Print calculated values

Report generated by:root, 16.05.2020 - 18:51:08

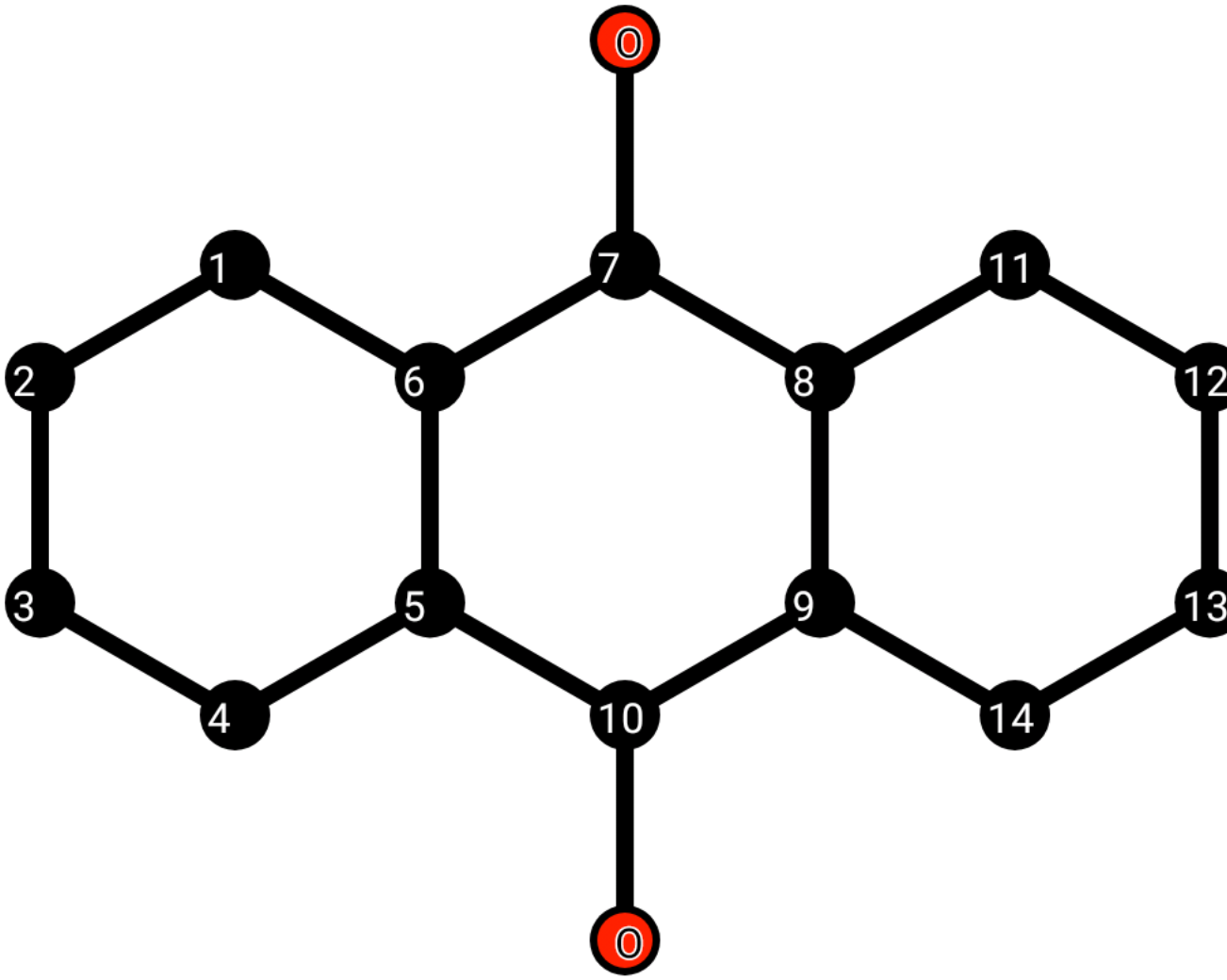
The following determinant is calculated:

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

It is about this molecule:

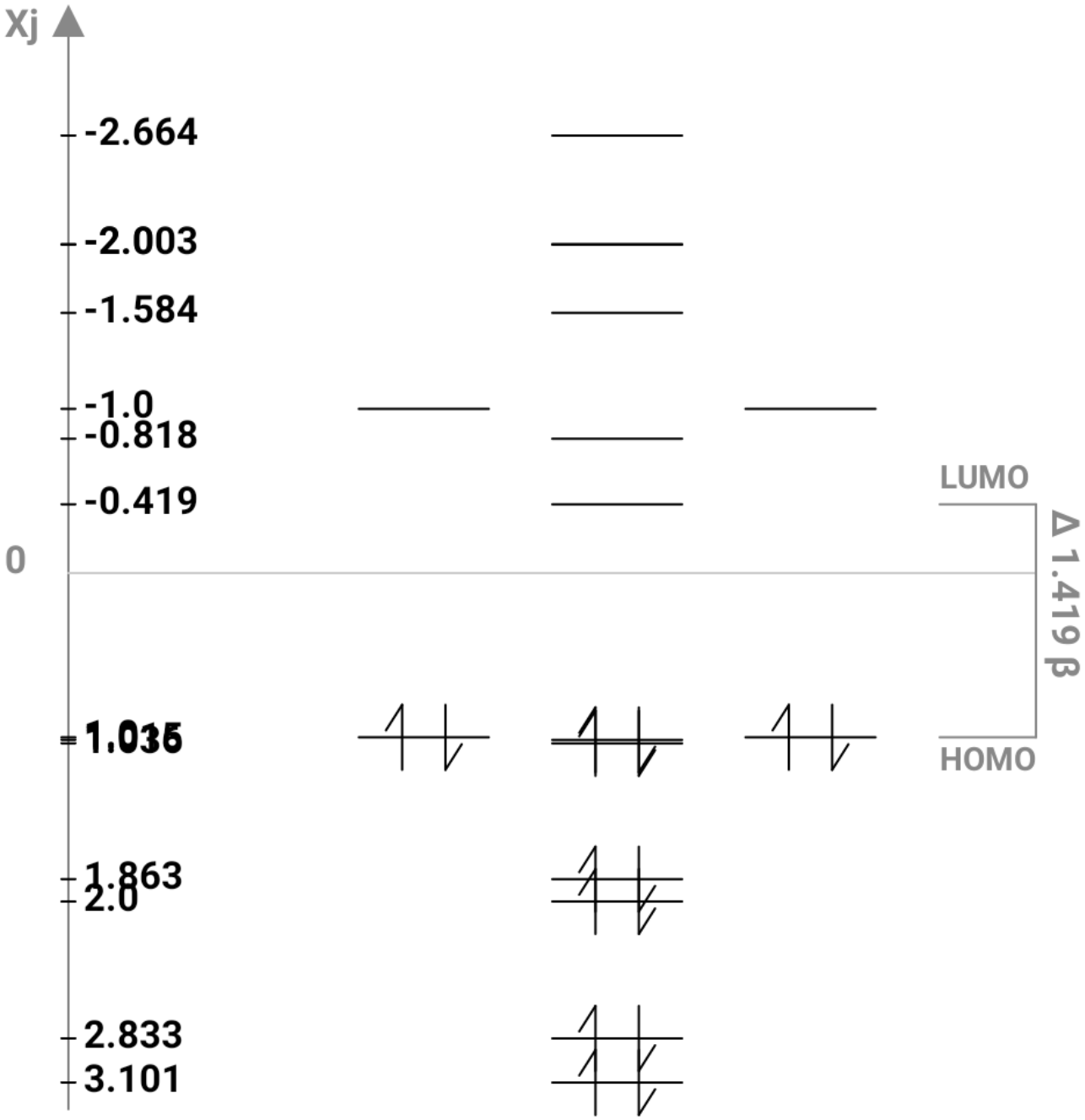
HMO-Energies

x1 = 3.101; x2 = 2.833; x3 = 2.0; x4 = 1.863; x5 = 1.036; x6 = 1.015; x7 = 1.0; x8 = 1.0;
x9 = -0.419; x10 = -0.818; x11 = -1.0; x12 = -1.0; x13 = -1.584; x14 = -2.0; x15 = -2.003; x16 = -2.664;


0
1
7
11
2
6
8
12
3
5
9
13
4
10
14
0

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 16α + 27.696β -

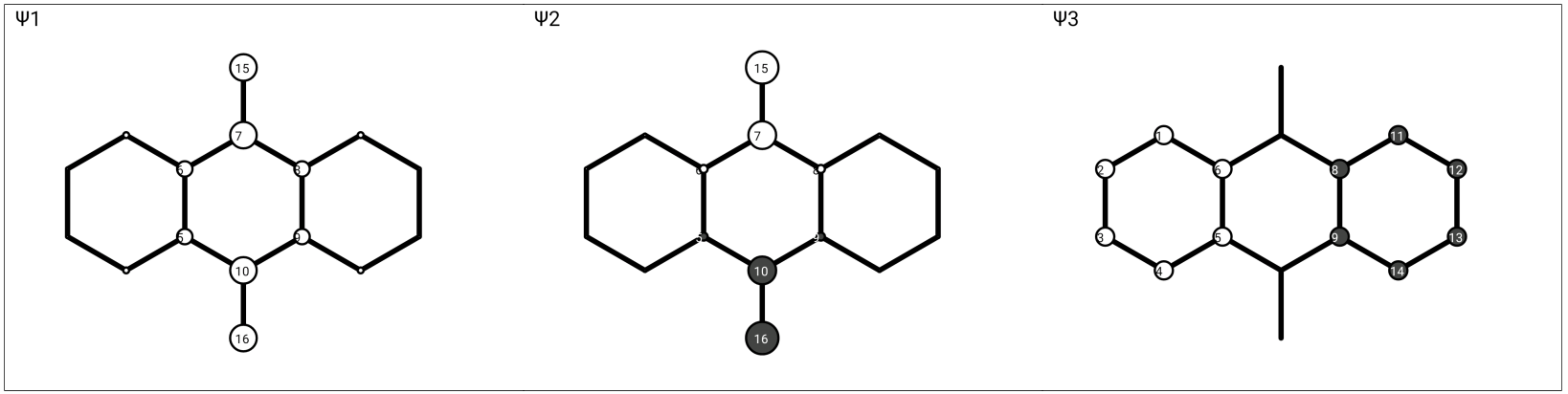
this corresponds to one πelectron: 1.731β

2. Hueckel-coefficient

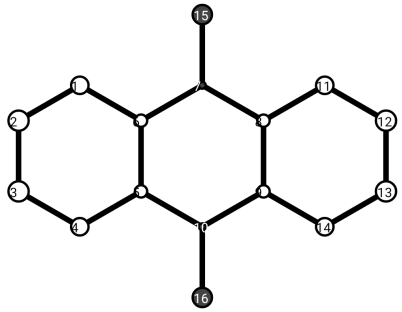
2.1. Calculated values:

	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
	x1= 3.101	x2= 2.833	x3= 2.0	x4= 1.863	x5= 1.036	x6= 1.015	x7= 1.0	x8= 1.0	x9= -0.419	x10= -0.818	x11= -1.0	x12= -1.0	x13= -1.584	x14= -2.0	x15= -2.003	x16= -2.664
1	0.093	0.05	0.289	0.266	0.012	0.389	0.108	-0.394	0.13	0.392	0.388	-0.128	-0.228	-0.289	-0.129	-0.164
2	0.044	0.013	0.289	0.308	0.323	0.193	0.395	-0.103	0.224	-0.216	-0.083	0.4	0.39	0.289	0.043	0.098
3	0.044	-0.013	0.289	0.308	0.323	-0.193	0.287	0.29	-0.224	-0.216	-0.305	-0.272	-0.39	-0.289	0.043	-0.098
4	0.093	-0.05	0.289	0.266	0.012	-0.389	-0.108	0.394	-0.13	0.392	0.388	-0.128	0.228	0.289	-0.129	0.164
5	0.245	-0.128	0.289	0.187	-0.311	-0.202	-0.395	0.103	0.279	-0.105	-0.083	0.4	0.029	-0.289	0.216	-0.338
6	0.245	0.128	0.289	0.187	-0.311	0.202	-0.287	-0.29	-0.279	-0.105	-0.305	-0.272	-0.029	0.289	0.216	0.338
7	0.422	0.442	0.0	-0.104	-0.023	0.017	0.0	0.0	-0.292	-0.201	0.0	0.0	0.245	0.0	-0.52	-0.399
8	0.245	0.128	-0.289	0.187	-0.311	0.202	0.287	0.29	-0.279	-0.105	0.305	0.272	-0.029	-0.289	0.216	0.338
9	0.245	-0.128	-0.289	0.187	-0.311	-0.202	0.395	-0.103	0.279	-0.105	0.083	-0.4	0.029	0.289	0.216	-0.338
10	0.422	-0.442	0.0	-0.104	-0.023	-0.017	0.0	0.0	0.292	-0.201	0.0	0.0	-0.245	0.0	-0.52	0.399
11	0.093	0.05	-0.289	0.266	0.012	0.389	-0.108	0.394	0.13	0.392	-0.388	0.128	-0.228	0.289	-0.129	-0.164
12	0.044	0.013	-0.289	0.308	0.323	0.193	-0.395	0.103	0.224	-0.216	0.083	-0.4	0.39	-0.289	0.043	0.098
13	0.044	-0.013	-0.289	0.308	0.323	-0.193	-0.287	-0.29	-0.224	-0.216	0.305	0.272	-0.39	0.289	0.043	-0.098
14	0.093	-0.05	-0.289	0.266	0.012	-0.389	0.108	-0.394	-0.13	0.392	-0.388	0.128	0.228	-0.289	-0.129	0.164
15	0.424	0.516	0.0	-0.295	0.31	-0.2	0.0	0.0	0.353	0.194	0.0	0.0	-0.171	0.0	0.315	0.2
16	0.424	-0.516	0.0	-0.295	0.31	0.2	0.0	0.0	-0.353	0.194	0.0	0.0	0.171	0.0	0.315	-0.2

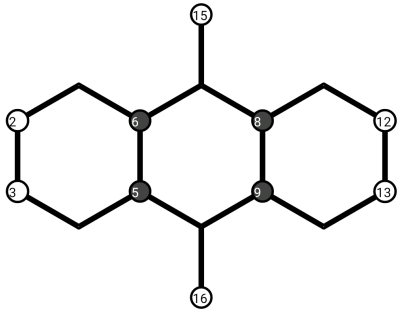
2.2. Molecule orbital presentation:



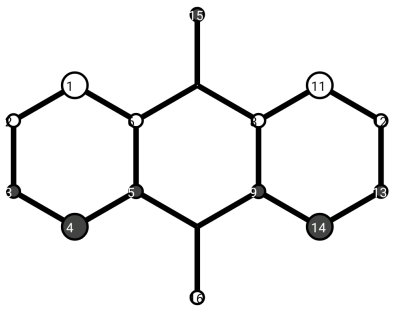
Ψ4



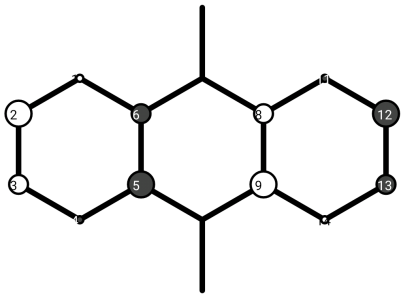
Ψ5



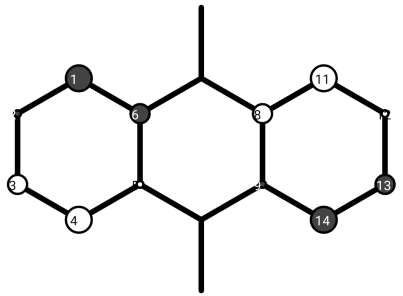
Ψ6



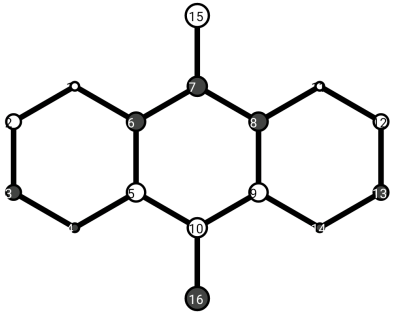
Ψ7



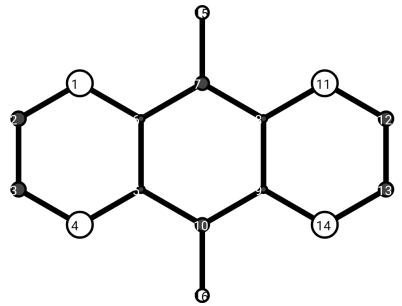
Ψ8



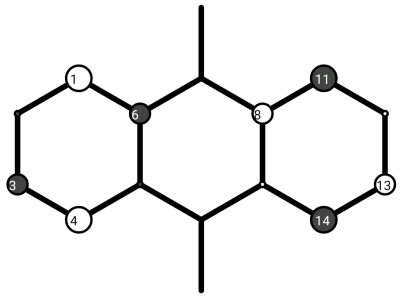
Ψ9



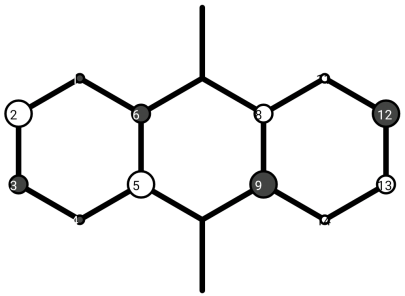
Ψ10



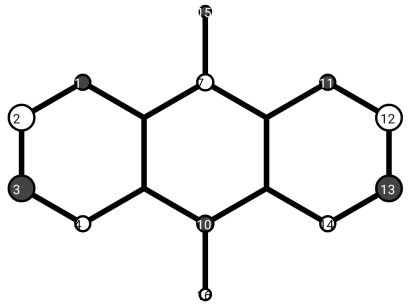
Ψ11



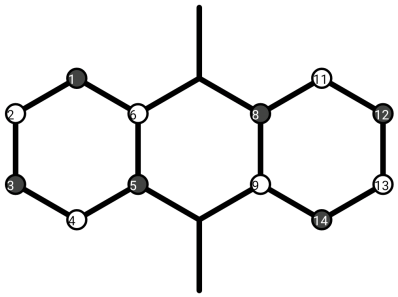
Ψ12



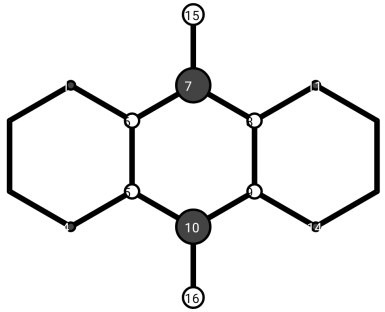
Ψ13



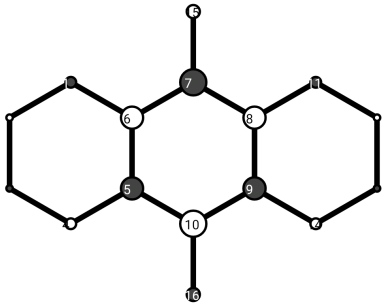
Ψ14



Ψ15



Ψ16

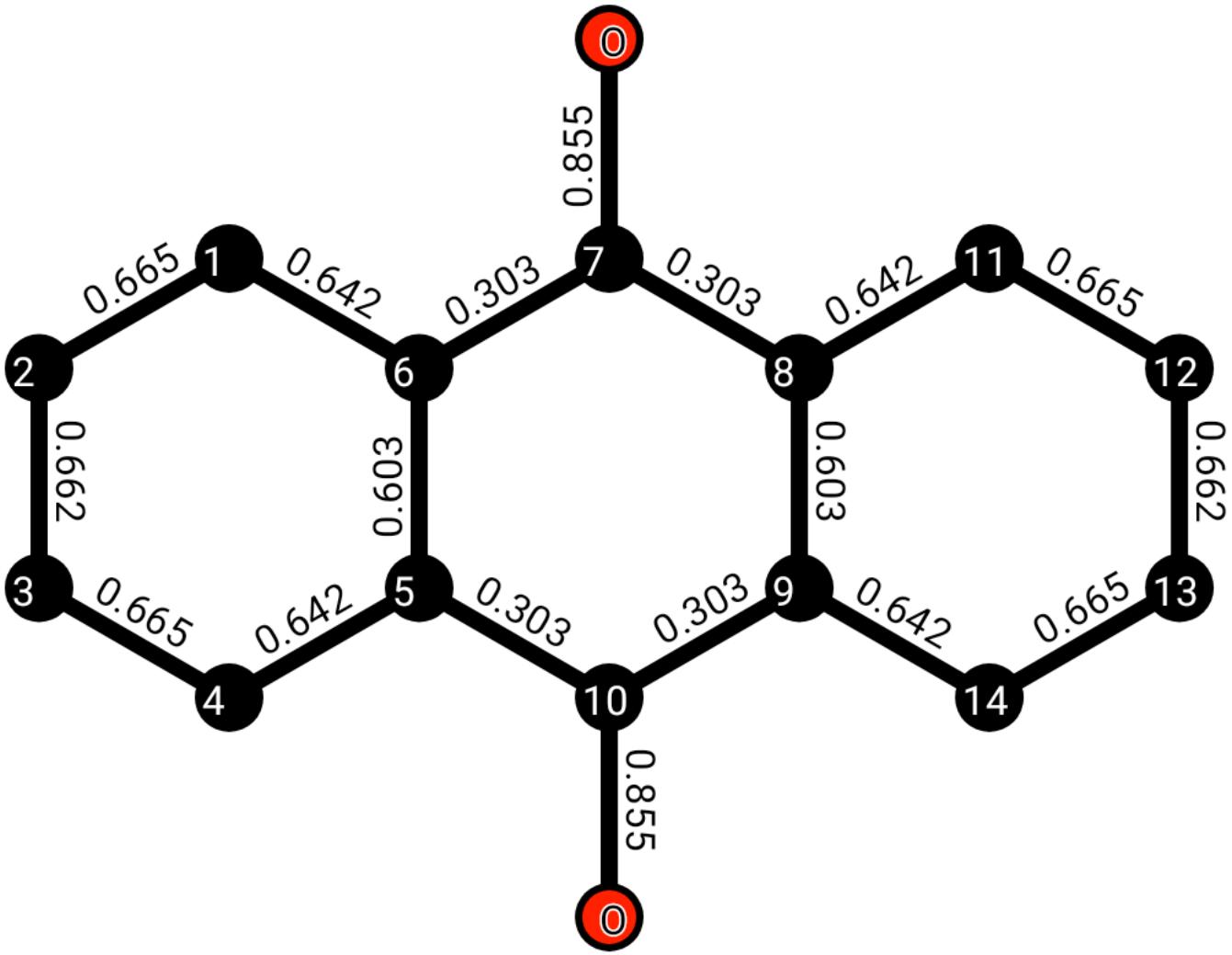


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
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	0.642	0.999											
6	0.642	0.017	-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	-0.032	-0.063	-0.001	0.303	0.999								
9	-0.032	0.021	0.017	-0.025	-0.001	-0.063	0.062	0.603	0.999							
10	-0.035	-0.06	-0.024	0.08	0.303	0.062	-0.012	0.062	0.303	0.771						
11	-0.032	-0.001	0.028	0.018	-0.032	-0.025	0.08	0.642	-0.032	-0.035	0.968					
12	-0.001	-0.022	-0.005	0.028	0.021	0.017	-0.024	0.017	-0.312	-0.06	0.665	0.978				
13	0.028	-0.005	-0.022	-0.001	0.017	0.021	-0.06	-0.312	0.017	-0.024	0.028	0.662	0.978			
14	0.018	0.028	-0.001	-0.032	-0.025	-0.032	-0.035	-0.032	0.642	0.08	-0.316	0.028	0.665	0.968		
15	-0.175	-0.008	0.12	0.034	-0.147	-0.044	0.855	-0.044	-0.147	-0.044	-0.175	-0.008	0.12	0.034	1.339	
16	0.034	0.12	-0.008	-0.175	-0.044	-0.147	-0.044	-0.147	-0.044	0.855	0.034	0.12	-0.008	-0.175	0.113	1.339

3.2. Presentation of bond order:

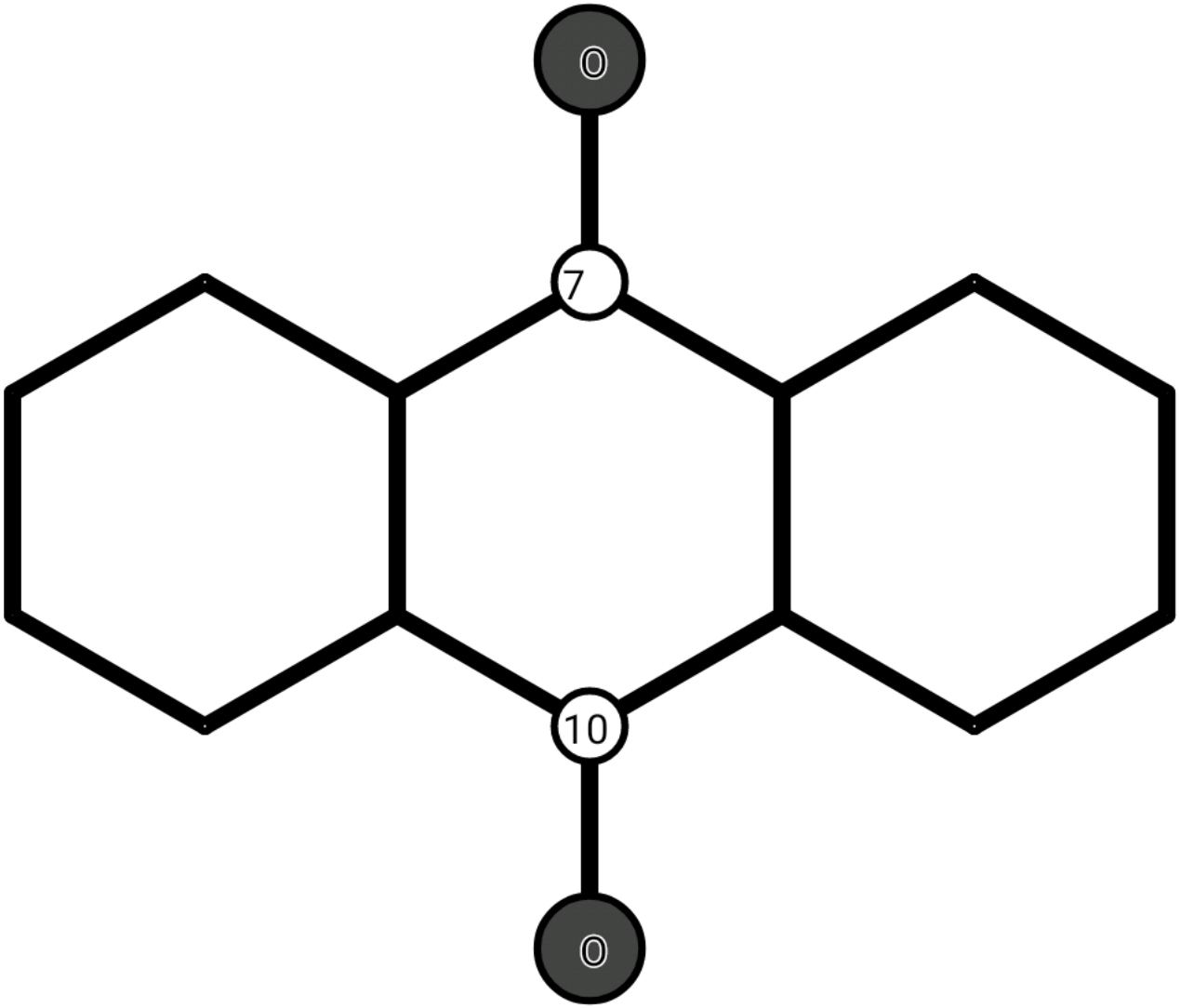

0
0.855
1
0.665
0.642
0.303
7
0.303
0.642
11
0.665
2
6
8
12
0.662
0.603
0.603
0.662
3
0.665
0.642
5
0.303
0.303
9
0.642
0.665
13
4
10
14
0.855
0

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.032															
2		0.022														
3			0.022													
4				0.032												
5					0.001											
6						0.001										
7							0.229									
8								0.001								
9									0.001							
10										0.229						
11											0.032					
12												0.022				
13													0.022			
14														0.032		
15															-0.339	
16																-0.339

4.2. Presentation of molecule:

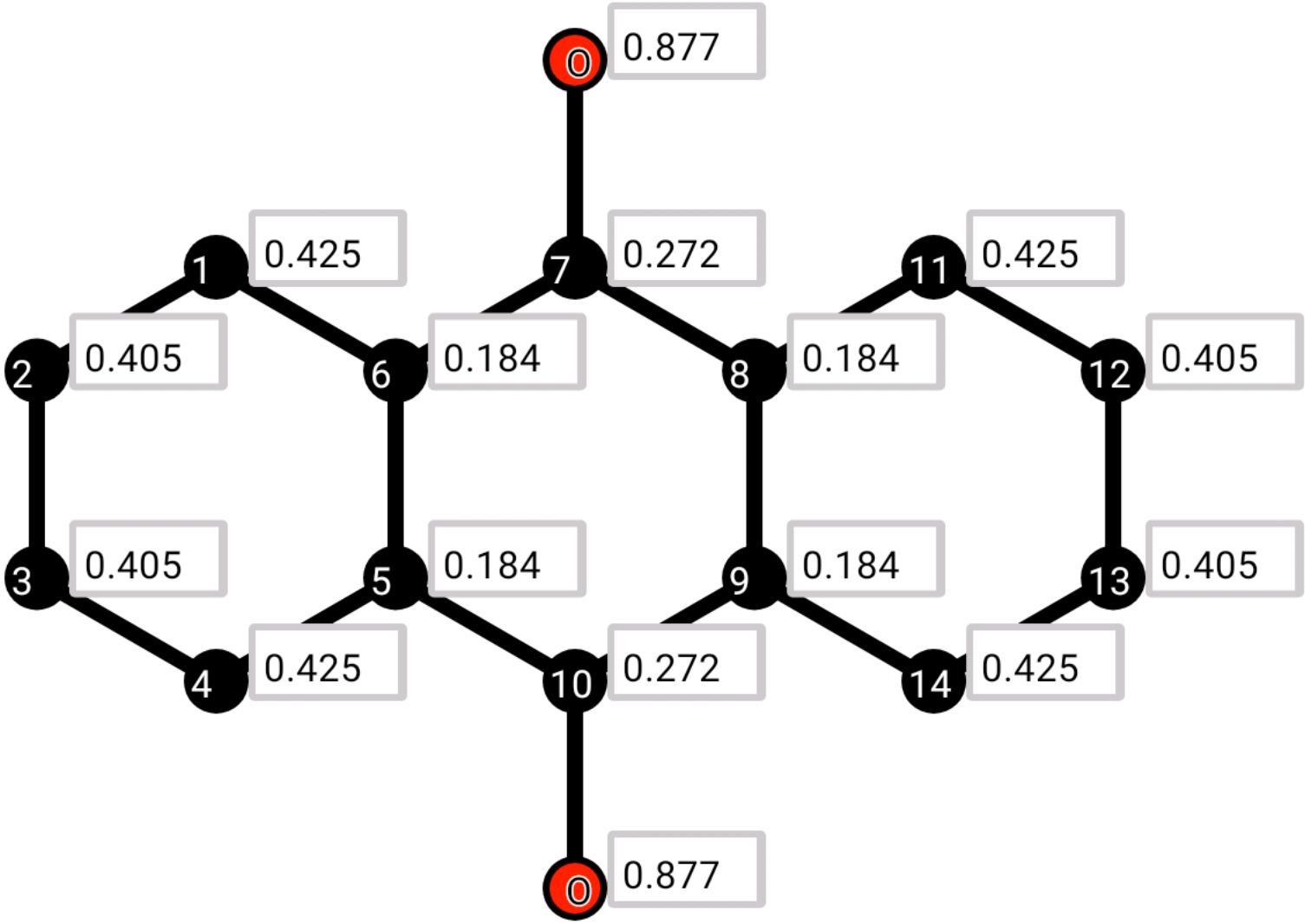

0
7
10
0

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
0.425	0.405	0.405	0.425	0.184	0.184	0.272	0.184	0.184	0.272	0.425	0.405	0.405	0.425	0.877	0.877

5.2. Presentation of molecule:

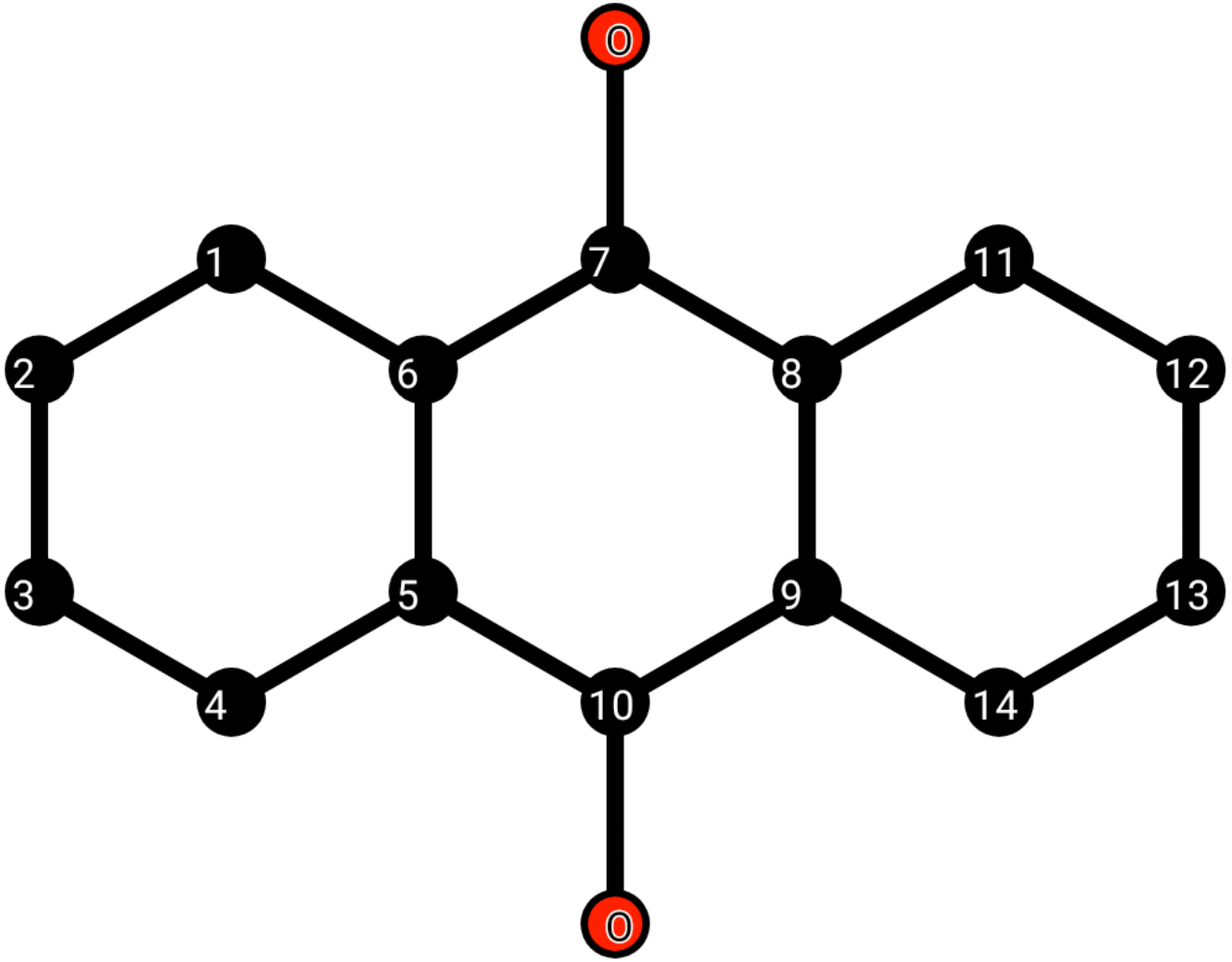

0
0.877
1
0.425
7
0.272
11
0.425
2
0.405
6
0.184
8
0.184
12
0.405
3
0.405
5
0.184
9
0.184
13
0.405
4
0.425
10
0.272
14
0.425
0
0.877

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.413															
2	-0.154	0.405														
3	0.012	-0.155	0.405													
4	-0.092	0.012	-0.154	0.413												
5	0.003	-0.094	0.01	-0.148	0.371											
6	-0.148	0.01	-0.094	0.003	-0.129	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	0.371								
9	-0.001	0.0	-0.001	0.0	0.0	-0.001	-0.001	-0.129	0.371							
10	-0.001	-0.004	0.0	-0.003	-0.011	-0.001	0.0	-0.001	-0.011	0.206						
11	-0.001	0.0	-0.001	0.0	-0.001	0.0	-0.003	-0.148	0.003	-0.001	0.413					
12	0.0	-0.001	0.0	-0.001	0.0	-0.001	0.0	0.01	-0.094	-0.004	-0.154	0.405				
13	-0.001	0.0	-0.001	0.0	-0.001	0.0	-0.004	-0.094	0.01	0.0	0.012	-0.155	0.405			
14	0.0	-0.001	0.0	-0.001	0.0	-0.001	-0.001	0.003	-0.148	-0.003	-0.092	0.012	-0.154	0.413		
15	-0.026	0.002	-0.019	-0.002	-0.018	0.018	-0.167	0.018	-0.018	-0.001	-0.026	0.002	-0.019	-0.002	0.271	
16	-0.002	-0.019	0.002	-0.026	0.018	-0.018	-0.001	-0.018	0.018	-0.167	-0.002	-0.019	0.002	-0.026	-0.015	0.271

6.2. Presentation of molecule:

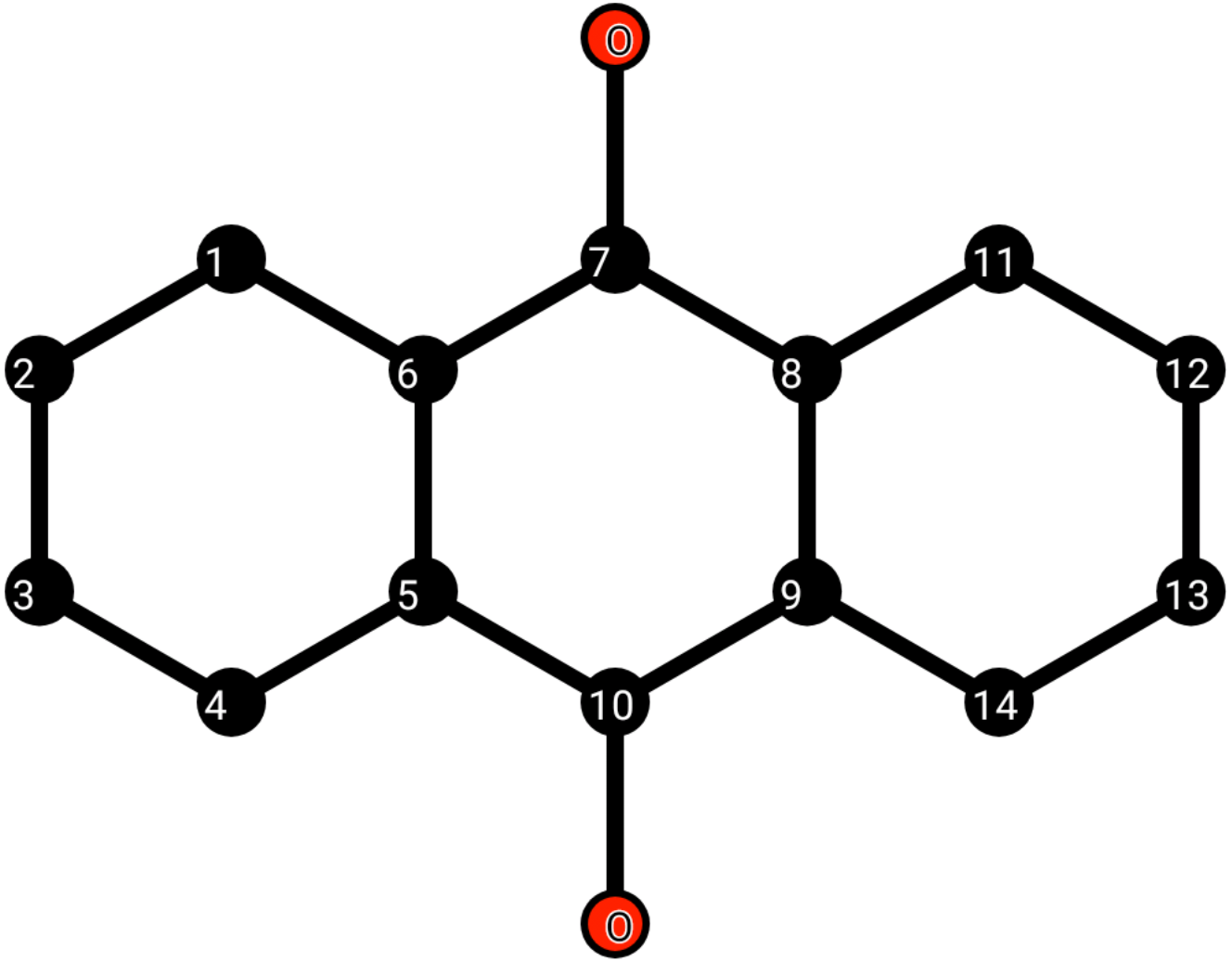

0
1
7
11
2
6
8
12
3
5
9
13
4
10
14
0

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1 2	0.016	0.012	-0.011	0.011	-0.013	-0.007	0.002	0.0	0.001	-0.002	0.0	0.0	0.0	-0.001	-0.001	-0.006
1 6	0.007	-0.009	0.009	-0.012	0.015	-0.002	-0.007	0.0	-0.002	0.002	-0.001	0.0	-0.001	0.001	-0.006	0.006
2 3	-0.013	0.006	0.006	-0.013	0.006	0.006	-0.001	0.0	0.0	-0.001	0.0	0.0	0.0	0.0	0.002	0.002
3 4	0.011	-0.011	0.012	0.016	-0.007	-0.013	-0.002	0.001	0.0	0.002	-0.001	0.0	0.0	0.0	-0.006	-0.001
4 5	-0.012	0.009	-0.009	0.007	-0.002	0.015	0.002	-0.002	0.0	-0.007	0.001	-0.001	0.0	-0.001	0.006	-0.006
5 6	0.014	0.006	0.006	0.014	-0.007	-0.007	-0.006	0.0	0.0	-0.006	-0.001	0.0	0.0	-0.001	-0.007	-0.007
5 10	-0.001	-0.022	0.002	-0.03	0.023	-0.022	0.001	0.004	-0.002	0.026	-0.001	0.002	0.0	0.002	-0.006	0.025
6 7	-0.03	0.002	-0.022	-0.001	-0.022	0.023	0.026	-0.002	0.004	0.001	0.002	0.0	0.002	-0.001	0.025	-0.006
7 8	0.002	0.0	0.002	-0.001	0.004	-0.002	0.026	0.023	-0.022	0.001	-0.03	0.002	-0.022	-0.001	0.025	-0.006
7 15	0.012	-0.001	0.009	0.001	0.008	-0.005	0.038	-0.005	0.008	0.0	0.012	-0.001	0.009	0.001	-0.091	0.006
8 9	-0.001	0.0	0.0	-0.001	0.0	0.0	-0.006	-0.007	-0.007	-0.006	0.014	0.006	0.006	0.014	-0.007	-0.007
8 11	-0.001	0.0	-0.001	0.001	-0.002	0.0	-0.007	-0.002	0.015	0.002	0.007	-0.009	0.009	-0.012	-0.006	0.006
9 10	-0.001	0.002	0.0	0.002	-0.002	0.004	0.001	-0.022	0.023	0.026	-0.001	-0.022	0.002	-0.03	-0.006	0.025
9 14	0.001	-0.001	0.0	-0.001	0.0	-0.002	0.002	0.015	-0.002	-0.007	-0.012	0.009	-0.009	0.007	0.006	-0.006
10 16	0.001	0.009	-0.001	0.012	-0.005	0.008	0.0	0.008	-0.005	0.038	0.001	0.009	-0.001	0.012	0.006	-0.091
11 12	0.0	0.0	0.0	-0.001	0.001	0.0	0.002	-0.007	-0.013	-0.002	0.016	0.012	-0.011	0.011	-0.001	-0.006
12 13	0.0	0.0	0.0	0.0	0.0	0.0	-0.001	0.006	0.006	-0.001	-0.013	0.006	0.006	-0.013	0.002	0.002
13 14	-0.001	0.0	0.0	0.0	0.0	0.001	-0.002	-0.013	-0.007	0.002	0.011	-0.011	0.012	0.016	-0.006	-0.001

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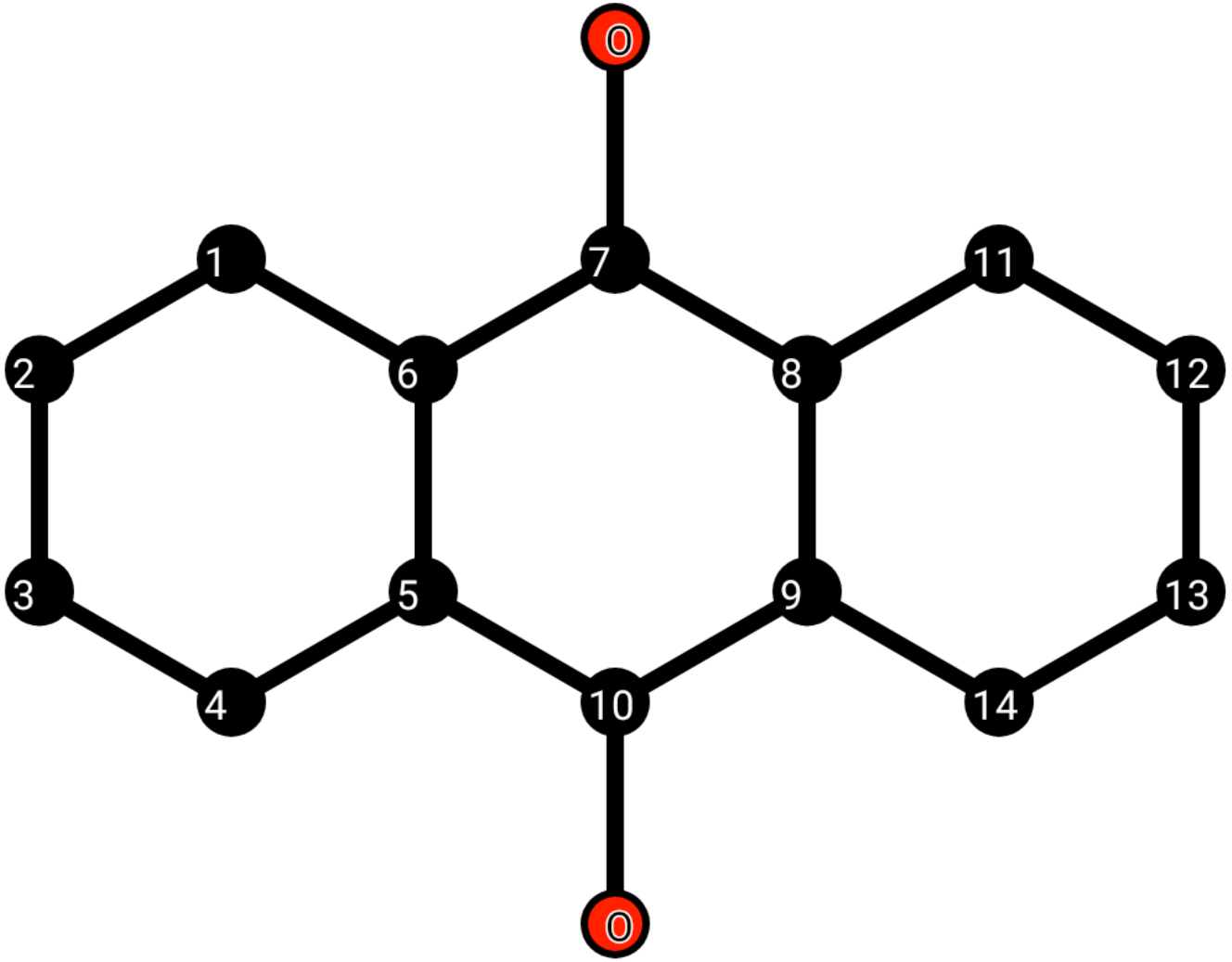
8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	2 3	3 4	4 5	5 6	5 10	6 7	7 8	7 15	8 9	8 11	9 10	9 14	10 16	11 12	12 13	13 14
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	0.243													
5 6	0.12	-0.172	-0.084	0.12	-0.172	0.242												
5 10	-0.014	0.017	-0.004	0.008	-0.063	-0.058	0.283											
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 15	-0.003	0.02	0.001	0.007	-0.007	0.018	0.003	-0.091	-0.091	0.108								
8 9	0.001	-0.001	-0.001	0.001	-0.001	-0.001	0.005	0.005	-0.058	0.018	0.242							
8 11	0.001	-0.001	-0.001	0.001	0.0	-0.001	0.0	0.004	-0.063	0.02	-0.172	0.243						
9 10	-0.001	0.0	0.001	-0.002	0.004	0.005	-0.024	0.0	-0.004	0.003	-0.058	0.017	0.283					
9 14	0.001	0.0	-0.001	0.001	-0.001	-0.001	0.004	0.0	0.017	-0.007	-0.172	0.108	-0.063	0.243				
10 16	0.007	-0.007	0.001	-0.003	0.02	0.018	-0.091	0.003	0.003	-0.003	0.018	-0.007	-0.091	0.02	0.108			
11 12	-0.001	0.001	0.001	-0.001	0.001	0.001	-0.001	-0.002	0.008	-0.003	0.12	-0.201	-0.014	-0.084	0.007	0.254		
12 13	0.001	-0.001	-0.001	0.001	-0.001	-0.001	0.001	0.001	-0.004	0.001	-0.084	0.124	-0.004	0.124	0.001	-0.208	0.249	
13 14	-0.001	0.001	0.001	-0.001	0.001	0.001	-0.002	-0.001	-0.014	0.007	0.12	-0.084	0.008	-0.201	-0.003	0.125	-0.208	0.254

8.2. Presentation of molecule: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