Print calculated values

Report generated by:root, 16.05.2020 - 18:53:12

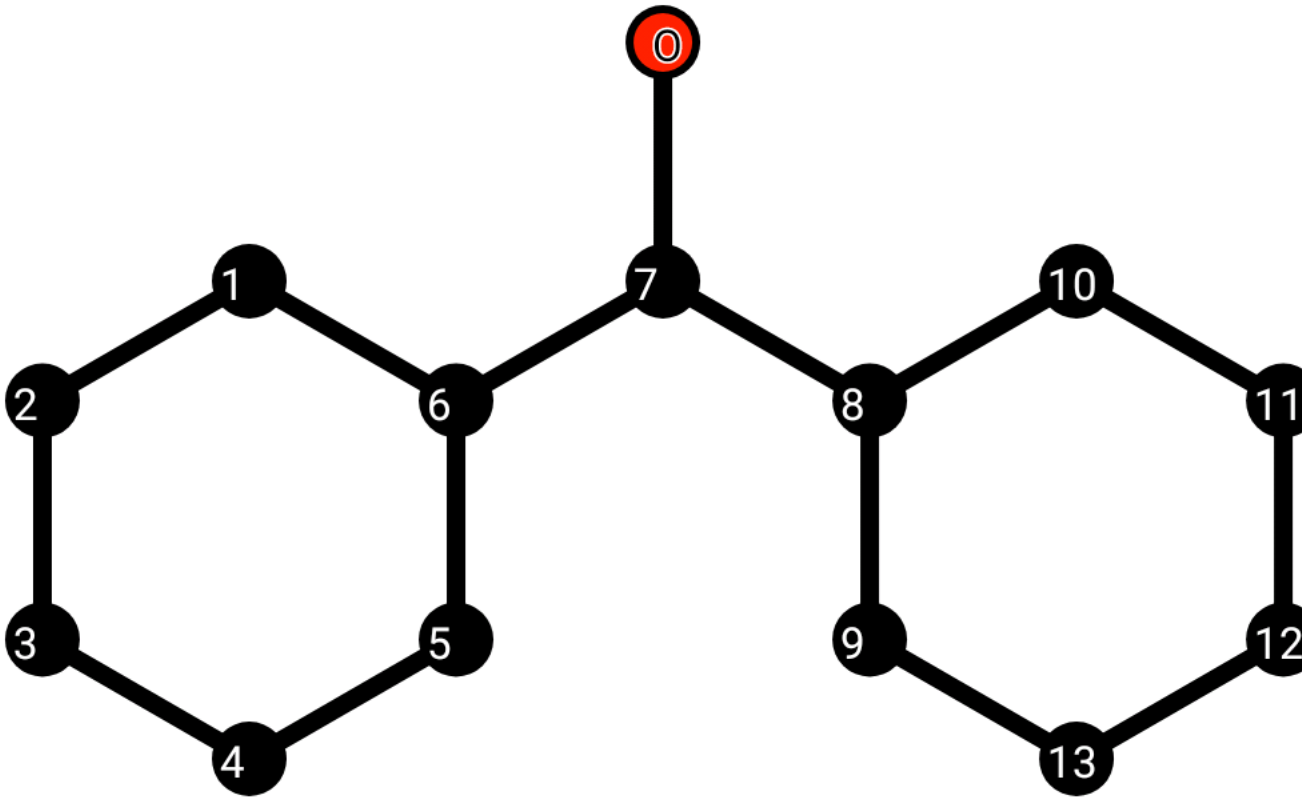
The following determinant is calculated:

-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
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	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	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	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	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	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	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	1.0	-x	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	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	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	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	1.0	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	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	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	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	1.95	0.0	-x+1.18

It is about this molecule:

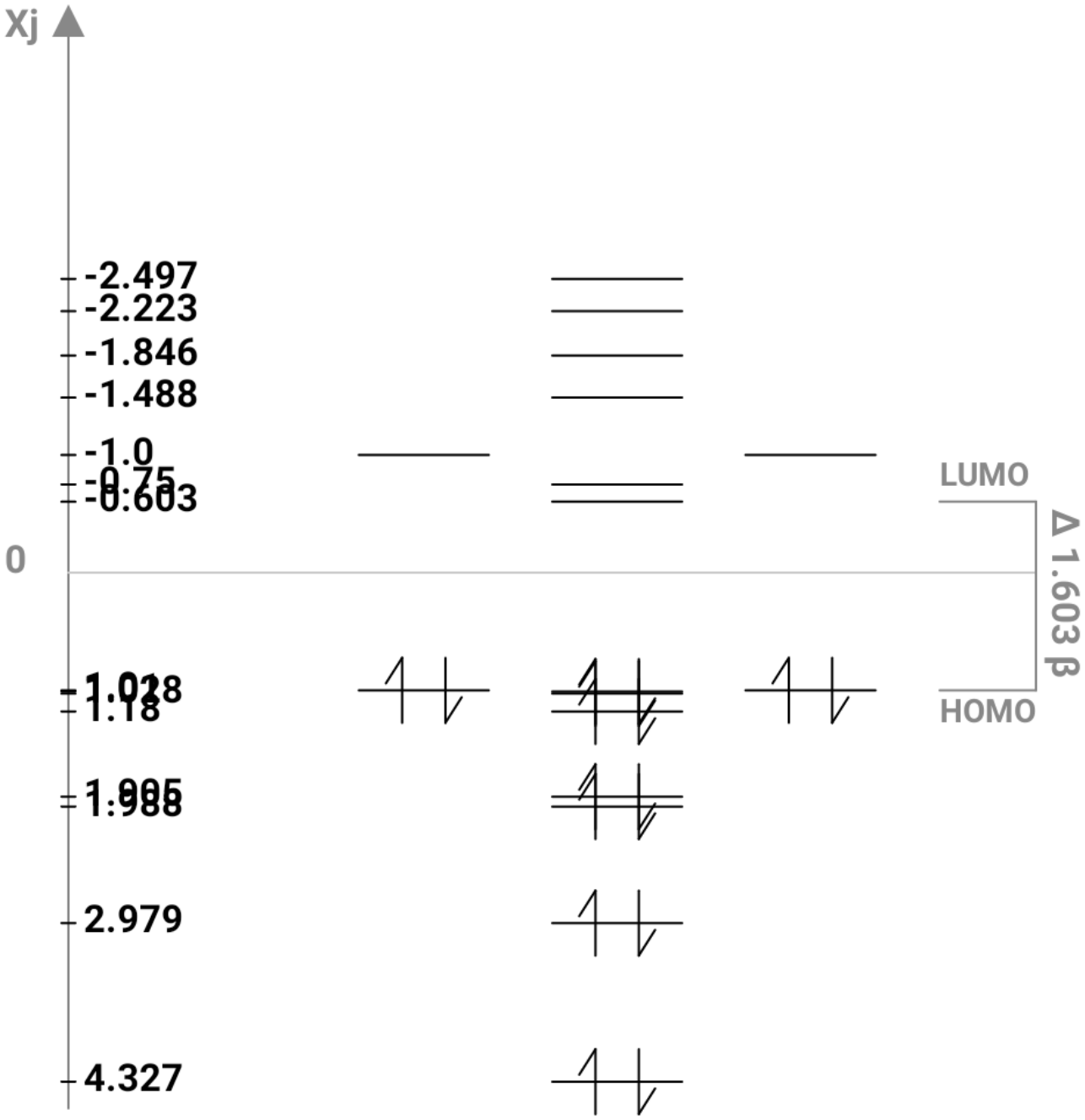
HMO-Energies

x1 = 4.327; x2 = 2.979; x3 = 1.988; x4 = 1.905; x5 = 1.18; x6 = 1.028; x7 = 1.01; x8 = 1.0; x9 = 1.0; x10 = -0.603; x11 = -0.75; x12 = -1.0; x13 = -1.0; x14 = -1.488; x15 = -1.846; x16 = -2.223; x17 = -2.497;


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

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 17α + 32.834β -

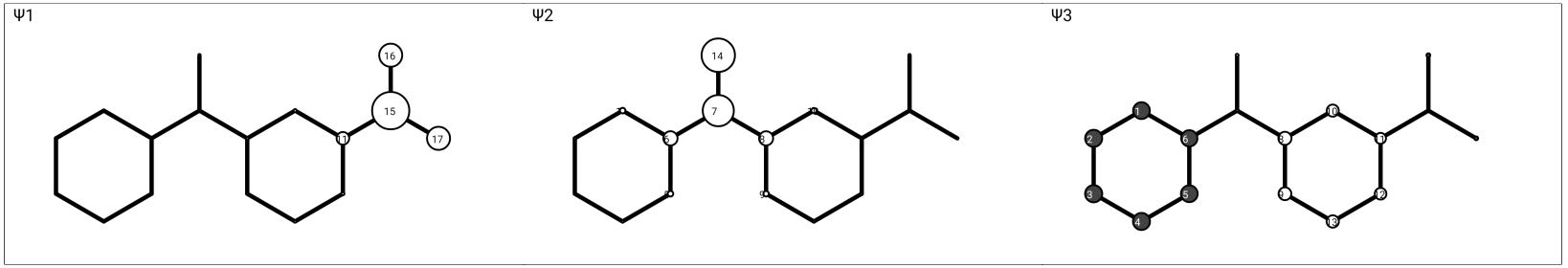
this corresponds to one πelectron: 1.824β

2. Hueckel-coefficient

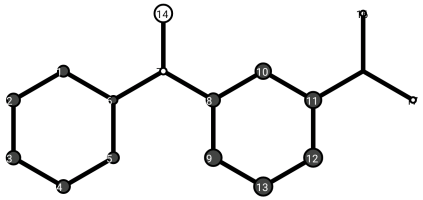
2.1. Calculated values:

	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= 4.327	x2= 2.979	x3= 1.988	x4= 1.905	x5= 1.18	x6= 1.028	x7= 1.01	x8= 1.0	x9= 1.0	x10= -0.603	x11= -0.75	x12= -1.0	x13= -1.0	x14= -1.488	x15= -1.846	x16= -2.223	x17= -2.497
1	0.0	0.109	-0.327	-0.206	0.0	0.16	0.112	0.527	-0.09	0.242	0.14	-0.261	0.466	0.028	-0.27	-0.212	0.181
2	0.0	0.047	-0.333	-0.241	0.0	-0.175	-0.116	0.336	-0.416	0.089	0.073	0.504	-0.177	-0.195	0.354	0.16	-0.107
3	0.0	0.032	-0.335	-0.253	0.0	-0.34	-0.229	-0.191	-0.326	-0.296	-0.195	-0.243	-0.289	0.262	-0.384	-0.144	0.085
4	0.0	0.047	-0.333	-0.241	0.0	-0.175	-0.116	-0.527	0.09	0.089	0.073	-0.261	0.466	-0.195	0.354	0.16	-0.107
5	0.0	0.109	-0.327	-0.206	0.0	0.16	0.112	-0.336	0.416	0.242	0.14	0.504	-0.177	0.028	-0.27	-0.212	0.181
6	0.002	0.277	-0.317	-0.151	0.0	0.34	0.229	0.191	0.326	-0.235	-0.178	-0.243	-0.289	0.153	0.144	0.311	-0.345
7	0.006	0.607	0.023	0.124	0.0	0.029	0.007	0.0	0.0	-0.342	-0.146	0.0	0.0	-0.284	0.274	-0.267	0.5
8	0.017	0.275	0.255	-0.25	0.0	0.4	-0.068	-0.191	-0.326	-0.273	0.005	0.243	0.289	-0.127	-0.313	-0.009	-0.397
9	0.008	0.107	0.249	-0.31	0.0	0.277	-0.475	0.0	0.0	0.368	-0.349	0.0	0.0	0.405	0.225	0.076	0.223
10	0.061	0.105	0.235	-0.29	0.0	0.105	0.4	-0.191	-0.326	0.138	0.492	-0.243	-0.289	0.068	0.079	0.212	0.269
11	0.246	0.037	0.212	-0.303	0.0	-0.291	0.472	0.0	0.0	0.19	-0.374	0.0	0.0	0.026	0.168	-0.461	-0.276
12	0.061	0.028	0.227	-0.338	0.0	-0.395	0.059	0.191	0.326	-0.399	0.157	0.243	0.289	0.302	-0.035	0.279	0.174
13	0.016	0.045	0.24	-0.34	0.0	-0.115	-0.412	0.191	0.326	0.051	0.257	-0.243	-0.289	-0.475	-0.103	-0.16	-0.159
14	0.004	0.651	0.056	0.33	0.0	-0.368	-0.08	0.0	0.0	0.37	0.146	0.0	0.0	0.205	-0.174	0.152	-0.262
15	0.726	-0.018	-0.031	0.039	0.0	-0.008	0.014	0.0	0.0	0.112	-0.283	0.0	0.0	-0.315	-0.272	0.411	0.189
16	0.45	-0.019	-0.075	0.105	0.707	0.098	-0.159	0.0	0.0	-0.123	0.286	0.0	0.0	0.23	0.175	-0.236	-0.1
17	0.45	-0.019	-0.075	0.105	-0.707	0.098	-0.159	0.0	0.0	-0.123	0.286	0.0	0.0	0.23	0.175	-0.236	-0.1

2.2. Molecule orbital presentation:



Ψ4



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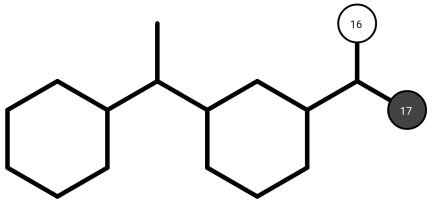

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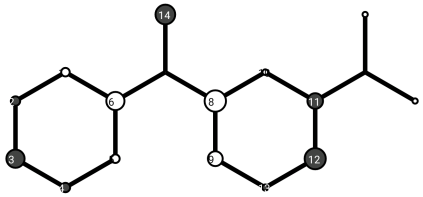

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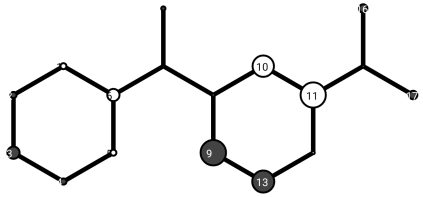

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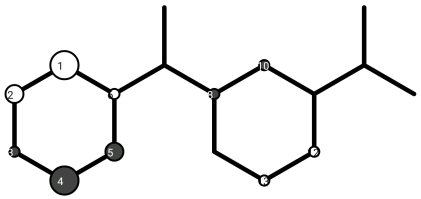
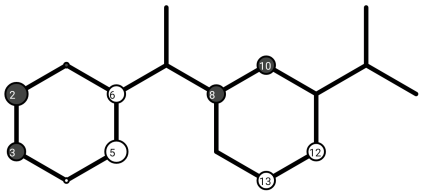


Ψ9



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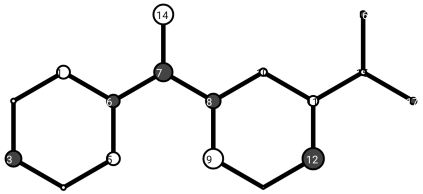

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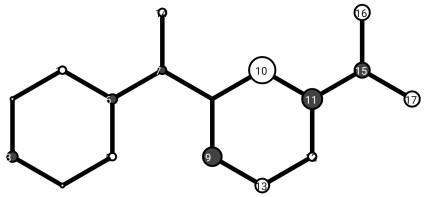

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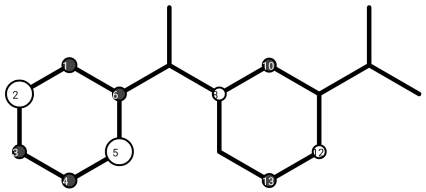
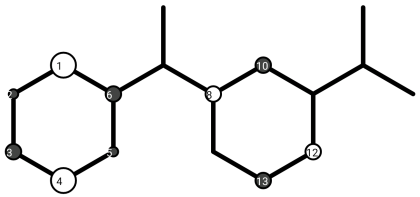
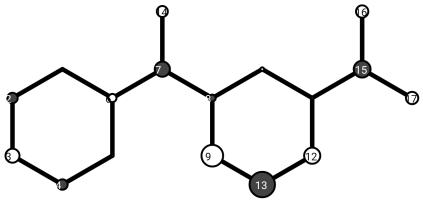


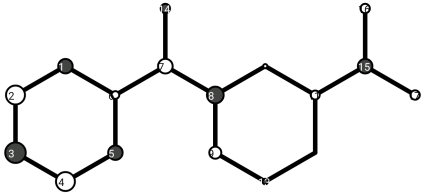
Ψ13



Ψ14



Ψ15



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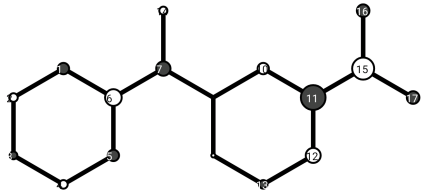
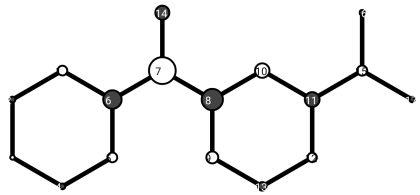


Ψ17

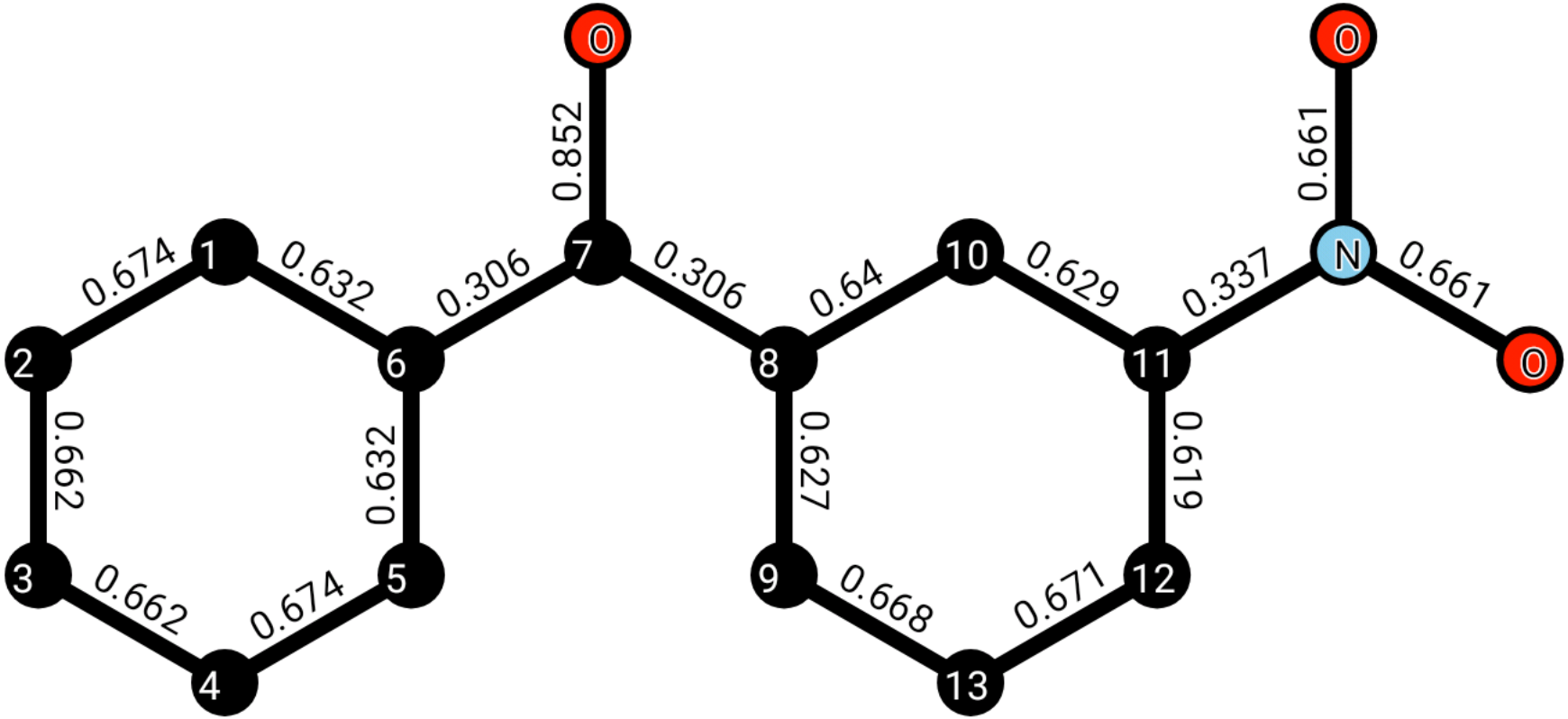


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	0.97																
2	0.674	1.001															
3	0.027	0.662	0.976														
4	-0.326	0.001	0.662	1.001													
5	-0.03	-0.326	0.027	0.674	0.97												
6	0.632	-0.005	-0.315	-0.005	0.632	1.02											
7	0.076	-0.03	-0.063	-0.03	0.076	0.306	0.77										
8	-0.034	-0.005	0.018	-0.005	-0.034	0.02	0.306	1.021									
9	-0.03	0.007	0.026	0.007	-0.03	-0.034	0.075	0.627	0.944								
10	-0.031	0.007	0.027	0.007	-0.031	-0.035	0.078	0.64	-0.001	0.936							
11	0.006	0.001	-0.004	0.001	0.006	-0.004	-0.028	-0.008	-0.305	0.629	1.013						
12	0.026	-0.004	-0.024	-0.004	0.026	0.018	-0.061	-0.307	0.055	-0.006	0.619	0.945					
13	0.007	0.001	-0.004	0.001	0.007	-0.005	-0.03	-0.004	0.668	-0.318	-0.003	0.671	1.003				
14	-0.167	0.012	0.123	0.012	-0.167	-0.062	0.852	-0.062	-0.165	-0.17	0.012	0.12	0.012	1.354			
15	0.002	0.0	-0.001	0.0	0.002	0.002	-0.005	-0.028	-0.05	0.057	0.337	0.054	-0.03	0.008	1.06		
16	-0.002	0.0	0.002	0.0	-0.002	0.0	0.008	0.014	0.105	-0.152	-0.083	-0.148	0.013	-0.007	0.661	1.508	
17	-0.002	0.0	0.002	0.0	-0.002	0.0	0.008	0.014	0.105	-0.152	-0.083	-0.148	0.013	-0.007	0.661	-0.492	1.508

3.2. Presentation of bond order:

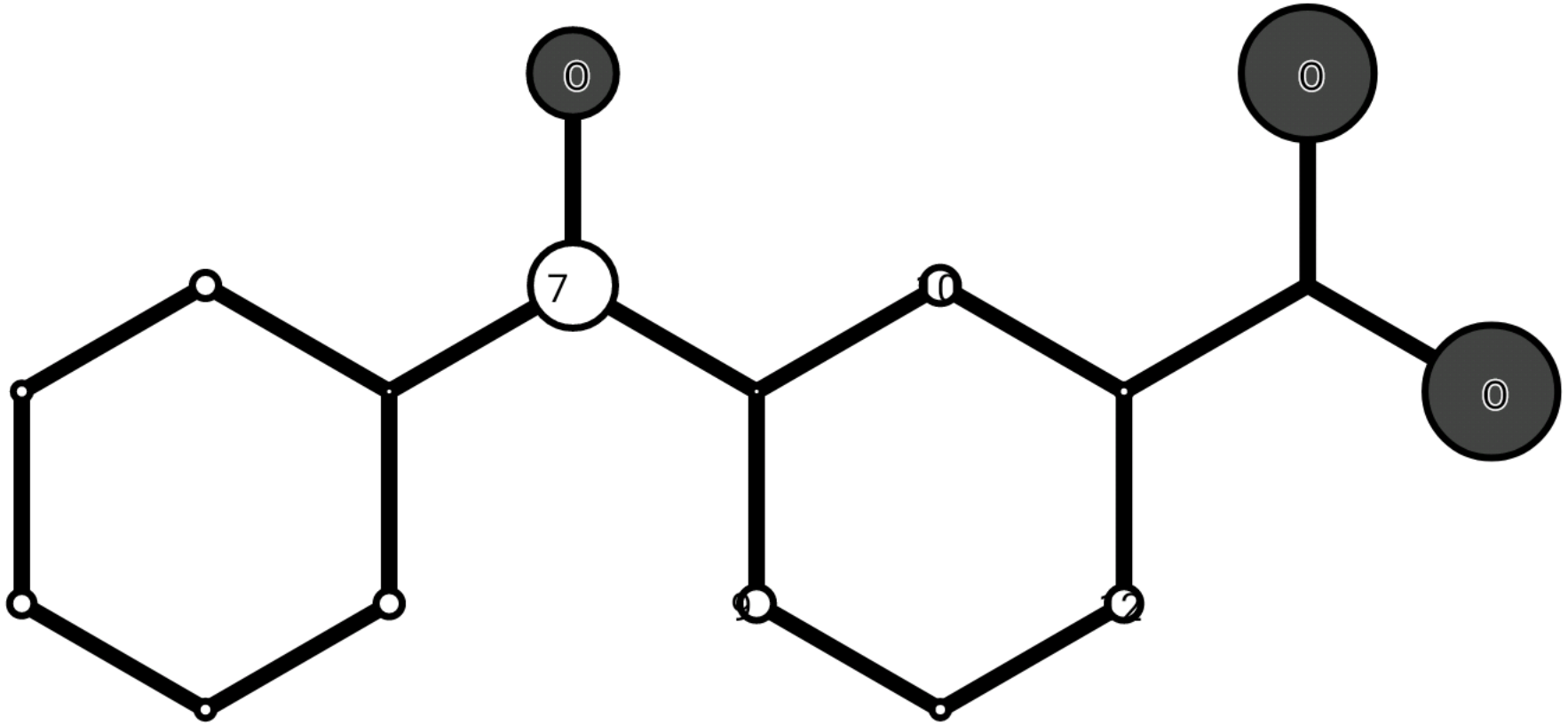

O
0.852
0.661
O
0.674
1
0.632
0.306
7
0.306
0.64
10
0.629
0.337
N
0.661
2
6
8
11
O
0.662
0.632
0.627
0.619
3
5
9
12
0.662
0.674
0.668
0.671
4
13

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	0.089																
2		0.058															
3			0.083														
4				0.058													
5					0.089												
6						0.038											
7							0.289										
8								0.037									
9									0.114								
10										0.123							
11											0.046						
12												0.114					
13													0.056				
14														-0.295			
15															-0.001		
16																-0.45	
17																	-0.45

4.2. Presentation of molecule:

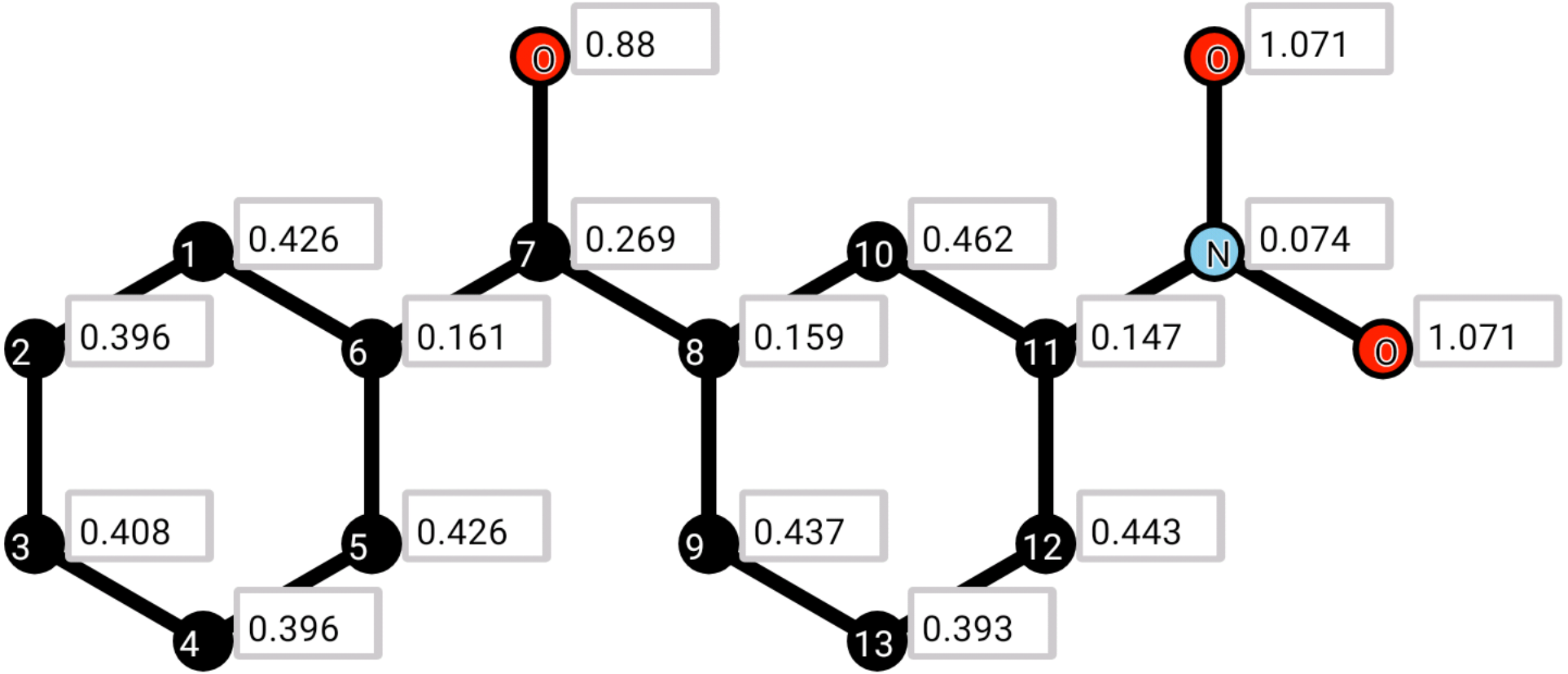

O
O
7
O

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
0.426	0.396	0.408	0.396	0.426	0.161	0.269	0.159	0.437	0.462	0.147	0.443	0.393	0.88	0.074	1.071	1.071

5.2. Presentation of molecule:

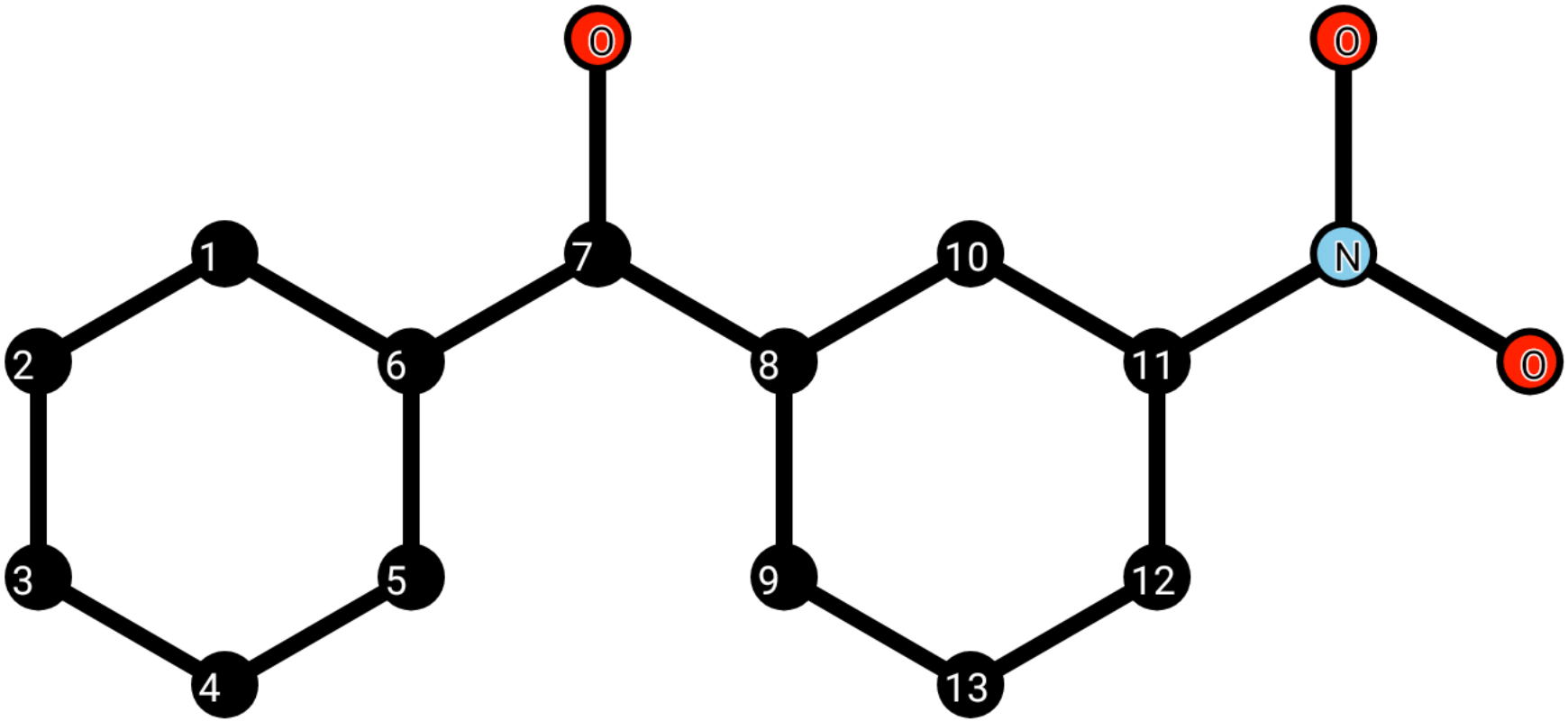

0
0.88
1
0.426
7
0.269
10
0.462
0
1.071
2
0.396
6
0.161
8
0.159
11
0.147
N
0.074
0
1.071
3
0.408
5
0.426
9
0.437
12
0.443
4
0.396
13
0.393

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	0.414																
2	-0.161	0.397															
3	0.011	-0.154	0.405														
4	-0.099	0.01	-0.154	0.397													
5	0.004	-0.099	0.011	-0.161	0.414												
6	-0.141	0.008	-0.094	0.008	-0.141	0.357											
7	-0.002	0.0	-0.004	0.0	-0.002	-0.012	0.205										
8	0.0	0.0	0.0	0.0	0.0	0.001	-0.012	0.356									
9	-0.001	0.0	-0.001	0.0	-0.001	0.0	-0.002	-0.138	0.42								
10	-0.001	0.0	-0.001	0.0	-0.001	0.0	-0.002	-0.146	0.009	0.431							
11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.006	-0.089	-0.141	0.344						
12	-0.001	0.0	-0.001	0.0	-0.001	0.0	-0.004	-0.09	0.012	0.007	-0.135	0.423					
13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.008	-0.158	-0.095	0.008	-0.159	0.395				
14	-0.023	0.001	-0.019	0.001	-0.023	0.014	-0.165	0.013	-0.022	-0.024	0.001	-0.018	0.001	0.262			
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	0.0	-0.013	-0.017	0.01	-0.016	0.001	0.0	-0.075	0.255	
17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.013	-0.017	0.01	-0.016	0.001	0.0	-0.075	-0.145	0.255

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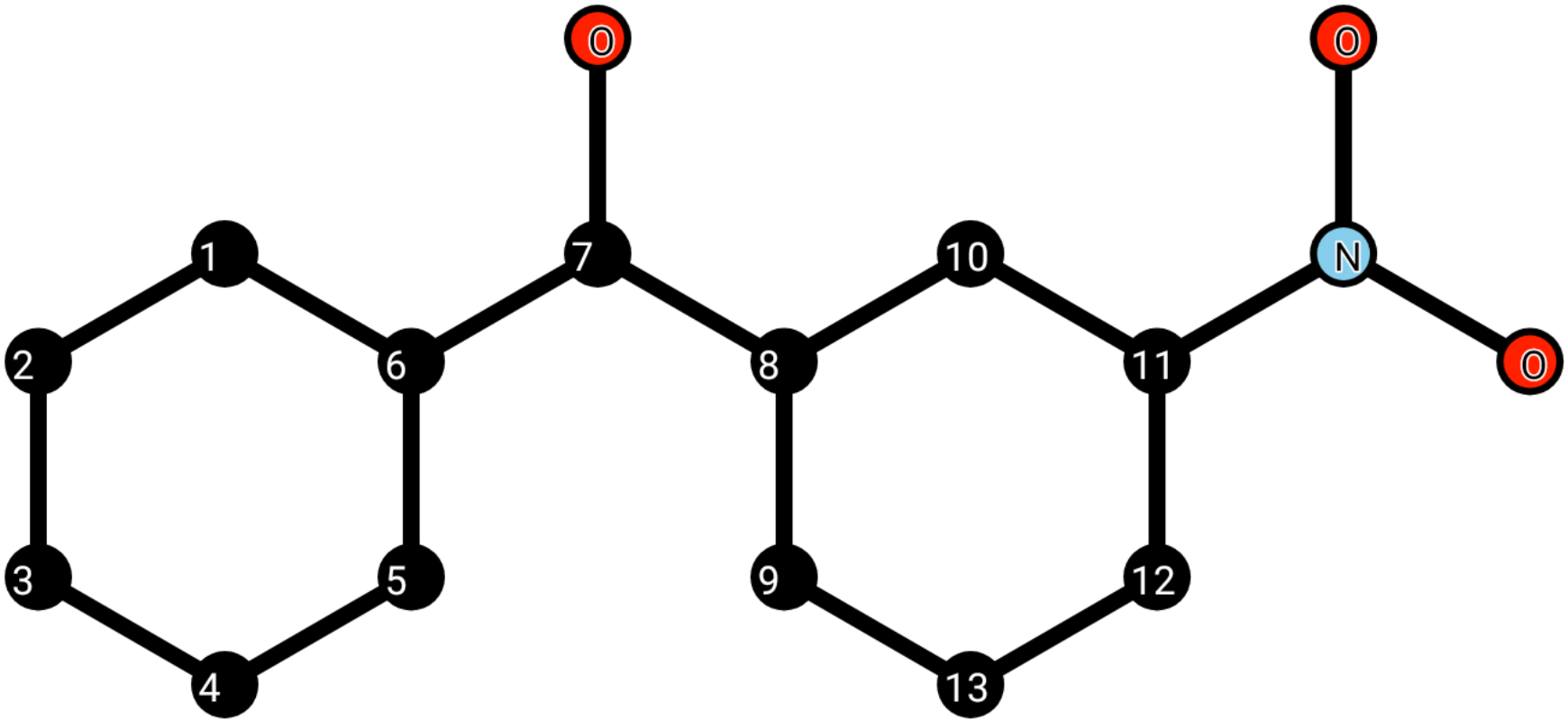
7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1 2	0.015	0.001	-0.011	0.0	-0.012	0.003	0.002	0.0	0.0	0.0	0.0	0.0	0.0	0.002	0.0	0.0	0.0
1 6	0.006	0.001	0.009	-0.002	0.014	-0.011	-0.007	0.001	-0.001	-0.001	0.0	-0.001	0.0	-0.009	0.0	0.0	0.0
2 3	-0.012	-0.002	0.01	0.0	0.01	-0.002	-0.001	0.0	0.0	0.0	0.0	0.0	0.0	-0.002	0.0	0.0	0.0
3 4	0.01	0.0	0.01	-0.002	-0.012	-0.002	-0.001	0.0	0.0	0.0	0.0	0.0	0.0	-0.002	0.0	0.0	0.0
4 5	-0.012	0.0	-0.011	0.001	0.015	0.003	0.002	0.0	0.0	0.0	0.0	0.0	0.0	0.002	0.0	0.0	0.0
5 6	0.014	-0.002	0.009	0.001	0.006	-0.011	-0.007	0.001	-0.001	-0.001	0.0	-0.001	0.0	-0.009	0.0	0.0	0.0
6 7	-0.028	0.001	-0.023	0.001	-0.028	0.017	0.025	-0.003	0.002	0.002	0.0	0.001	0.0	0.031	0.0	0.0	0.0
7 8	0.002	0.0	0.002	0.0	0.002	-0.003	0.025	0.017	-0.027	-0.029	0.001	-0.022	0.001	0.031	0.0	0.0	0.0
7 14	0.01	0.0	0.01	0.0	0.01	-0.002	0.038	-0.002	0.01	0.011	0.0	0.009	0.0	-0.094	0.0	0.0	0.0
8 9	-0.001	0.0	-0.001	0.0	-0.001	0.001	-0.007	-0.012	0.016	0.001	-0.003	0.019	0.001	-0.009	-0.001	-0.002	-0.002
8 10	-0.001	0.0	-0.001	0.0	-0.001	0.001	-0.007	-0.01	0.002	0.022	0.004	-0.003	-0.002	-0.009	0.001	0.002	0.002
9 13	0.0	0.0	0.0	0.0	0.0	0.0	0.002	0.003	0.025	-0.001	-0.002	-0.024	-0.001	0.002	-0.001	-0.002	-0.002
10 11	0.0	0.0	0.0	0.0	0.0	0.0	0.002	0.004	-0.001	0.022	-0.009	0.004	-0.002	0.002	-0.005	-0.008	-0.008
11 12	0.0	0.0	0.0	0.0	0.0	0.0	-0.001	-0.003	0.019	0.003	-0.011	0.016	0.001	-0.002	-0.004	-0.008	-0.008
11 15	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.001	-0.018	-0.024	0.007	-0.022	0.001	0.0	0.005	0.025	0.025
12 13	0.0	0.0	0.0	0.0	0.0	0.0	-0.001	-0.002	-0.024	-0.003	0.003	0.025	0.0	-0.002	0.001	0.002	0.002
15 16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.006	0.007	0.002	0.007	0.0	0.0	-0.008	-0.133	0.119
15 17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.006	0.007	0.002	0.007	0.0	0.0	-0.008	0.119	-0.133

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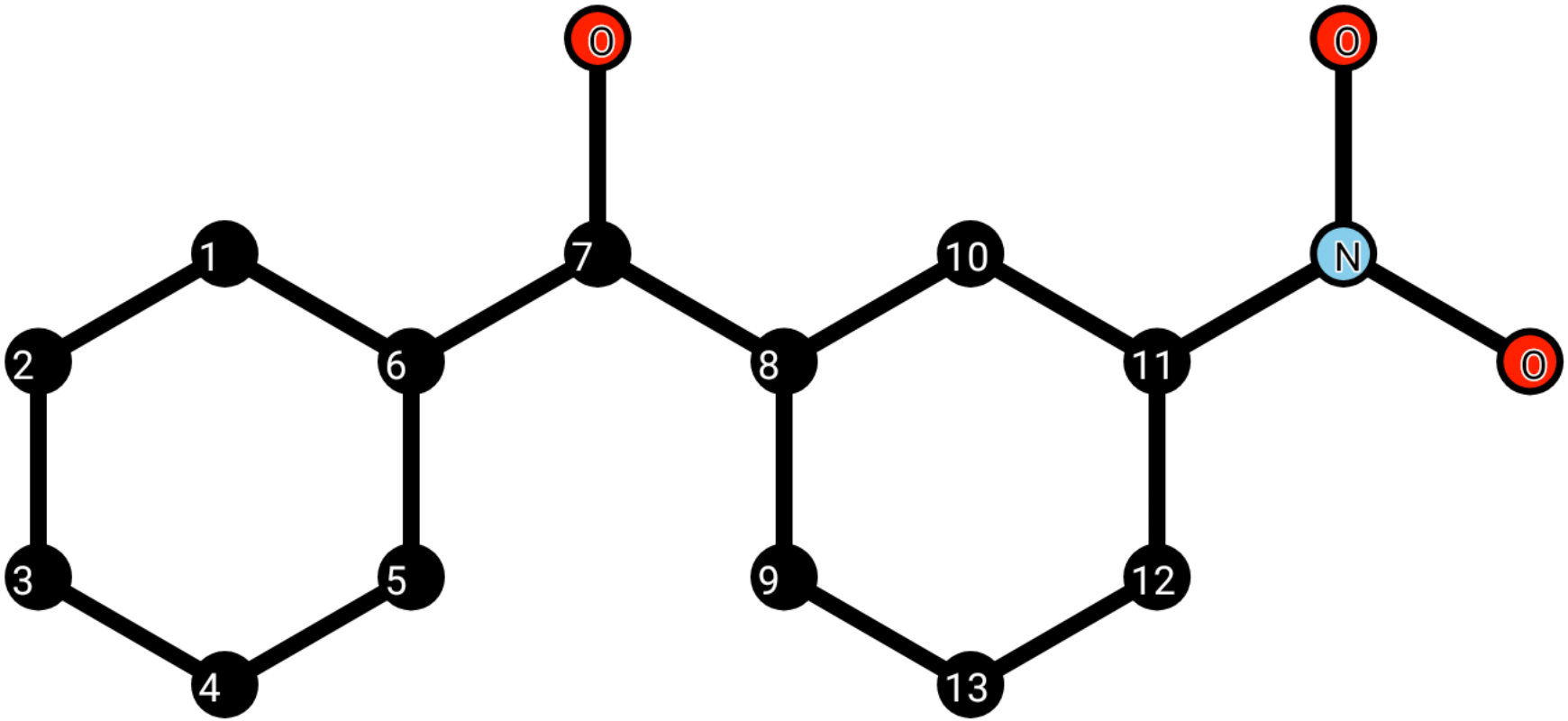
8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	2 3	3 4	4 5	5 6	6 7	7 8	7 14	8 9	8 10	9 13	10 11	11 12	11 15	12 13	15 16	15 17
1 2	0.244																	
1 6	-0.196	0.244																
2 3	-0.21	0.126	0.247															
3 4	0.128	-0.086	-0.203	0.247														
4 5	-0.092	0.119	0.128	-0.21	0.244													
5 6	0.119	-0.176	-0.086	0.126	-0.196	0.244												
6 7	0.013	-0.066	-0.009	-0.009	0.013	-0.066	0.283											
7 8	0.0	0.003	0.0	0.0	0.0	0.003	-0.023	0.282										
7 14	-0.005	0.022	0.004	0.004	-0.005	0.022	-0.093	-0.092	0.112									
8 9	0.0	-0.001	0.0	0.0	0.0	-0.001	0.003	-0.065	0.022	0.251								
8 10	0.0	-0.001	0.0	0.0	0.0	-0.001	0.003	-0.066	0.022	-0.183	0.249							
9 13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.013	-0.005	-0.195	0.118	0.252						
10 11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.013	-0.005	0.116	-0.186	-0.084	0.246					
11 12	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.008	0.004	-0.079	0.114	0.124	-0.176	0.249				
11 15	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.007	0.012	-0.008	-0.063	-0.063	0.232			
12 13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.009	0.004	0.125	-0.085	-0.217	0.116	-0.193	0.012	0.251		
15 16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.003	-0.004	0.003	0.019	0.018	-0.065	-0.004	0.189	
15 17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.003	-0.004	0.003	0.019	0.018	-0.065	-0.004	-0.149	0.189

8.2. Presentation of molecule: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