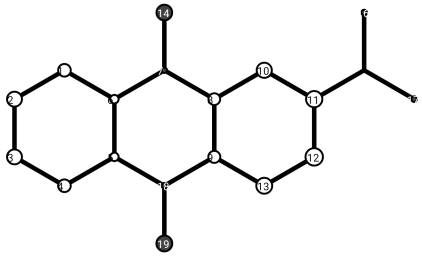

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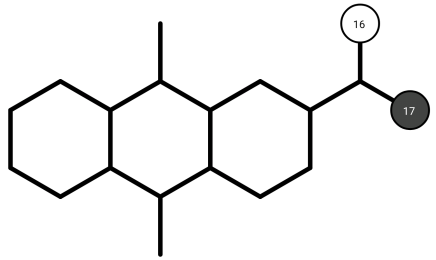

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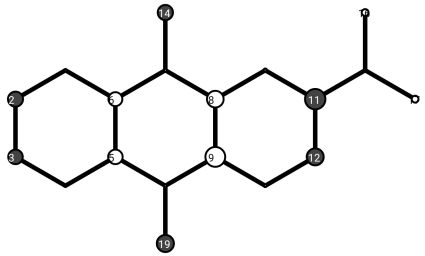

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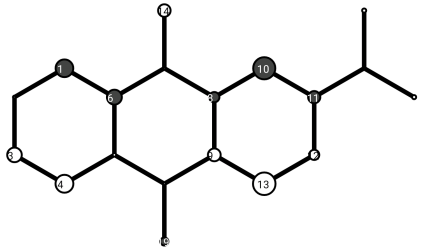

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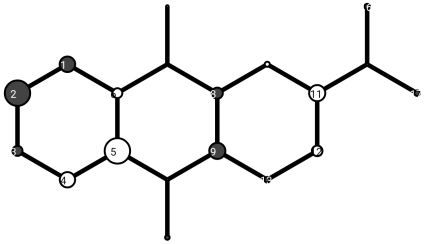

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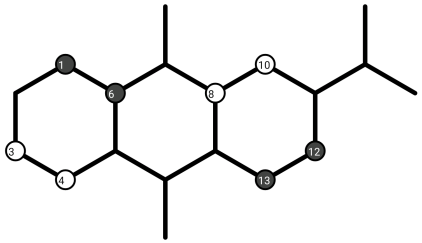

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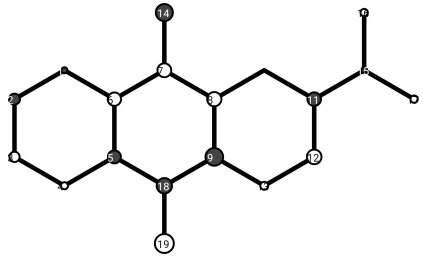

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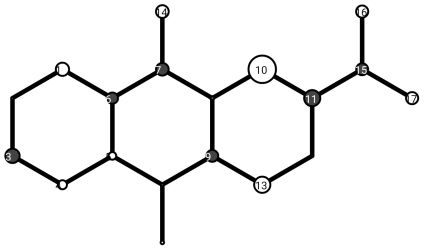

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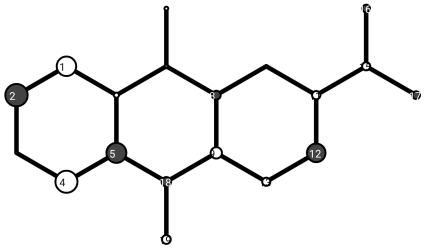

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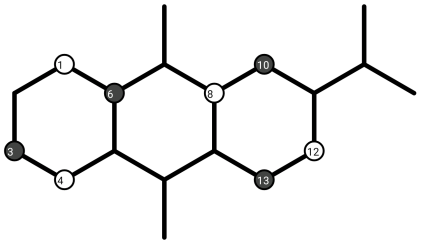

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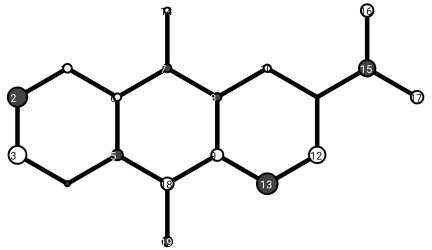

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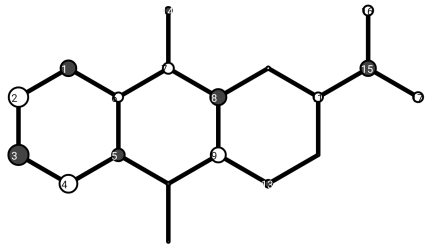

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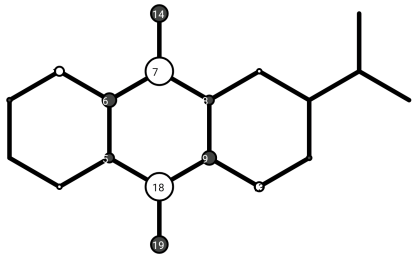

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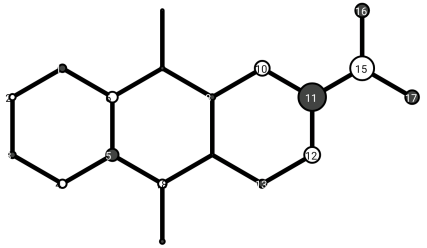

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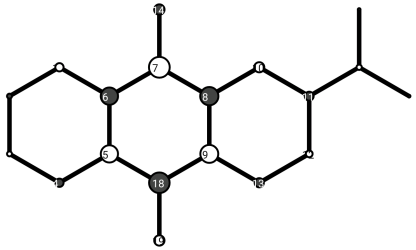
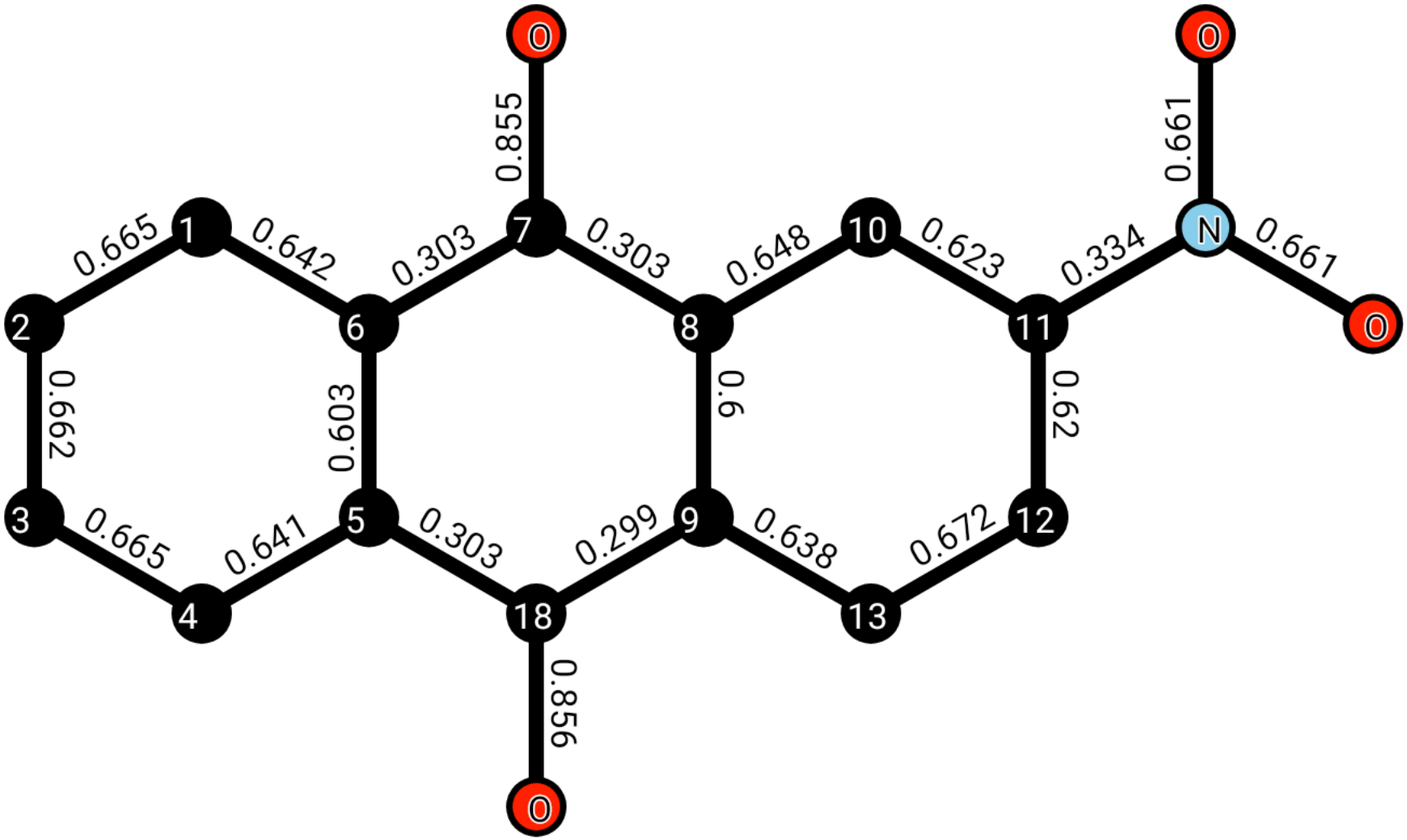


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
1	0.968																		
2	0.665	0.978																	
3	0.028	0.662	0.978																
4	-0.316	0.028	0.665	0.968															
5	-0.032	-0.312	0.017	0.641	0.999														
6	0.642	0.018	-0.312	-0.032	0.603	0.999													
7	0.08	-0.024	-0.06	-0.035	0.062	0.303	0.771												
8	-0.025	0.017	0.021	-0.031	-0.063	-0.001	0.303	1.001											
9	-0.032	0.019	0.017	-0.023	0.001	-0.062	0.061	0.6	0.976										
10	-0.032	0.001	0.029	0.016	-0.034	-0.027	0.082	0.648	-0.005	0.936									
11	-0.001	-0.02	-0.005	0.026	0.021	0.017	-0.022	0.012	-0.293	0.623	0.993								
12	0.028	-0.003	-0.021	-0.003	0.015	0.019	-0.058	-0.305	0.044	-0.003	0.62	0.948							
13	0.018	0.028	-0.001	-0.032	-0.025	-0.032	-0.035	-0.03	0.638	-0.309	0.021	0.672	0.97						
14	-0.175	-0.007	0.12	0.034	-0.147	-0.044	0.855	-0.045	-0.146	-0.176	-0.005	0.119	0.033	1.339					
15	0.0	-0.003	-0.002	0.002	0.006	0.004	-0.005	-0.026	-0.046	0.056	0.334	0.053	-0.027	0.006	1.06				
16	0.0	0.007	0.002	-0.009	-0.008	-0.007	0.007	0.007	0.101	-0.15	-0.076	-0.148	0.005	-0.001	0.661	1.506			
17	0.0	0.007	0.002	-0.009	-0.008	-0.007	0.007	0.007	0.101	-0.15	-0.076	-0.148	0.005	-0.001	0.661	-0.494	1.506		
18	-0.035	-0.06	-0.024	0.081	0.303	0.062	-0.012	0.061	0.299	-0.031	-0.055	-0.021	0.079	-0.044	-0.002	0.017	0.017	0.771	
19	0.034	0.121	-0.007	-0.176	-0.045	-0.148	-0.044	-0.146	-0.034	0.024	0.113	-0.018	-0.173	0.113	0.017	-0.04	-0.04	0.856	1.335

3.2. Presentation of bond order:

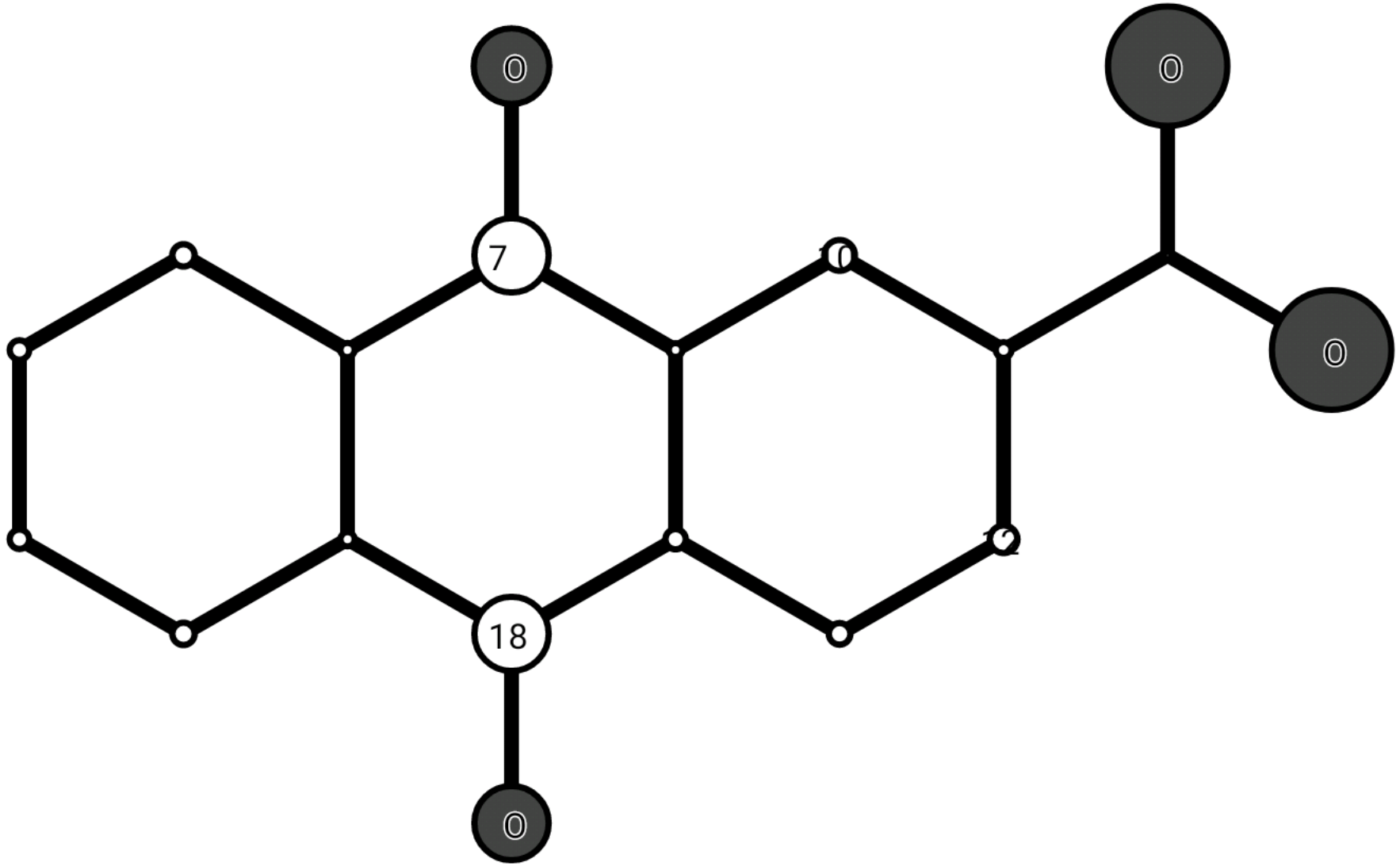

O
0.855
0.661
O
0.665
1
0.642
0.303
7
0.303
0.648
10
0.623
0.334
N
0.661
2
6
8
11
O
0.662
0.603
0.6
0.62
3
0.665
0.641
5
0.303
0.299
9
0.638
0.672
12
4
18
13
0.856
O

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	19
1	0.085																		
2		0.074																	
3			0.074																
4				0.085															
5					0.054														
6						0.054													
7							0.282												
8								0.052											
9									0.077										
10										0.117									
11											0.06								
12												0.105							
13													0.082						
14														-0.287					
15															-0.007				
16																-0.453			
17																	-0.453		
18																		0.282	
19																			-0.282

4.2. Presentation of molecule: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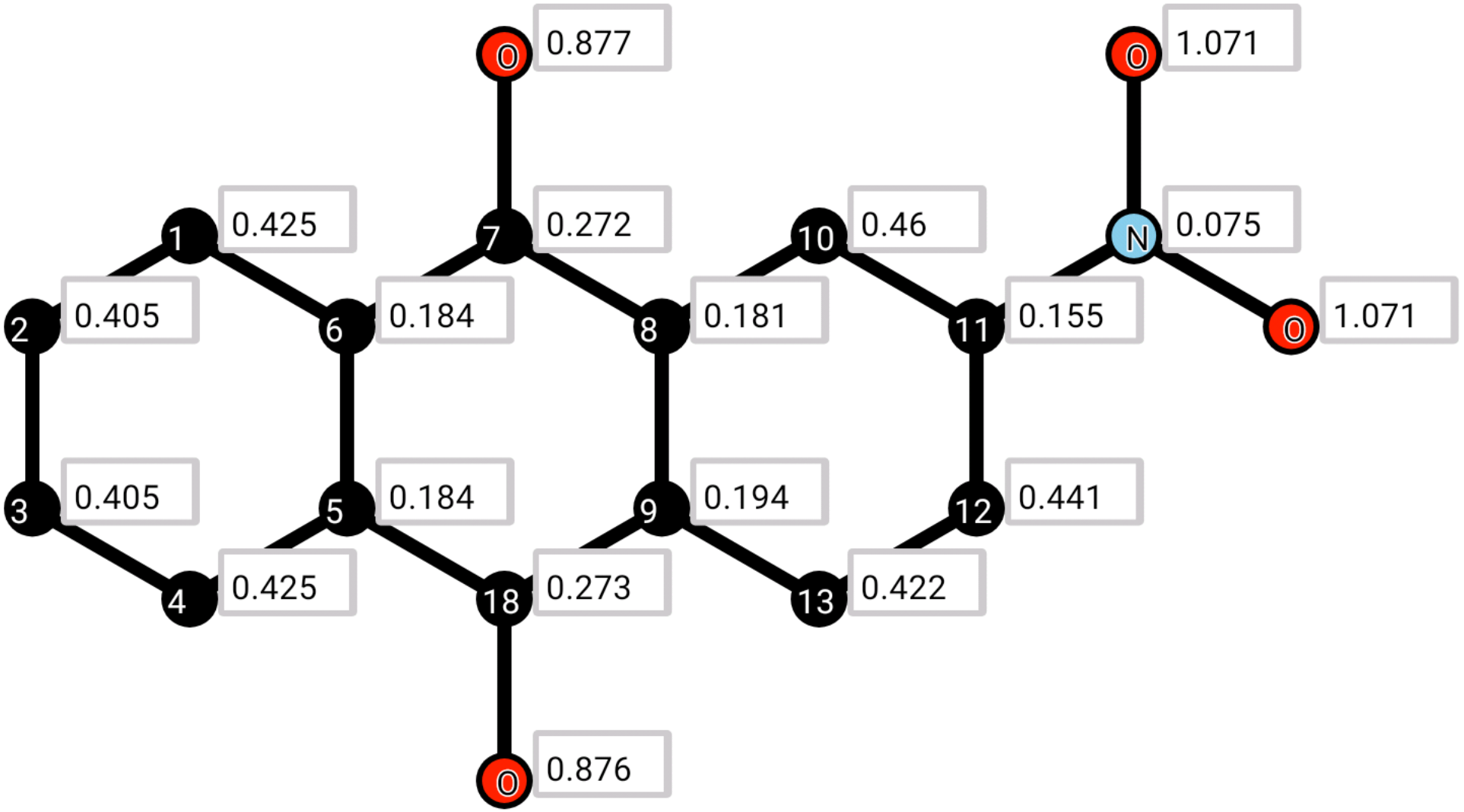
5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
0.425	0.405	0.405	0.425	0.184	0.184	0.272	0.181	0.194	0.46	0.155	0.441	0.422	0.877	0.075	1.071	1.071	0.273	0.876

5.2. Presentation of molecule: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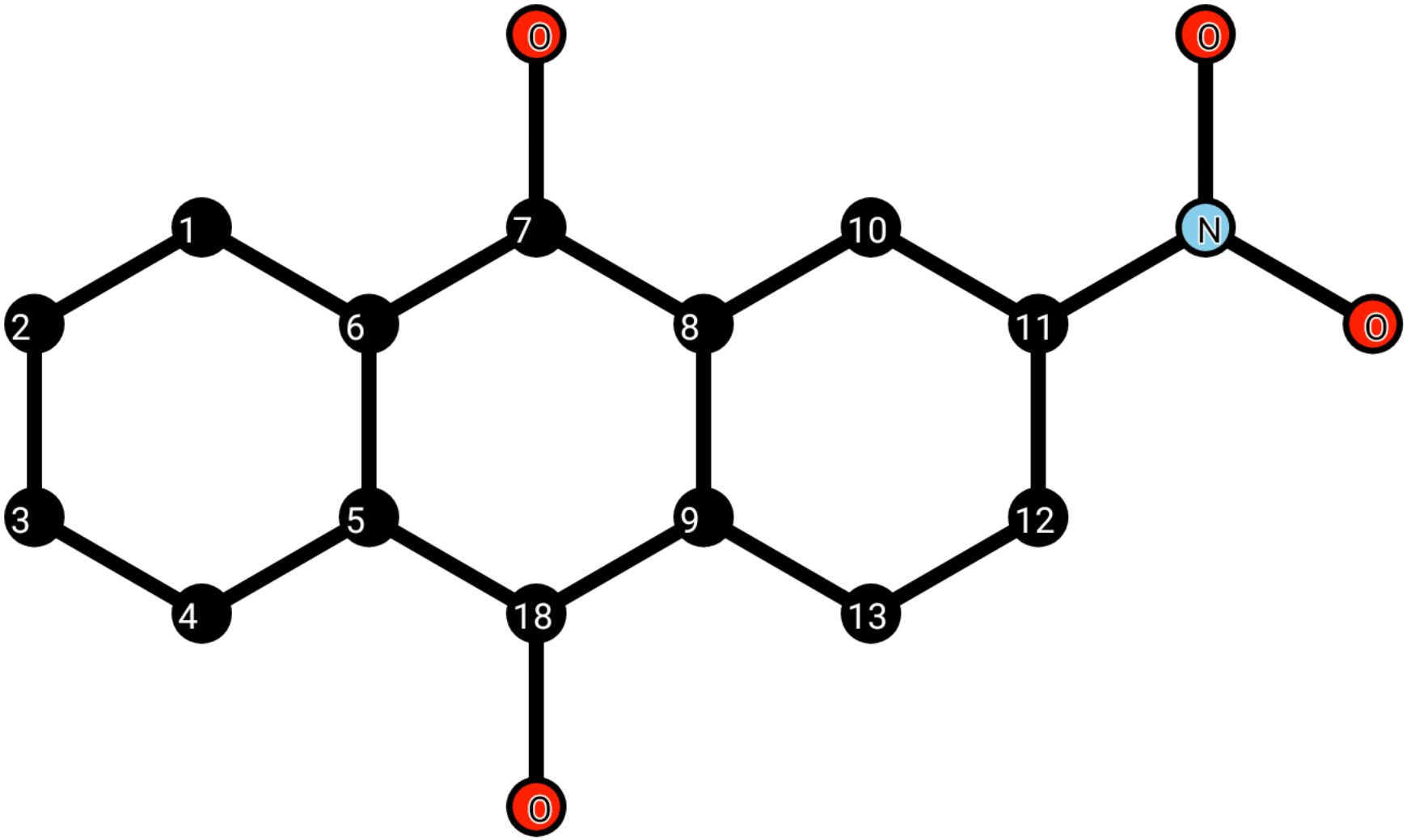
6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
1	0.413																		
2	-0.154	0.405																	
3	0.012	-0.155	0.404																
4	-0.092	0.012	-0.155	0.413															
5	0.003	-0.094	0.01	-0.148	0.371														
6	-0.148	0.01	-0.094	0.003	-0.128	0.371													
7	-0.003	0.0	-0.004	-0.001	-0.001	-0.011	0.206												
8	0.0	-0.001	0.0	-0.001	-0.001	0.0	-0.011	0.369											
9	-0.001	0.0	-0.001	0.0	0.0	-0.001	-0.001	-0.127	0.378										
10	-0.001	0.0	-0.001	0.0	-0.001	0.0	-0.003	-0.151	0.007	0.43									
11	0.0	-0.001	0.0	-0.001	0.0	-0.001	0.0	0.009	-0.086	-0.137	0.351								
12	-0.001	0.0	-0.001	0.0	-0.001	0.0	-0.003	-0.092	0.011	0.008	-0.137	0.422							
13	0.0	-0.001	0.0	-0.001	0.0	-0.001	-0.001	0.003	-0.147	-0.09	0.01	-0.157	0.411						
14	-0.026	0.002	-0.019	-0.002	-0.018	0.018	-0.167	0.018	-0.018	-0.026	0.001	-0.018	-0.001	0.271					
15	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.002	-0.001	-0.013	0.0	0.0	0.0	0.167				
16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.001	-0.012	-0.017	0.012	-0.016	0.001	0.0	-0.075	0.257			
17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.001	-0.012	-0.017	0.012	-0.016	0.001	0.0	-0.075	-0.147	0.257		
18	-0.001	-0.004	0.0	-0.003	-0.011	-0.001	0.0	-0.001	-0.01	0.0	-0.003	0.0	-0.002	-0.001	0.0	0.0	0.0	0.206	
19	-0.002	-0.019	0.002	-0.026	0.018	-0.018	-0.001	-0.018	0.02	0.0	-0.017	0.001	-0.025	-0.014	0.0	-0.002	-0.002	-0.168	0.272

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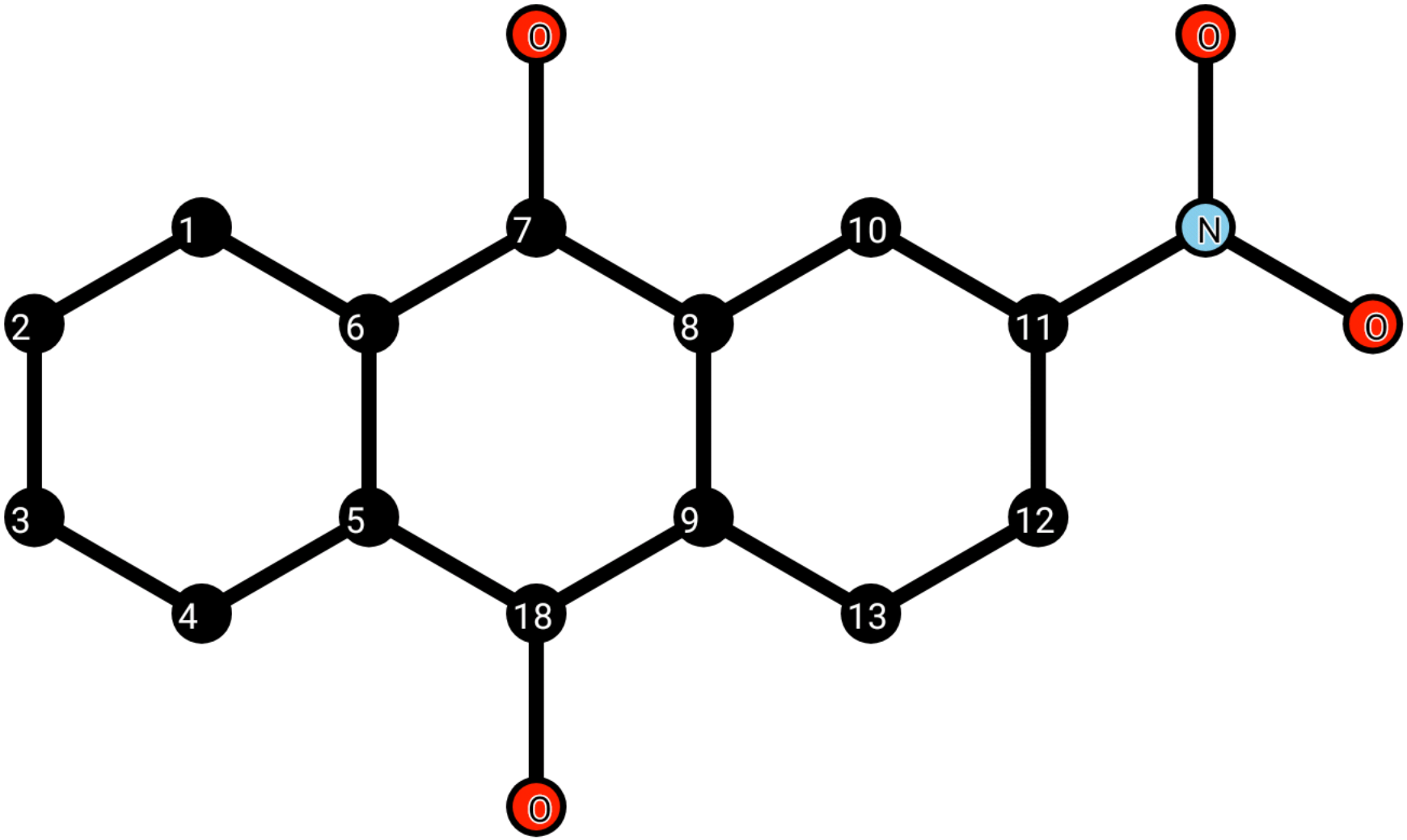
7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
1 2	0.016	0.012	-0.011	0.011	-0.013	-0.007	0.002	0.0	0.001	0.0	0.0	0.0	-0.001	-0.001	0.0	0.0	0.0	-0.002	-0.006
1 6	0.007	-0.009	0.009	-0.012	0.015	-0.002	-0.007	0.0	-0.002	-0.001	0.0	-0.001	0.001	-0.006	0.0	0.0	0.0	0.002	0.006
2 3	-0.013	0.007	0.006	-0.013	0.006	0.006	-0.001	0.0	0.0	0.0	0.0	0.0	0.0	0.002	0.0	0.0	0.0	-0.001	0.002
3 4	0.011	-0.011	0.012	0.016	-0.007	-0.013	-0.002	0.001	0.0	-0.001	0.0	0.0	0.0	-0.006	0.0	0.0	0.0	0.002	-0.001
4 5	-0.012	0.009	-0.009	0.007	-0.002	0.015	0.002	-0.002	0.0	0.001	-0.001	0.0	-0.001	0.006	0.0	0.0	0.0	-0.007	-0.006
5 6	0.014	0.006	0.006	0.015	-0.007	-0.007	-0.006	0.0	0.0	-0.001	0.0	0.0	-0.001	-0.007	0.0	0.0	0.0	-0.006	-0.007
5 18	-0.001	-0.022	0.002	-0.03	0.023	-0.022	0.001	0.004	-0.002	-0.001	0.002	0.0	0.002	-0.006	0.0	0.0	0.0	0.026	0.026
6 7	-0.03	0.002	-0.022	-0.001	-0.022	0.023	0.026	-0.002	0.004	0.002	0.0	0.002	-0.001	0.025	0.0	0.0	0.0	0.001	-0.006
7 8	0.002	0.0	0.002	-0.001	0.004	-0.002	0.026	0.023	-0.021	-0.031	0.002	-0.021	-0.001	0.026	0.0	0.0	0.0	0.001	-0.006
7 14	0.012	-0.001	0.009	0.001	0.008	-0.005	0.038	-0.004	0.007	0.012	-0.001	0.009	0.001	-0.091	0.0	0.0	0.0	0.0	0.006
8 9	-0.001	0.0	0.0	-0.001	0.0	0.0	-0.006	-0.009	0.001	0.002	0.003	0.016	0.014	-0.007	-0.001	-0.001	-0.001	-0.006	-0.005
8 10	-0.001	0.0	-0.001	0.001	-0.002	0.0	-0.007	-0.001	0.004	0.023	-0.005	-0.003	-0.012	-0.006	0.001	0.001	0.001	0.002	0.004
9 13	0.001	-0.001	0.0	0.0	0.0	-0.002	0.002	0.014	0.006	-0.002	0.006	-0.022	0.004	0.006	-0.001	0.0	0.0	-0.007	-0.004
9 18	-0.001	0.002	0.0	0.002	-0.002	0.004	0.001	-0.021	0.026	0.0	-0.019	0.003	-0.029	-0.006	0.0	-0.002	-0.002	0.026	0.022
10 11	0.0	0.0	0.0	-0.001	0.001	0.0	0.001	-0.005	-0.004	0.021	-0.001	0.004	0.008	-0.001	-0.004	-0.007	-0.007	-0.001	-0.004
11 12	0.0	0.0	0.0	0.0	0.0	0.0	-0.001	0.004	0.014	0.002	-0.005	0.012	-0.011	0.001	-0.004	-0.008	-0.008	-0.001	0.003
11 15	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.001	-0.016	-0.023	0.009	-0.021	0.002	0.0	0.005	0.024	0.024	0.0	-0.003
12 13	-0.001	0.0	0.0	0.0	0.0	0.001	-0.002	-0.013	-0.017	-0.002	-0.007	0.028	0.017	-0.006	0.001	0.001	0.001	0.001	-0.003
15 16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.006	0.007	0.001	0.006	0.0	0.0	-0.008	-0.133	0.12	0.0	0.001
15 17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.006	0.007	0.001	0.006	0.0	0.0	-0.008	0.12	-0.133	0.0	0.001
18 19	0.001	0.009	-0.001	0.012	-0.004	0.008	0.0	0.007	-0.006	0.0	0.008	-0.001	0.011	0.006	0.0	0.001	0.001	0.038	-0.09

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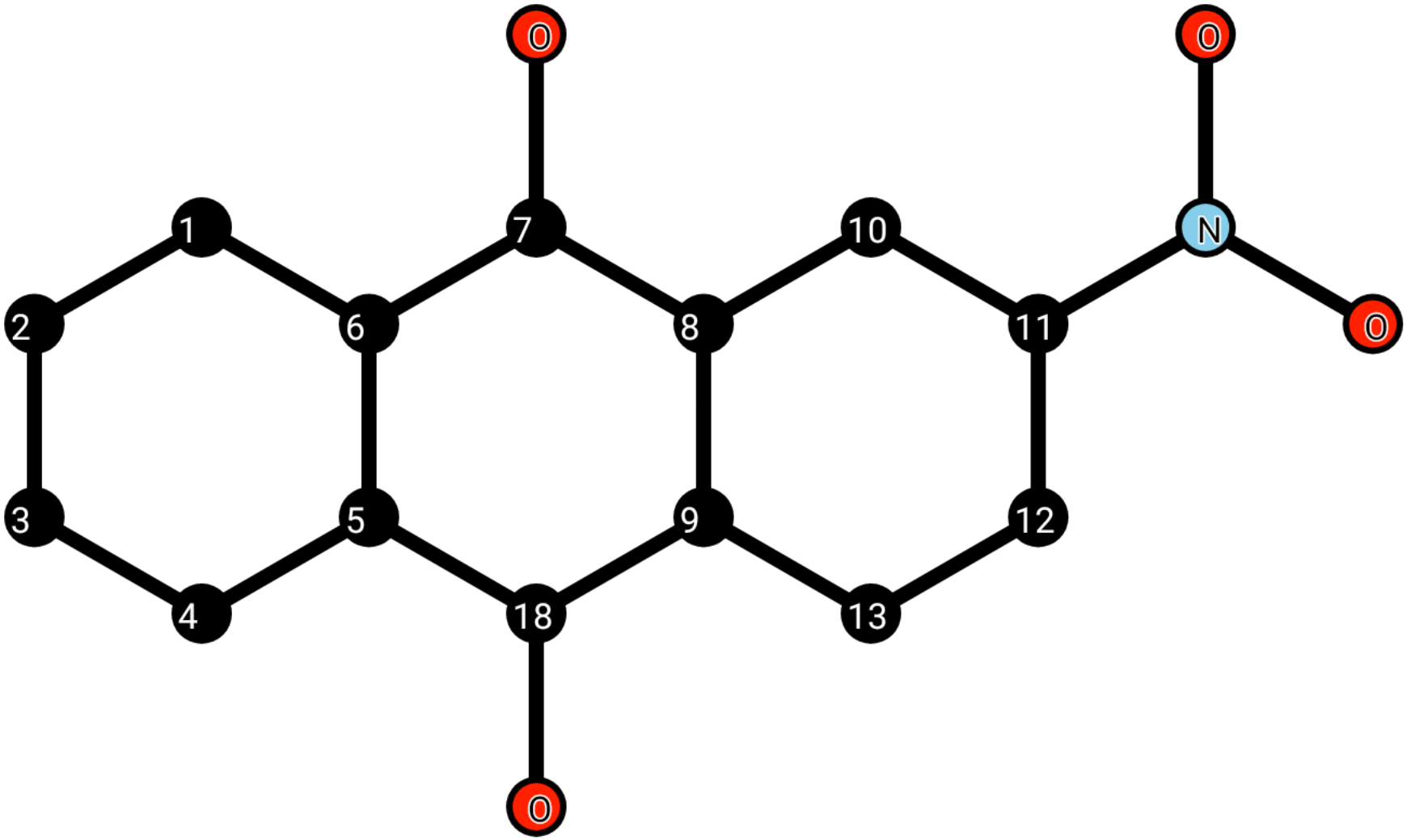
8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	2 3	3 4	4 5	5 6	5 18	6 7	7 8	7 14	8 9	8 10	9 13	9 18	10 11	11 12	11 15	12 13	15 16	15 17	18 19
1 2	0.254																				
1 6	-0.201	0.243																			
2 3	-0.208	0.124	0.249																		
3 4	0.125	-0.084	-0.208	0.254																	
4 5	-0.084	0.108	0.124	-0.201	0.244																
5 6	0.12	-0.172	-0.084	0.12	-0.172	0.242															
5 18	-0.014	0.017	-0.004	0.009	-0.064	-0.059	0.284														
6 7	0.008	-0.063	-0.004	-0.014	0.017	-0.058	-0.004	0.283													
7 8	-0.002	0.004	0.001	-0.001	0.0	0.005	0.0	-0.024	0.283												
7 14	-0.003	0.02	0.001	0.007	-0.007	0.018	0.002	-0.091	-0.091	0.108											
8 9	0.001	-0.001	0.0	0.001	-0.001	0.0	0.005	0.005	-0.059	0.018	0.248										
8 10	0.001	-0.001	-0.001	0.001	0.0	-0.001	0.0	0.004	-0.064	0.02	-0.178	0.249									
9 13	0.001	0.0	-0.001	0.001	-0.001	-0.001	0.003	0.0	0.017	-0.007	-0.174	0.109	0.248								
9 18	-0.001	0.0	0.001	-0.002	0.003	0.005	-0.023	0.0	-0.004	0.002	-0.055	0.014	-0.06	0.281							
10 11	-0.001	0.001	0.001	-0.001	0.001	0.001	-0.001	-0.002	0.008	-0.002	0.116	-0.19	-0.079	-0.01	0.253						
11 12	0.001	-0.001	-0.001	0.001	-0.001	0.0	0.001	0.001	-0.004	0.001	-0.079	0.114	0.119	0.0	-0.176	0.249					
11 15	0.0	0.0	0.0	0.0	0.0	0.0	0.001	0.0	0.0	0.0	-0.005	0.009	-0.005	-0.005	-0.06	-0.06	0.231				
12 13	-0.001	0.001	0.001	-0.001	0.001	0.001	-0.002	-0.001	-0.014	0.007	0.121	-0.085	-0.207	0.005	0.116	-0.197	0.01	0.26			
15 16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.002	-0.003	0.002	0.002	0.017	0.017	-0.063	-0.004	0.189		
15 17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.002	-0.003	0.002	0.002	0.017	0.017	-0.063	-0.004	-0.15	0.189	
18 19	0.007	-0.007	0.001	-0.003	0.021	0.018	-0.092	0.003	0.002	-0.002	0.017	-0.006	0.019	-0.089	0.005	0.0	0.002	-0.001	-0.001	-0.001	0.107

8.2. Presentation of molecule: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