Print calculated values

Report generated by:root, 16.05.2020 - 18:59:39

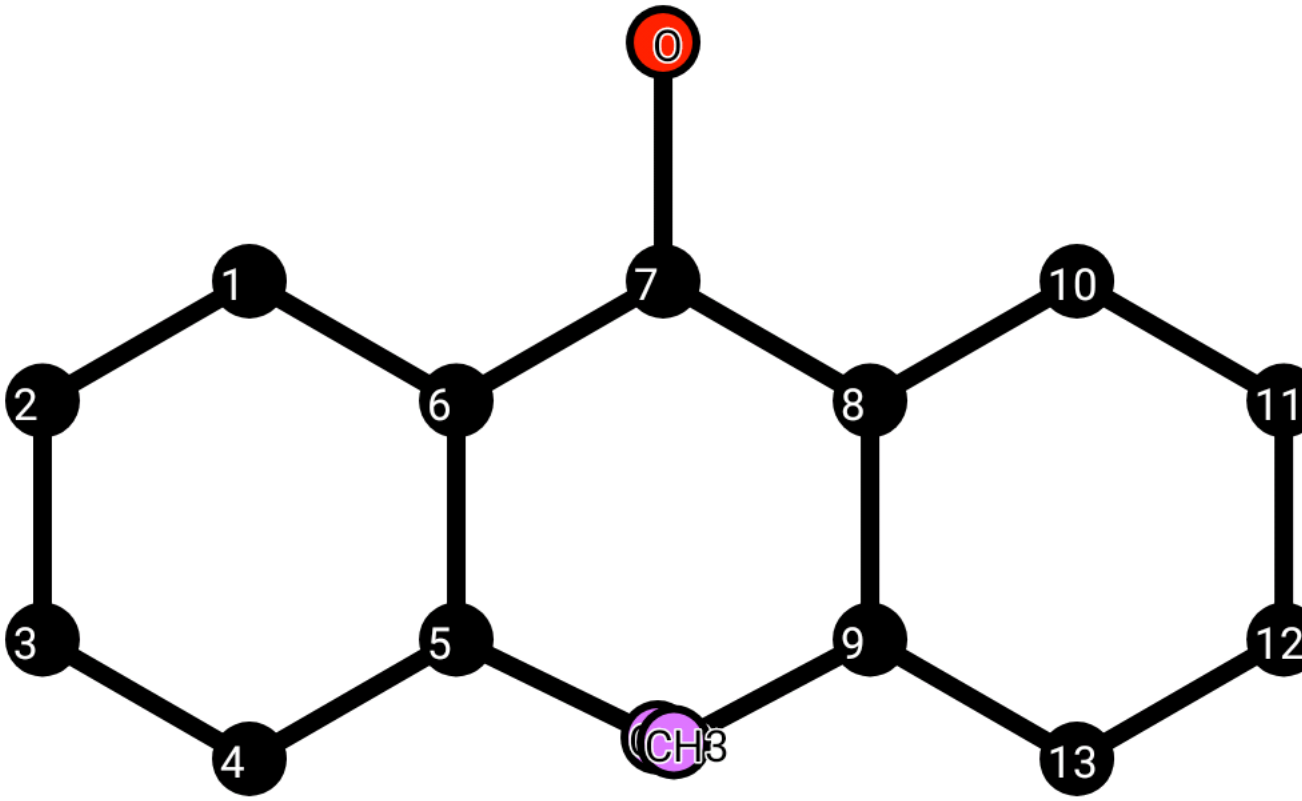
The following determinant is calculated:

-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	0.0	0.0	0.0	0.0	0.0	0.18	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	1.93	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	1.0	-x	0.0	0.0	0.0	1.0	0.0	0.0	0.18
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	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	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	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	0.18	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-x+0.88	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.18	0.0	0.0	0.0	0.0	0.0	0.0	-x+0.88

It is about this molecule:

HMO-Energies

x1 = 2.981; x2 = 2.005; x3 = 1.924; x4 = 1.064; x5 = 1.06; x6 = 1.019; x7 = 1.0; x8 = 0.827;
x9 = 0.822; x10 = -0.622; x11 = -1.0; x12 = -1.004; x13 = -1.006; x14 = -1.664; x15 = -2.002; x16 = -2.465;


0
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11
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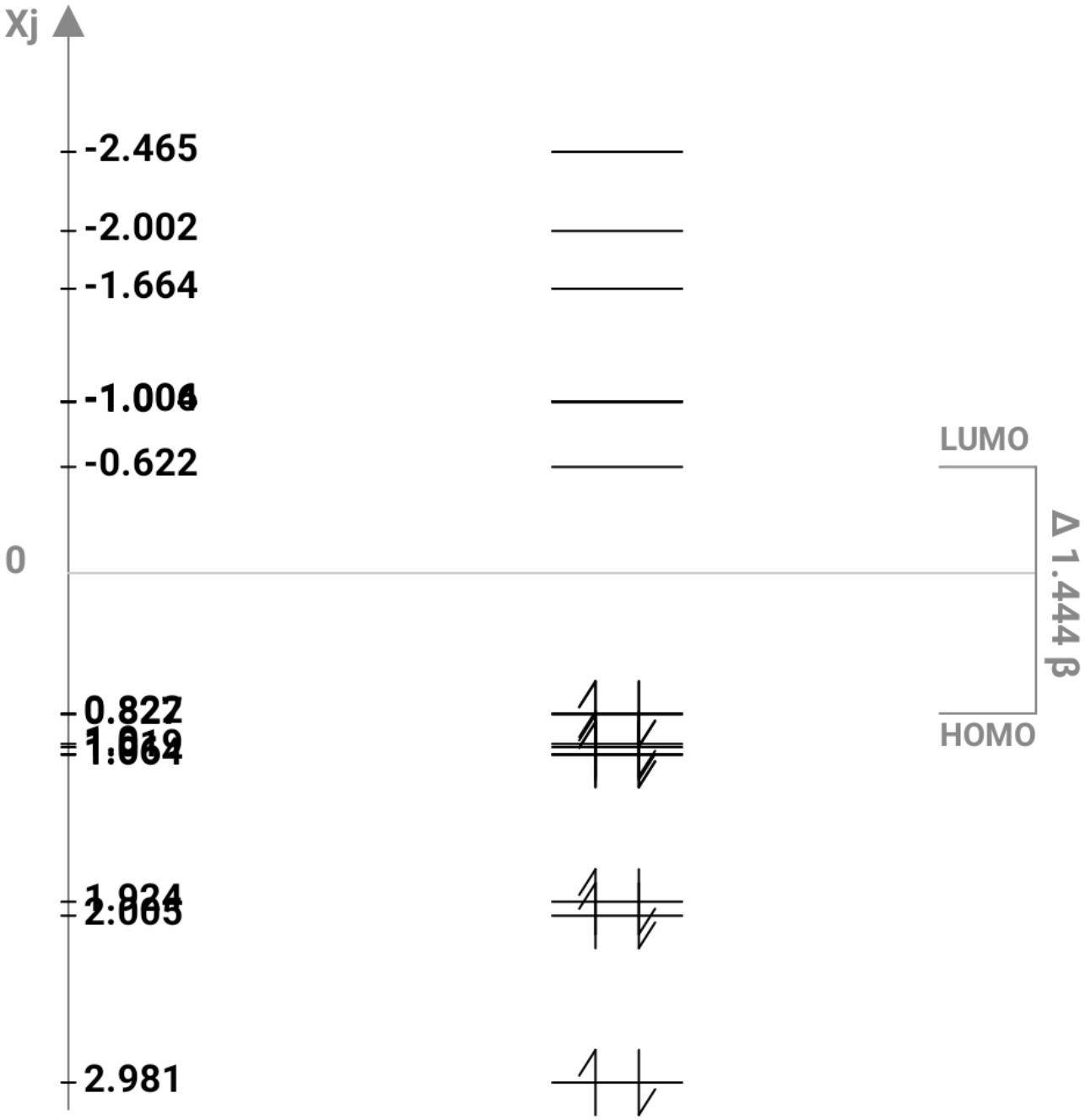
13
CH3

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 16α + 25.404β -

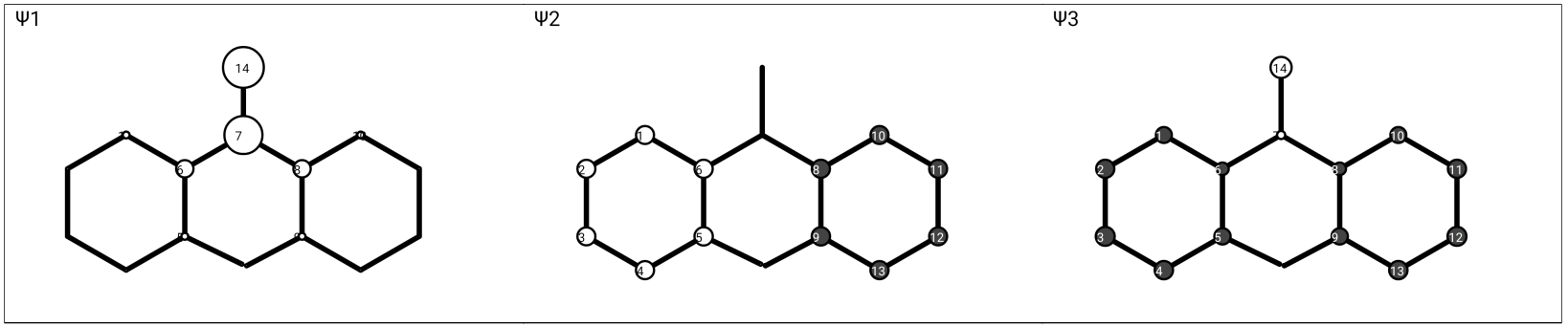
this corresponds to one πelectron: 1.411β

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= 2.981	x2= 2.005	x3= 1.924	x4= 1.064	x5= 1.06	x6= 1.019	x7= 1.0	x8= 0.827	x9= 0.822	x10= -0.622	x11= -1.0	x12= -1.004	x13= -1.006	x14= -1.664	x15= -2.002	x16= -2.465
1	0.108	0.287	-0.254	0.141	-0.189	-0.355	0.354	-0.11	0.084	-0.272	-0.354	0.352	-0.205	0.143	-0.288	0.216
2	0.047	0.286	-0.289	0.352	-0.357	-0.057	0.0	-0.196	0.204	-0.099	0.0	-0.354	0.408	-0.31	0.288	-0.131
3	0.032	0.287	-0.302	0.233	-0.189	0.298	-0.354	-0.052	0.084	0.334	0.354	0.004	-0.205	0.373	-0.288	0.106
4	0.047	0.289	-0.292	-0.104	0.156	0.36	-0.354	0.153	-0.135	-0.109	-0.354	0.35	-0.202	-0.311	0.289	-0.131
5	0.109	0.292	-0.26	-0.343	0.355	0.069	0.0	0.179	-0.195	-0.267	0.0	-0.356	0.408	0.145	-0.29	0.217
6	0.276	0.289	-0.2	-0.201	0.156	-0.305	0.354	0.105	-0.135	0.269	0.354	0.001	-0.202	0.072	0.289	-0.402
7	0.606	0.0	0.13	-0.012	0.0	-0.025	0.0	0.018	0.0	0.372	0.0	0.003	0.0	-0.408	0.0	0.557
8	0.276	-0.289	-0.2	-0.201	-0.156	-0.305	-0.354	0.105	0.135	0.269	-0.354	0.001	0.202	0.072	-0.289	-0.402
9	0.109	-0.292	-0.26	-0.343	-0.355	0.069	0.0	0.179	0.195	-0.267	0.0	-0.356	-0.408	0.145	0.29	0.217
10	0.108	-0.287	-0.254	0.141	0.189	-0.355	-0.354	-0.11	-0.084	-0.272	0.354	0.352	0.205	0.143	0.288	0.216
11	0.047	-0.286	-0.289	0.352	0.357	-0.057	0.0	-0.196	-0.204	-0.099	0.0	-0.354	-0.408	-0.31	-0.288	-0.131
12	0.032	-0.287	-0.302	0.233	0.189	0.298	0.354	-0.052	-0.084	0.334	-0.354	0.004	0.205	0.373	0.288	0.106
13	0.047	-0.289	-0.292	-0.104	-0.156	0.36	0.354	0.153	0.135	-0.109	0.354	0.35	0.202	-0.311	-0.289	-0.131
14	0.649	0.0	0.337	0.202	0.0	0.303	0.0	-0.101	0.0	-0.398	0.0	-0.003	0.0	0.277	0.0	-0.295
15	0.009	0.047	-0.045	-0.336	0.355	0.09	0.0	-0.612	0.609	0.032	0.0	0.034	-0.039	-0.01	0.018	-0.012
16	0.009	-0.047	-0.045	-0.336	-0.355	0.09	0.0	-0.612	-0.609	0.032	0.0	0.034	0.039	-0.01	-0.018	-0.012

2.2. Molecule orbital presentation:



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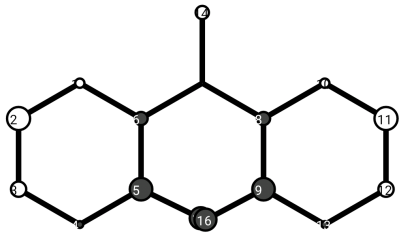

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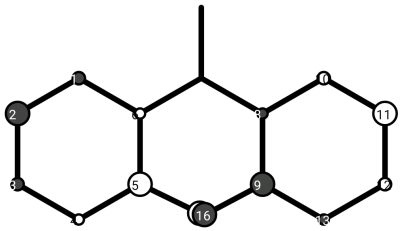
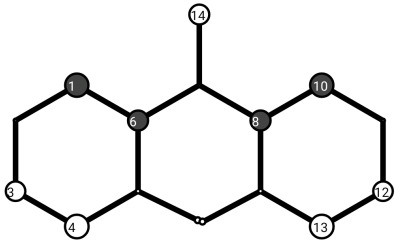
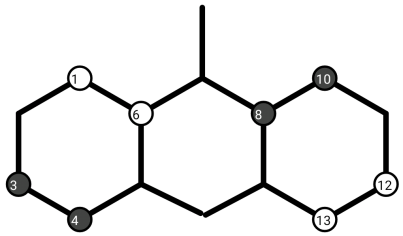


Ψ6



Ψ7



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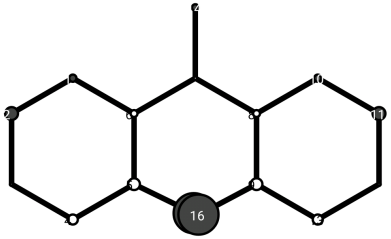

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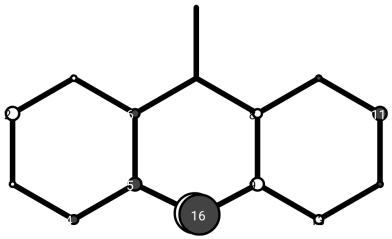

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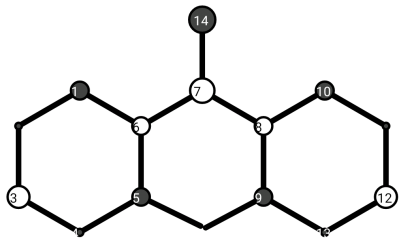

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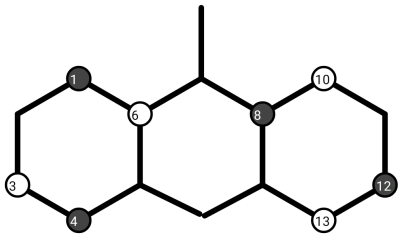
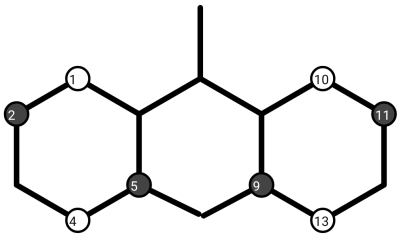
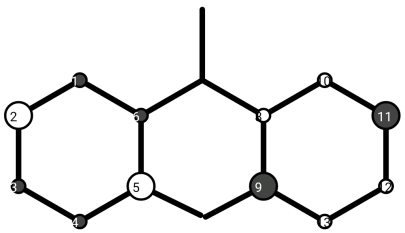


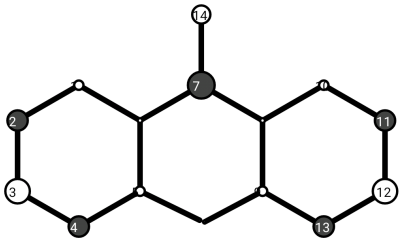
Ψ12



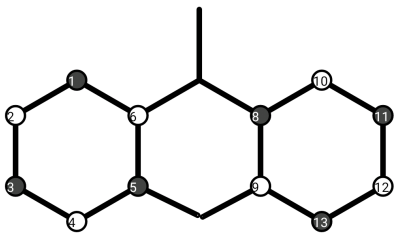
Ψ13

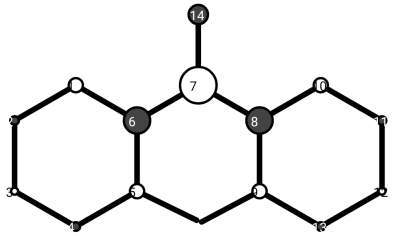


Ψ14



Ψ15



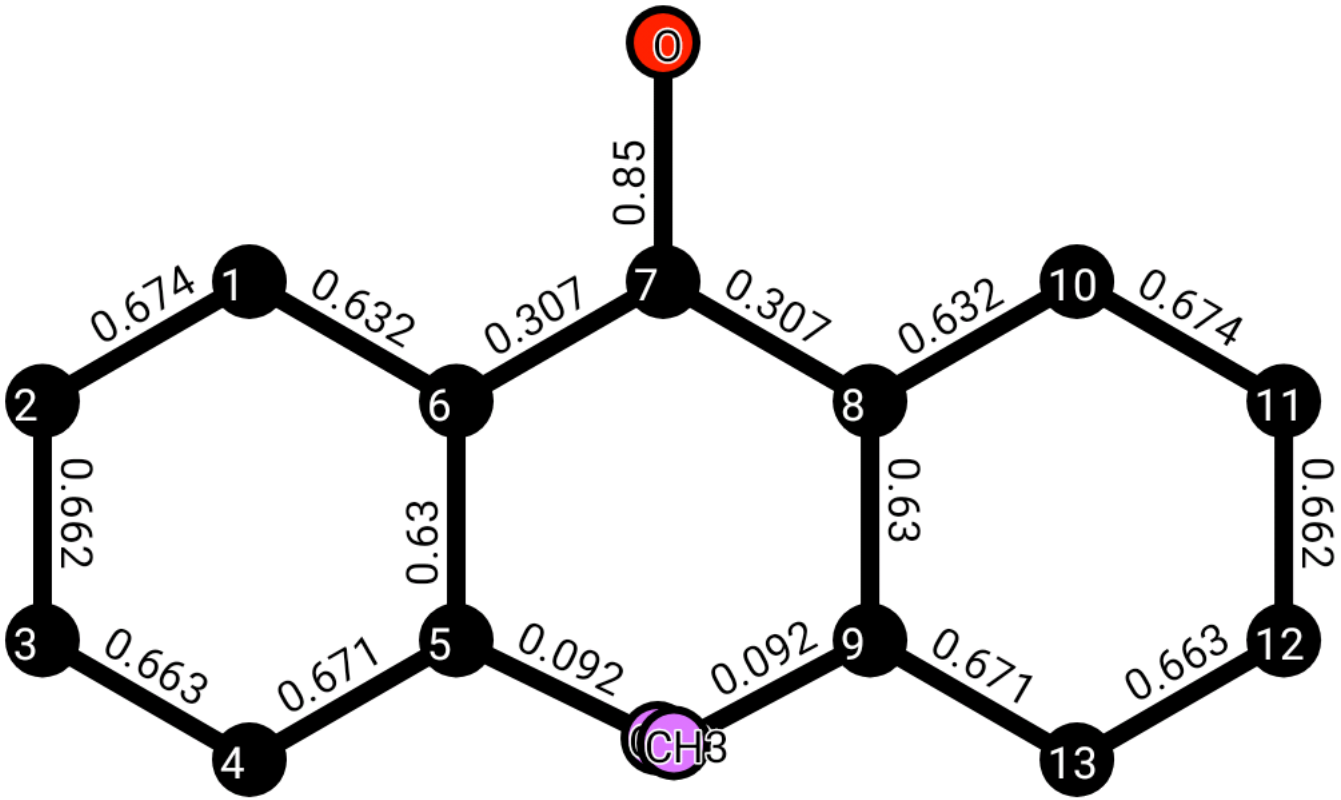
Ψ16 		

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.97															
2	0.674	1.004														
3	0.026	0.662	0.976													
4	-0.326	-0.002	0.663	1.005												
5	-0.03	-0.325	0.027	0.671	0.967											
6	0.632	-0.008	-0.314	-0.001	0.63	1.024										
7	0.076	-0.031	-0.063	-0.029	0.076	0.307	0.77									
8	-0.035	-0.005	0.018	-0.005	-0.035	0.02	0.307	1.024								
9	-0.03	0.007	0.027	0.006	-0.03	-0.035	0.076	0.63	0.967							
10	-0.03	0.007	0.027	0.006	-0.03	-0.035	0.076	0.632	-0.03	0.97						
11	0.007	0.001	-0.005	0.001	0.007	-0.005	-0.031	-0.008	-0.325	0.674	1.004					
12	0.027	-0.005	-0.024	-0.004	0.027	0.018	-0.063	-0.314	0.027	0.026	0.662	0.976				
13	0.006	0.001	-0.004	0.001	0.006	-0.005	-0.029	-0.001	0.671	-0.326	-0.002	0.663	1.005			
14	-0.166	0.013	0.122	0.01	-0.166	-0.063	0.85	-0.063	-0.166	-0.166	0.013	0.122	0.01	1.356		
15	-0.004	0.042	-0.017	-0.052	0.092	-0.051	-0.019	0.001	0.007	0.007	0.0	-0.006	0.0	0.024	1.991	
16	0.007	0.0	-0.006	0.0	0.007	0.001	-0.019	-0.051	0.092	-0.004	0.042	-0.017	-0.052	0.024	-0.001	1.991

3.2. Presentation of bond order:


0
0.85
1
2
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4
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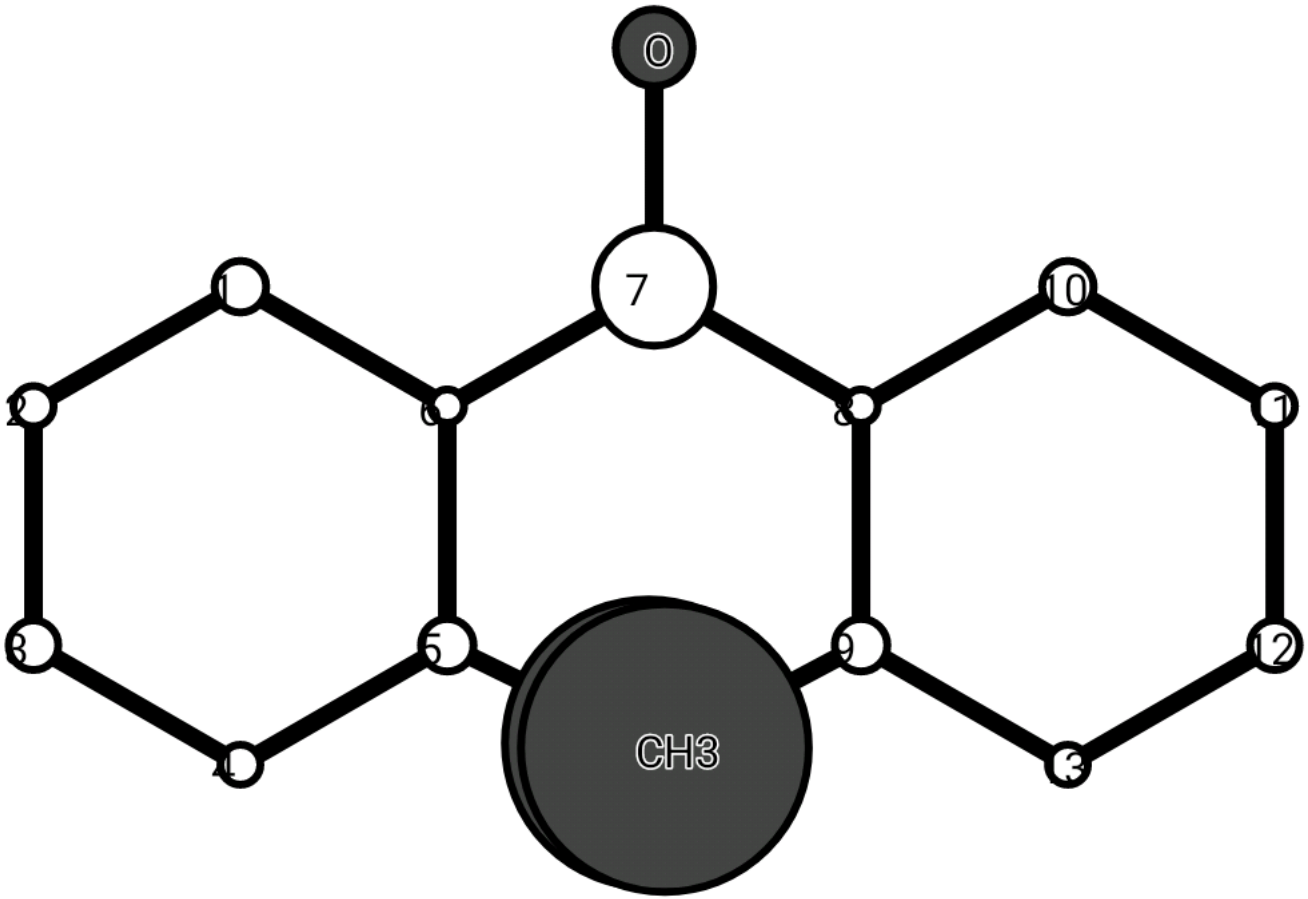
10
11
12
13
0.674
0.632
0.307
0.307
0.632
0.674
0.662
0.63
0.63
0.662
0.663
0.671
0.092
0.092
0.671
0.663
CH3

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.155															
2		0.121														
3			0.149													
4				0.12												
5					0.158											
6						0.101										
7							0.355									
8								0.101								
9									0.158							
10										0.155						
11											0.121					
12												0.149				
13													0.12			
14														-0.231		
15															-0.866	
16																-0.866

4.2. Presentation of molecule:

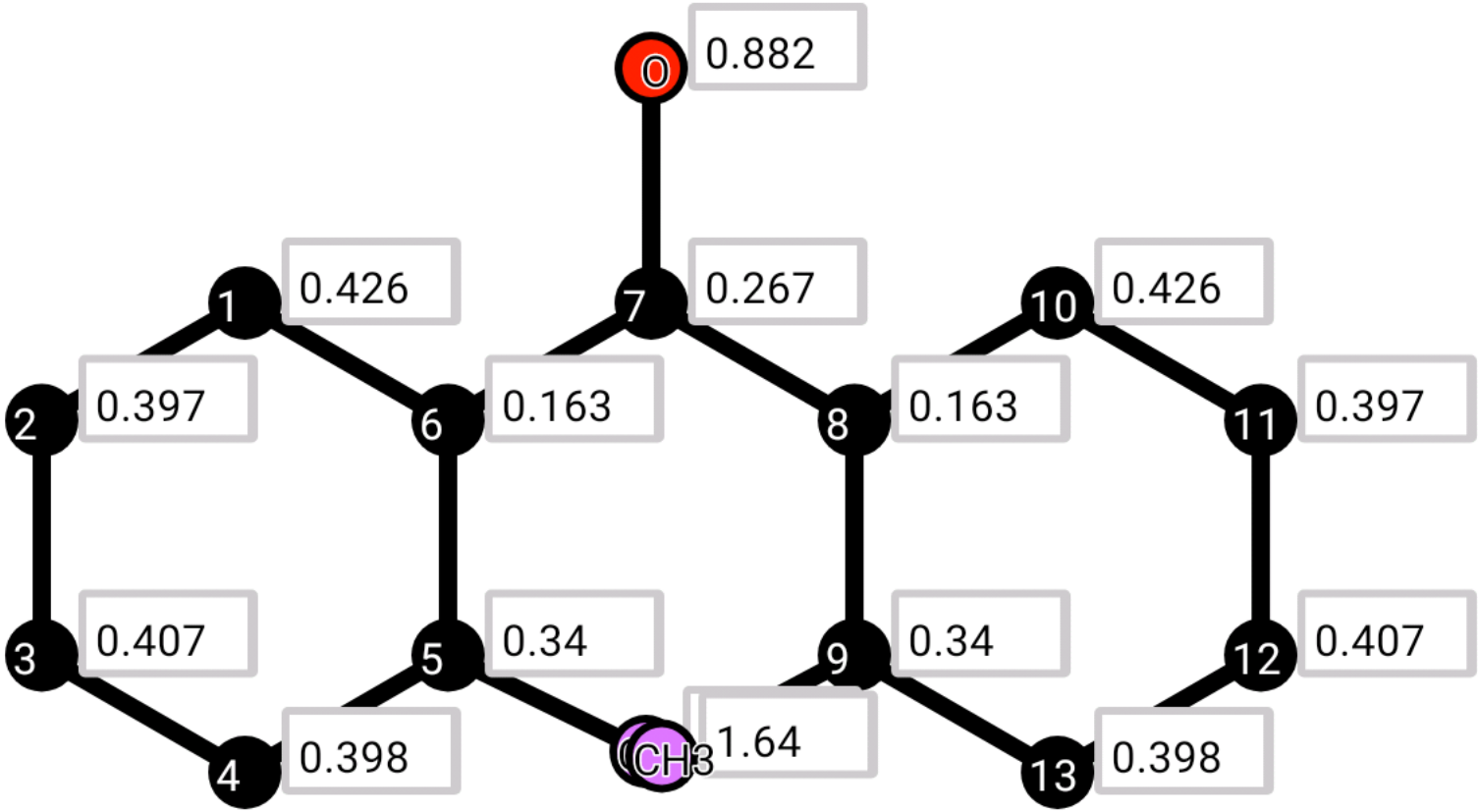

0
7
10
1
5
9
12
CH3
3

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
0.426	0.397	0.407	0.398	0.34	0.163	0.267	0.163	0.34	0.426	0.397	0.407	0.398	0.882	1.64	1.64

5.2. Presentation of molecule:

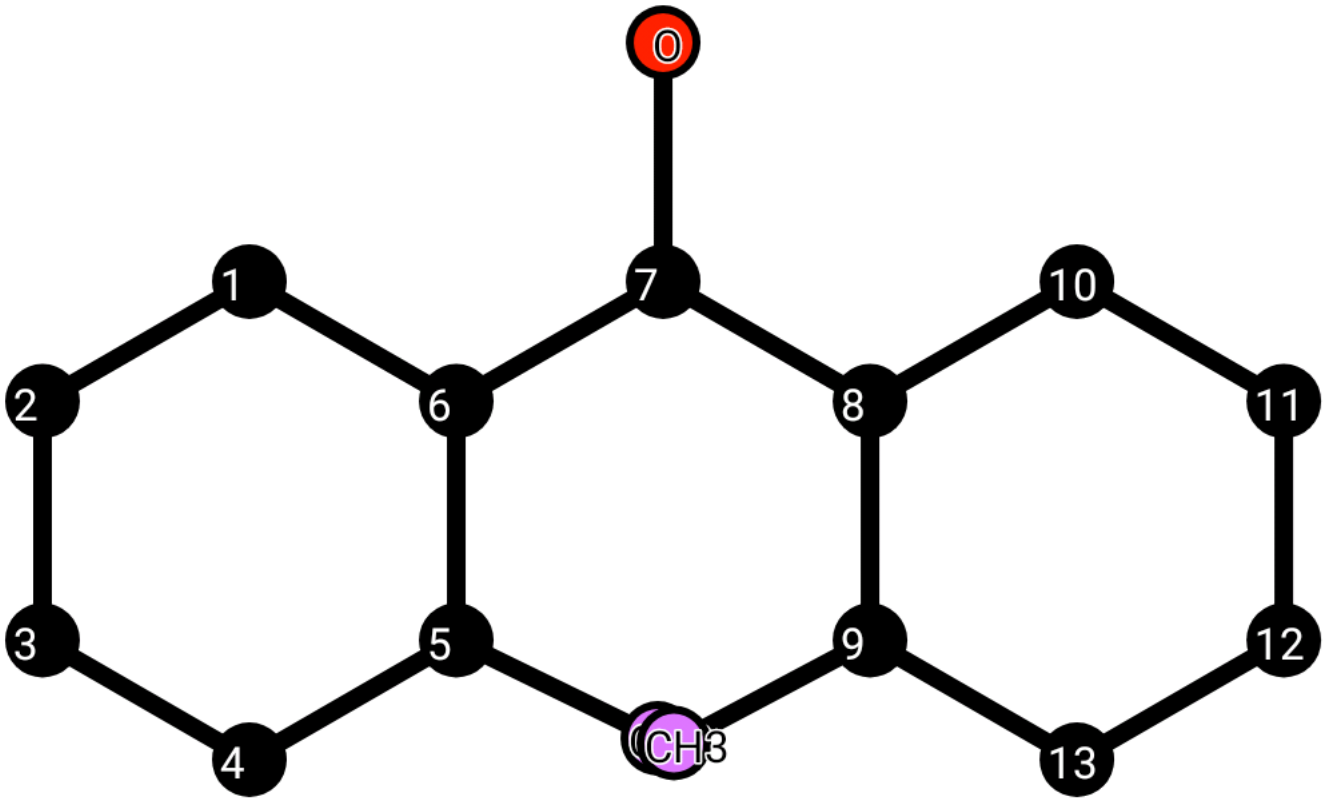

0
0.882
1
0.426
7
0.267
10
0.426
2
0.397
6
0.163
8
0.163
11
0.397
3
0.407
5
0.34
9
0.34
12
0.407
4
0.398
CH3
1.64
13
0.398

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	0.414															
2	-0.162	0.397														
3	0.011	-0.154	0.405													
4	-0.099	0.01	-0.155	0.398												
5	0.004	-0.098	0.011	-0.16	0.411											
6	-0.141	0.008	-0.093	0.008	-0.14	0.358										
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	0.358								
9	-0.001	0.0	-0.001	0.0	-0.001	0.0	-0.002	-0.14	0.411							
10	-0.001	0.0	-0.001	0.0	-0.001	0.0	-0.002	-0.141	0.004	0.414						
11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.008	-0.098	-0.162	0.397					
12	-0.001	0.0	-0.001	0.0	-0.001	0.0	-0.004	-0.093	0.011	0.011	-0.154	0.405				
13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.008	-0.16	-0.099	0.01	-0.155	0.398			
14	-0.022	0.001	-0.018	0.001	-0.022	0.014	-0.164	0.014	-0.022	-0.022	0.001	-0.018	0.001	0.262		
15	0.0	-0.002	0.0	-0.002	-0.001	-0.003	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.001	0.009	
16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.003	-0.001	0.0	-0.002	0.0	-0.002	-0.001	0.0	0.009

6.2. Presentation of molecule:

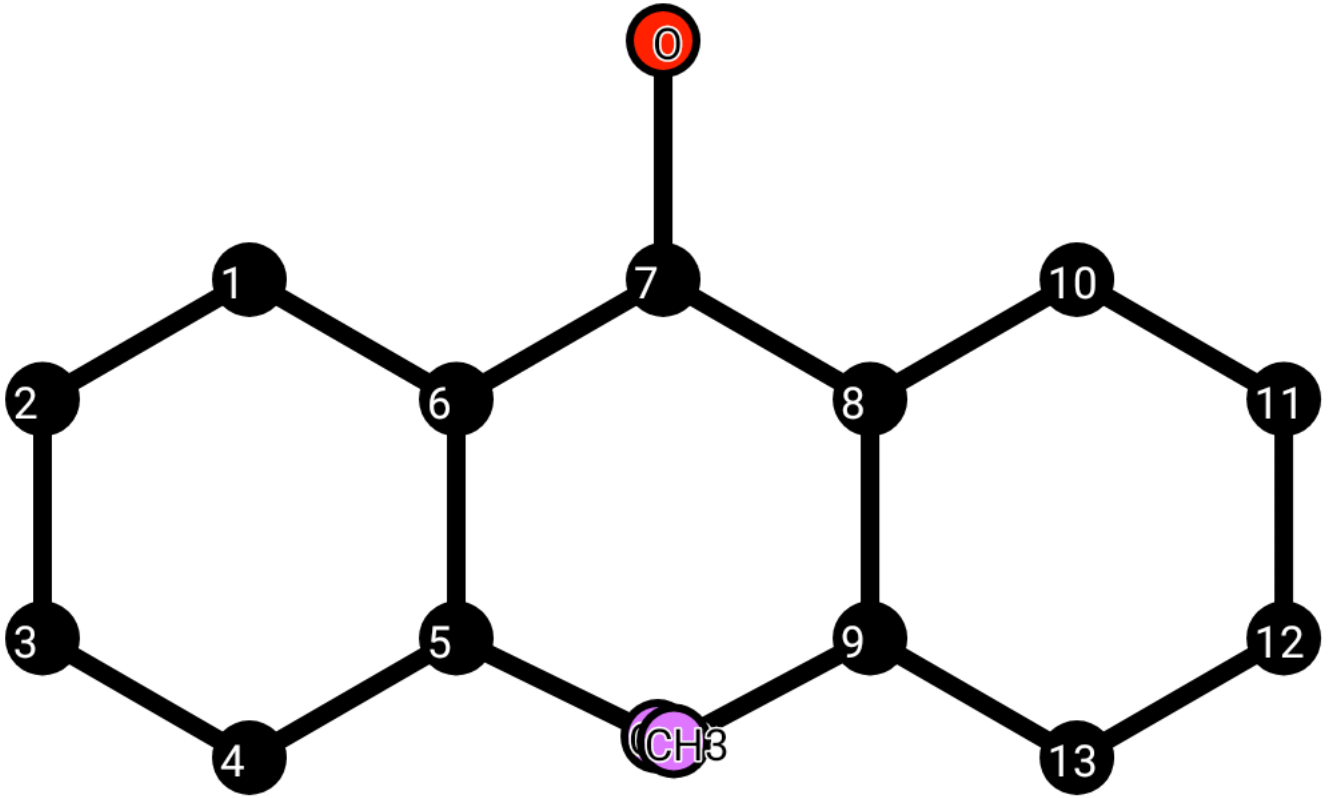

0
1
2
3
4
5
6
7
8
9
10
11
12
13
CH3

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	0.015	0.0	-0.011	-0.001	-0.012	0.004	0.002	0.0	0.0	0.0	0.0	0.0	0.0	0.003	0.0	0.0
1 6	0.006	0.003	0.009	0.0	0.013	-0.013	-0.007	0.001	-0.001	-0.001	0.0	-0.001	0.0	-0.009	0.0	0.0
2 3	-0.012	-0.003	0.01	0.001	0.011	-0.003	-0.002	0.0	0.0	0.0	0.0	0.0	0.0	-0.002	0.001	0.0
3 4	0.01	0.001	0.009	-0.003	-0.013	-0.001	-0.001	0.0	0.0	0.0	0.0	0.0	0.0	-0.001	-0.001	0.0
4 5	-0.012	-0.001	-0.011	0.0	0.016	0.001	0.002	0.0	0.0	0.0	0.0	0.0	0.0	0.002	0.003	0.0
5 6	0.013	-0.003	0.009	-0.001	0.008	-0.012	-0.007	0.001	-0.001	-0.001	0.0	-0.001	0.0	-0.009	0.002	0.0
5 15	0.0	0.016	-0.001	0.02	-0.015	0.02	0.001	0.0	0.0	0.0	0.0	0.0	0.0	0.005	-0.047	0.0
6 7	-0.028	0.001	-0.023	0.001	-0.028	0.017	0.026	-0.003	0.002	0.002	0.0	0.002	0.0	0.031	-0.001	0.0
7 8	0.002	0.0	0.002	0.0	0.002	-0.003	0.026	0.017	-0.028	-0.028	0.001	-0.023	0.001	0.031	0.0	-0.001
7 14	0.01	0.0	0.009	0.0	0.01	-0.002	0.038	-0.002	0.01	0.01	0.0	0.009	0.0	-0.095	0.001	0.001
8 9	-0.001	0.0	-0.001	0.0	-0.001	0.001	-0.007	-0.012	0.008	0.013	-0.003	0.009	-0.001	-0.009	0.0	0.002
8 10	-0.001	0.0	-0.001	0.0	-0.001	0.001	-0.007	-0.013	0.013	0.006	0.003	0.009	0.0	-0.009	0.0	0.0
9 13	0.0	0.0	0.0	0.0	0.0	0.0	0.002	0.001	0.016	-0.012	-0.001	-0.011	0.0	0.002	0.0	0.003
9 16	0.0	0.0	0.0	0.0	0.0	0.0	0.001	0.02	-0.015	0.0	0.016	-0.001	0.02	0.005	0.0	-0.047
10 11	0.0	0.0	0.0	0.0	0.0	0.0	0.002	0.004	-0.012	0.015	0.0	-0.011	-0.001	0.003	0.0	0.0
11 12	0.0	0.0	0.0	0.0	0.0	0.0	-0.002	-0.003	0.011	-0.012	-0.003	0.01	0.001	-0.002	0.0	0.001
12 13	0.0	0.0	0.0	0.0	0.0	0.0	-0.001	-0.001	-0.013	0.01	0.001	0.009	-0.003	-0.001	0.0	-0.001

7.2. Presentation of molecule: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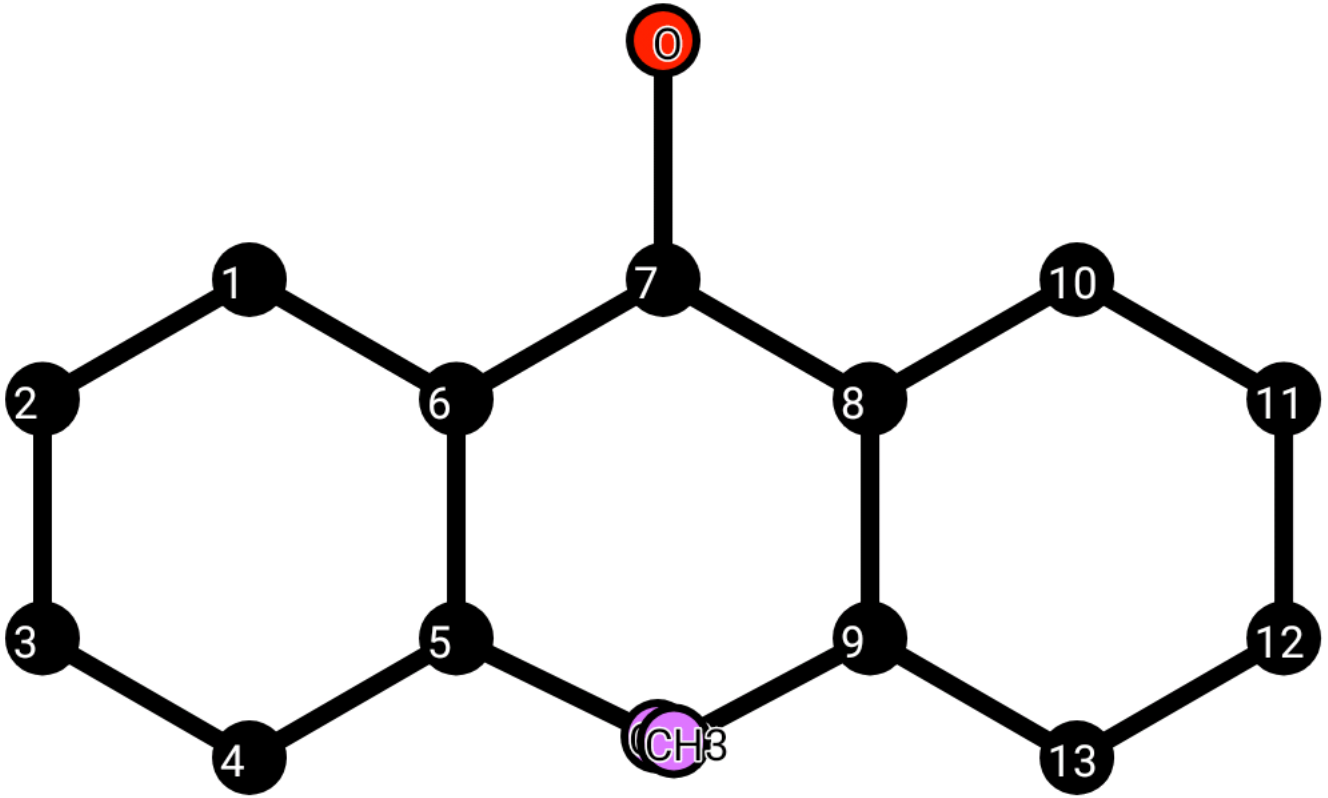
CH3

8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	2 3	3 4	4 5	5 6	5 15	6 7	7 8	7 14	8 9	8 10	9 13	9 16	10 11	11 12	12 13
1 2	0.245																
1 6	-0.196	0.245															
2 3	-0.21	0.126	0.248														
3 4	0.128	-0.086	-0.203	0.247													
4 5	-0.091	0.119	0.128	-0.209	0.246												
5 6	0.119	-0.175	-0.085	0.125	-0.193	0.245											
5 15	0.001	-0.001	-0.008	0.011	-0.033	-0.028	0.507										
6 7	0.014	-0.067	-0.009	-0.008	0.012	-0.066	0.013	0.283									
7 8	-0.001	0.003	0.0	0.0	0.0	0.003	-0.001	-0.024	0.283								
7 14	-0.006	0.022	0.004	0.003	-0.005	0.022	-0.006	-0.094	-0.094	0.113							
8 9	0.0	-0.001	0.0	0.0	0.0	-0.001	0.0	0.003	-0.066	0.022	0.245						
8 10	0.0	-0.001	0.0	0.0	0.0	-0.001	0.0	0.003	-0.067	0.022	-0.175	0.245					
9 13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.012	-0.005	-0.193	0.119	0.246				
9 16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.001	0.013	-0.006	-0.028	-0.001	-0.033	0.507			
10 11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.001	0.014	-0.006	0.119	-0.196	-0.091	0.001	0.245		
11 12	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.009	0.004	-0.085	0.126	0.128	-0.008	-0.21	0.248	
12 13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.008	0.003	0.125	-0.086	-0.209	0.011	0.128	-0.203	0.247

8.2. Presentation of molecule: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CH3