Print calculated values

Report generated by:root, 18.02.2020 - 15:24:15

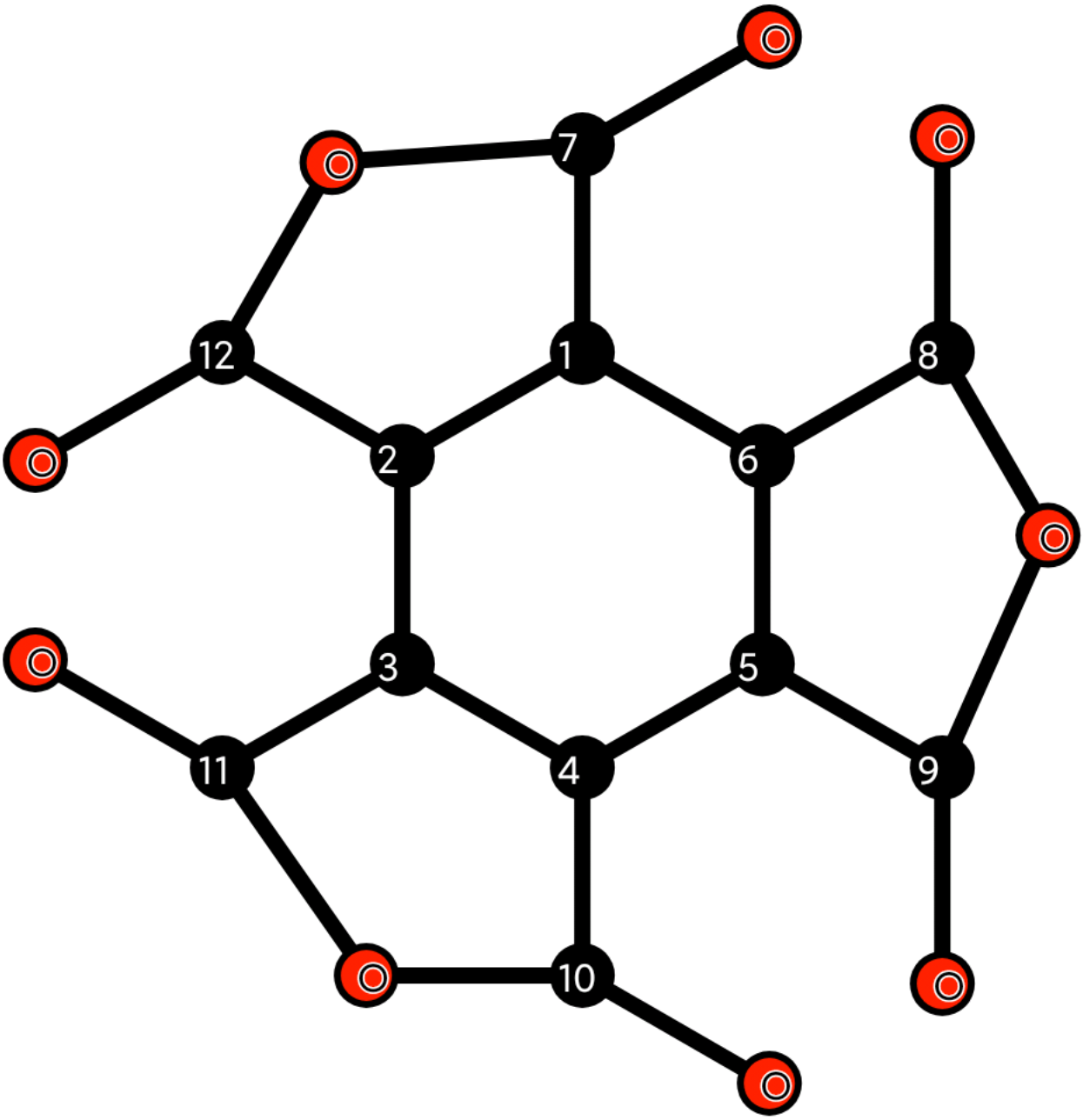
The following determinant is calculated:

-x	1.0	0.0	0.0	0.0	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	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	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	1.0	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	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	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	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	0.0	0.0	0.0
1.0	0.0	0.0	0.0	0.0	0.0	-x	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.19	1.93	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	0.0	0.0	0.0	0.0	0.19	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.93
0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	-x	0.0	0.0	0.0	0.19	0.0	0.0	0.0	0.0	0.0	0.0	1.93	0.0
0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	-x	0.0	0.0	0.0	0.19	0.0	0.0	0.0	0.0	1.93	0.0	0.0
0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-x	0.0	0.0	0.19	0.0	0.0	0.0	1.93	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	0.0	-x	0.0	0.0	0.19	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	0.19	0.19	0.0	0.0	0.0	-x+2.06	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	0.19	0.19	0.0	0.0	-x+2.06	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	0.19	0.0	0.0	0.0	0.0	0.19	0.0	0.0	-x+2.06	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	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	0.0	1.93	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	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	1.93	0.0	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	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	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	-x+1.18

It is about this molecule:

HMO-Energies

x1 = 3.039; x2 = 2.848; x3 = 2.848; x4 = 2.716; x5 = 2.716; x6 = 2.686; x7 = 2.056; x8 = 2.037; x9 = 2.037; x10 = 1.768; x11 = 1.037; x12 = 1.037; x13 = -0.454; x14 = -0.454; x15 = -0.893; x16 = -1.624; x17 = -1.686; x18 = -1.686; x19 = -2.077; x20 = -2.077; x21 = -2.613;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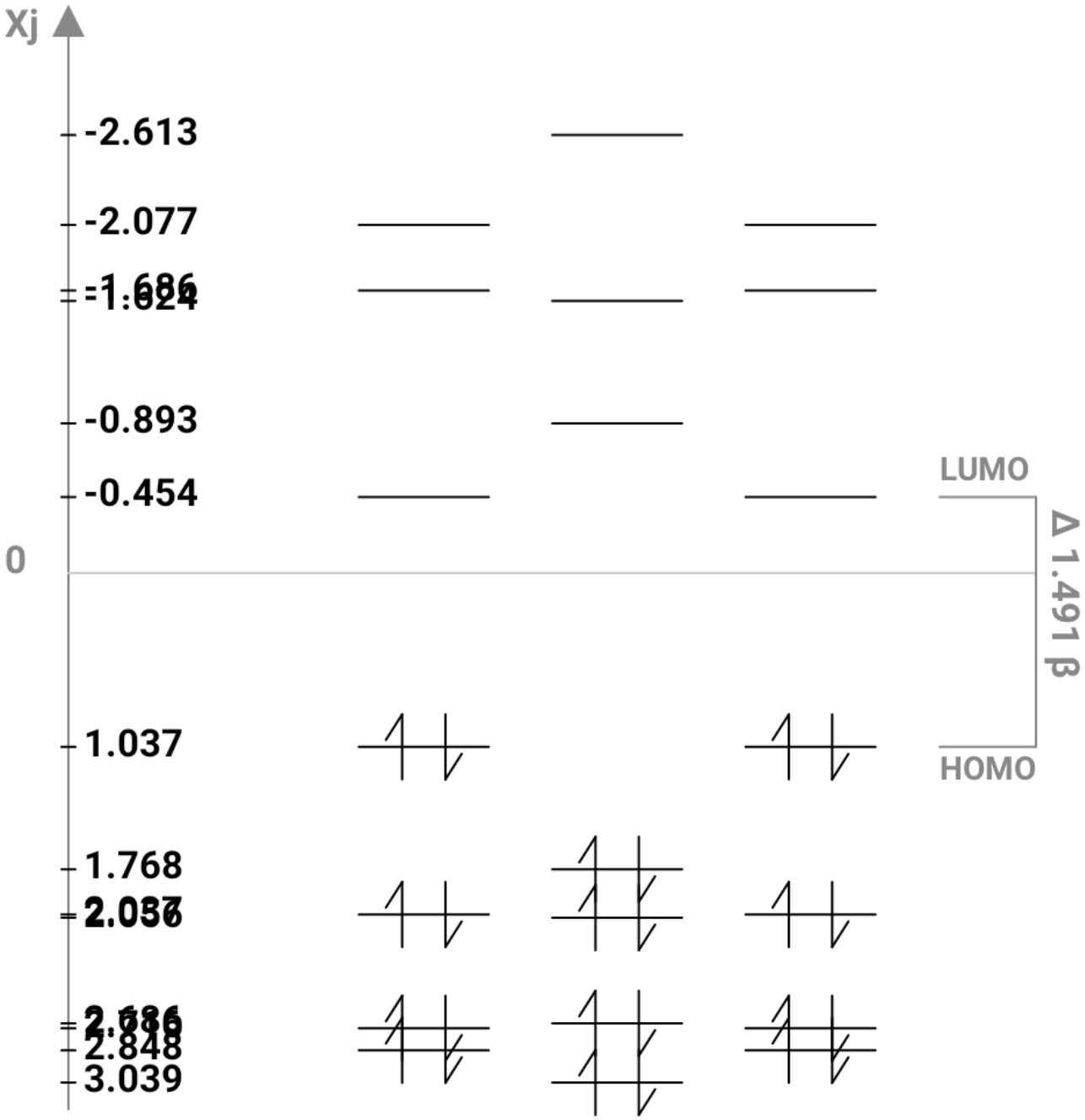
1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 21α + 53.65β -

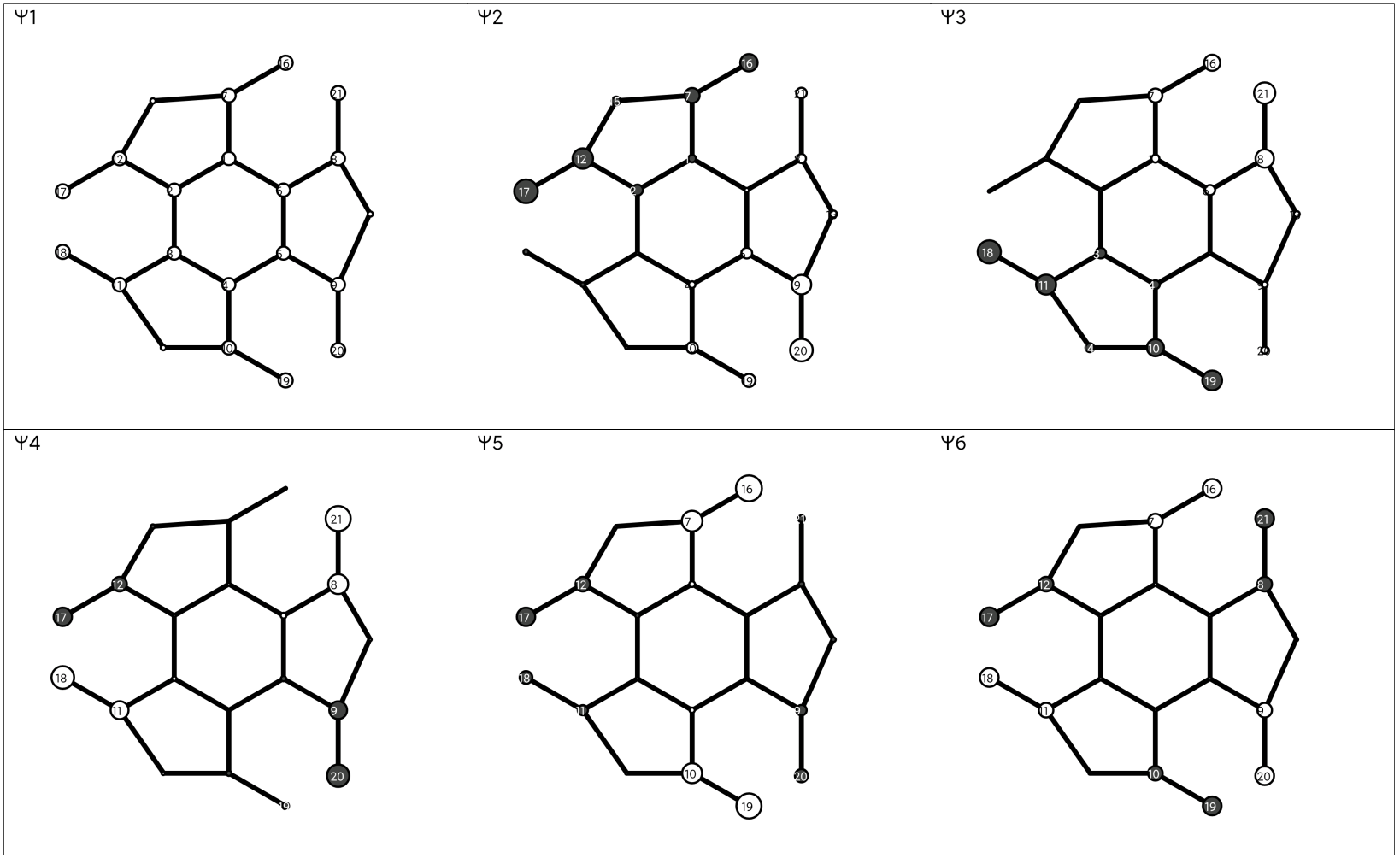
this corresponds to one πelectron: 2.235β

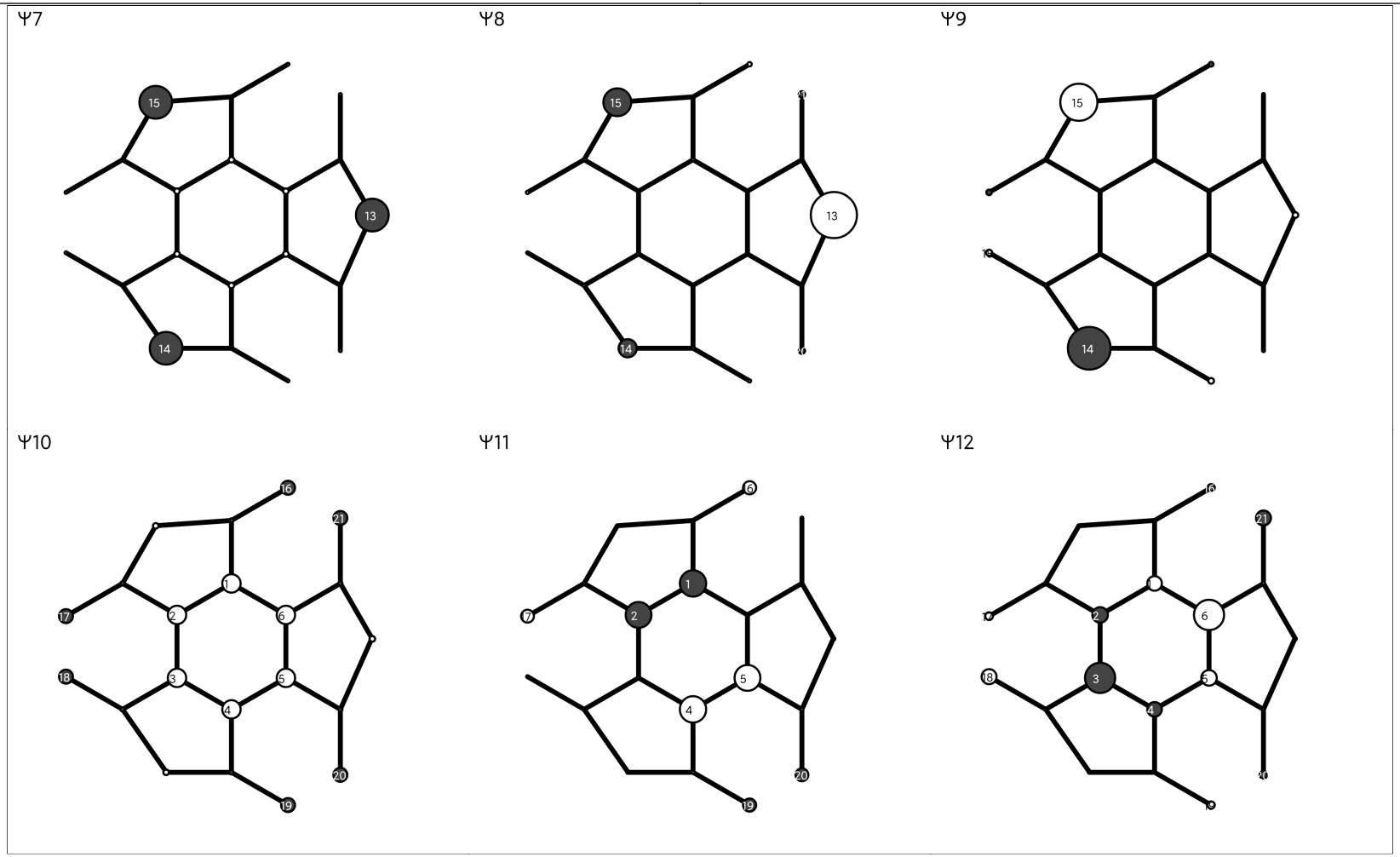
2. Hueckel-coefficient

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	Psi 20	Psi 21
	x1= 3.039	x2= 2.848	x3= 2.848	x4= 2.716	x5= 2.716	x6= 2.686	x7= 2.056	x8= 2.037	x9= 2.037	x10= 1.768	x11= 1.037	x12= 1.037	x13= - 0.454	x14= - 0.454	x15= - 0.893	x16= - 1.624	x17= - 1.686	x18= - 1.686	x19= - 2.077	x20= - 2.077	x21= - 2.613
1	0.224	-0.13	0.136	0.013	0.097	0.053	0.095	0.014	-0.037	0.315	-0.452	0.25	0.383	-0.219	0.225	0.09	-0.091	-0.144	-0.183	-0.31	0.336
2	0.224	-0.187	-0.023	-0.059	-0.078	-0.053	0.095	0.032	-0.024	0.315	-0.443	-0.266	-0.38	-0.223	-0.225	0.09	0.088	-0.145	-0.18	0.312	-0.336
3	0.224	-0.053	-0.181	0.077	-0.06	0.053	0.095	0.025	0.031	0.315	0.009	-0.517	-0.001	0.441	0.225	0.09	0.17	-0.006	0.36	-0.003	0.336
4	0.224	0.113	-0.15	-0.038	0.09	-0.053	0.095	0.005	0.039	0.315	0.452	-0.25	0.383	-0.218	-0.225	0.09	0.082	0.149	-0.18	-0.312	-0.336
5	0.224	0.183	0.044	-0.09	-0.037	0.053	0.095	-0.039	0.006	0.315	0.443	0.266	-0.381	-0.222	0.225	0.09	-0.079	0.151	-0.178	0.313	0.336
6	0.224	0.073	0.173	0.097	-0.012	-0.053	0.095	-0.037	-0.016	0.315	-0.009	0.517	-0.003	0.441	-0.225	0.09	-0.17	-0.004	0.36	0.0	-0.336
7	0.233	-0.256	0.238	-0.003	0.353	0.249	0.005	0.033	-0.036	-0.073	-0.017	0.009	0.21	-0.118	0.249	-0.327	0.235	0.392	0.2	0.333	-0.206
8	0.233	0.156	0.313	0.341	-0.091	-0.249	0.005	-0.049	-0.001	-0.073	0.0	0.019	0.0	0.241	-0.249	-0.327	0.457	0.0	-0.388	-0.003	0.206
9	0.233	0.334	0.103	-0.304	-0.179	0.249	0.005	-0.048	-0.011	-0.073	0.016	0.01	-0.207	-0.122	0.249	-0.327	0.222	-0.399	0.188	-0.339	-0.206
10	0.233	0.193	-0.291	-0.091	0.341	-0.249	0.005	0.024	0.043	-0.073	0.017	-0.009	0.208	-0.12	-0.249	-0.327	-0.229	-0.396	0.191	0.338	0.206
11	0.233	-0.078	-0.341	0.307	-0.174	0.249	0.005	0.015	0.047	-0.073	0.0	-0.019	-0.002	0.241	0.249	-0.327	-0.457	0.007	-0.388	0.006	-0.206
12	0.233	-0.349	-0.021	-0.249	-0.249	-0.249	0.005	0.026	-0.042	-0.073	-0.016	-0.01	-0.208	-0.12	-0.249	-0.327	-0.229	0.396	0.197	-0.334	0.206
13	0.09	0.118	0.1	0.011	-0.078	0.0	-0.561	0.79	0.096	0.095	-0.003	-0.005	0.016	-0.009	0.0	0.034	-0.034	0.02	0.009	0.016	0.0
14	0.09	0.028	-0.152	0.062	0.048	0.0	-0.561	-0.312	-0.733	0.095	-0.003	0.005	-0.016	-0.009	0.0	0.034	0.035	0.02	0.009	-0.016	0.0
15	0.09	-0.146	0.052	-0.073	0.03	0.0	-0.561	-0.478	0.637	0.095	0.006	0.0	0.0	0.018	0.0	0.034	0.0	-0.04	-0.018	0.0	0.0
16	0.242	-0.297	0.275	-0.004	0.443	0.319	0.012	0.075	-0.082	-0.24	0.225	-0.125	-0.248	0.14	-0.232	0.225	-0.158	-0.264	-0.118	-0.197	0.105
17	0.242	-0.404	-0.025	-0.313	-0.313	-0.319	0.012	0.058	-0.095	-0.24	0.22	0.133	0.246	0.142	0.232	0.225	0.154	-0.267	-0.117	0.198	-0.105
18	0.242	-0.09	-0.394	0.386	-0.218	0.319	0.012	0.033	0.106	-0.24	-0.004	0.257	0.003	-0.284	-0.232	0.225	0.308	-0.005	0.23	-0.004	0.105
19	0.242	0.223	-0.337	-0.115	0.428	-0.319	0.012	0.053	0.097	-0.24	-0.225	0.124	-0.246	0.142	0.232	0.225	0.154	0.267	-0.113	-0.2	-0.105
20	0.242	0.387	0.119	-0.382	-0.225	0.319	0.012	-0.108	-0.024	-0.24	-0.22	-0.132	0.245	0.145	-0.232	0.225	-0.15	0.269	-0.112	0.201	0.105
21	0.242	0.18	0.362	0.428	-0.115	-0.319	0.012	-0.111	-0.003	-0.24	0.005	-0.257	0.0	-0.284	0.232	0.225	-0.308	0.0	0.23	0.002	-0.105

2.2. Molecule orbital presentation:


Ψ1
Ψ2
Ψ3
Ψ4
Ψ5
Ψ6


Ψ7
15
13
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Ψ8
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13
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Ψ9
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14
Ψ10
16
21
1
17
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18
3
5
4
20
19
Ψ11
6
1
7
2
5
4
20
19
Ψ12
21
2
6
18
3
5
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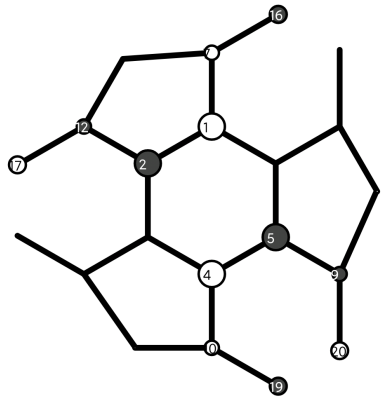
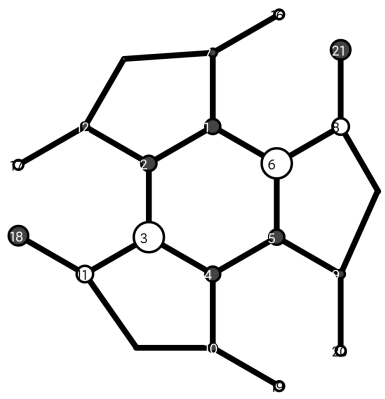
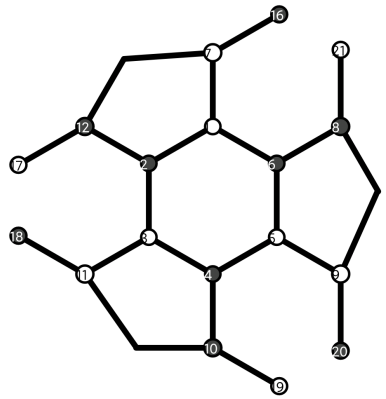
Ψ13



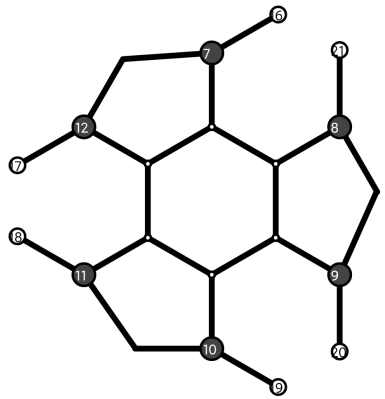
Ψ14



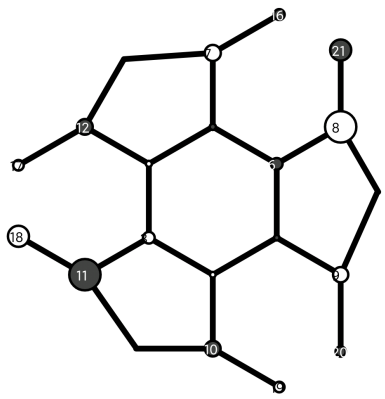
Ψ15



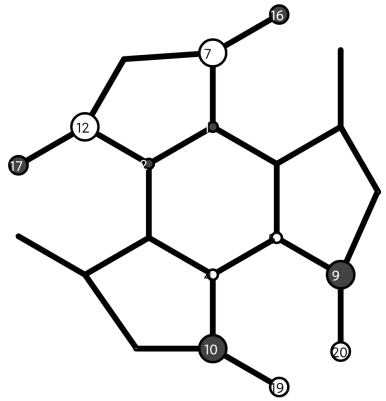
Ψ16



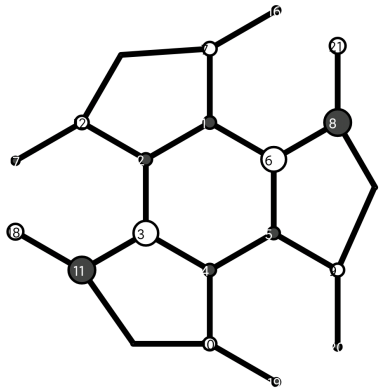
Ψ17



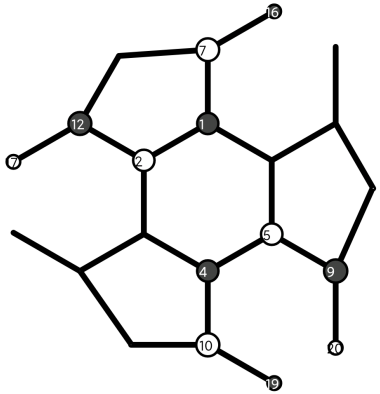
Ψ18



Ψ19



Ψ20



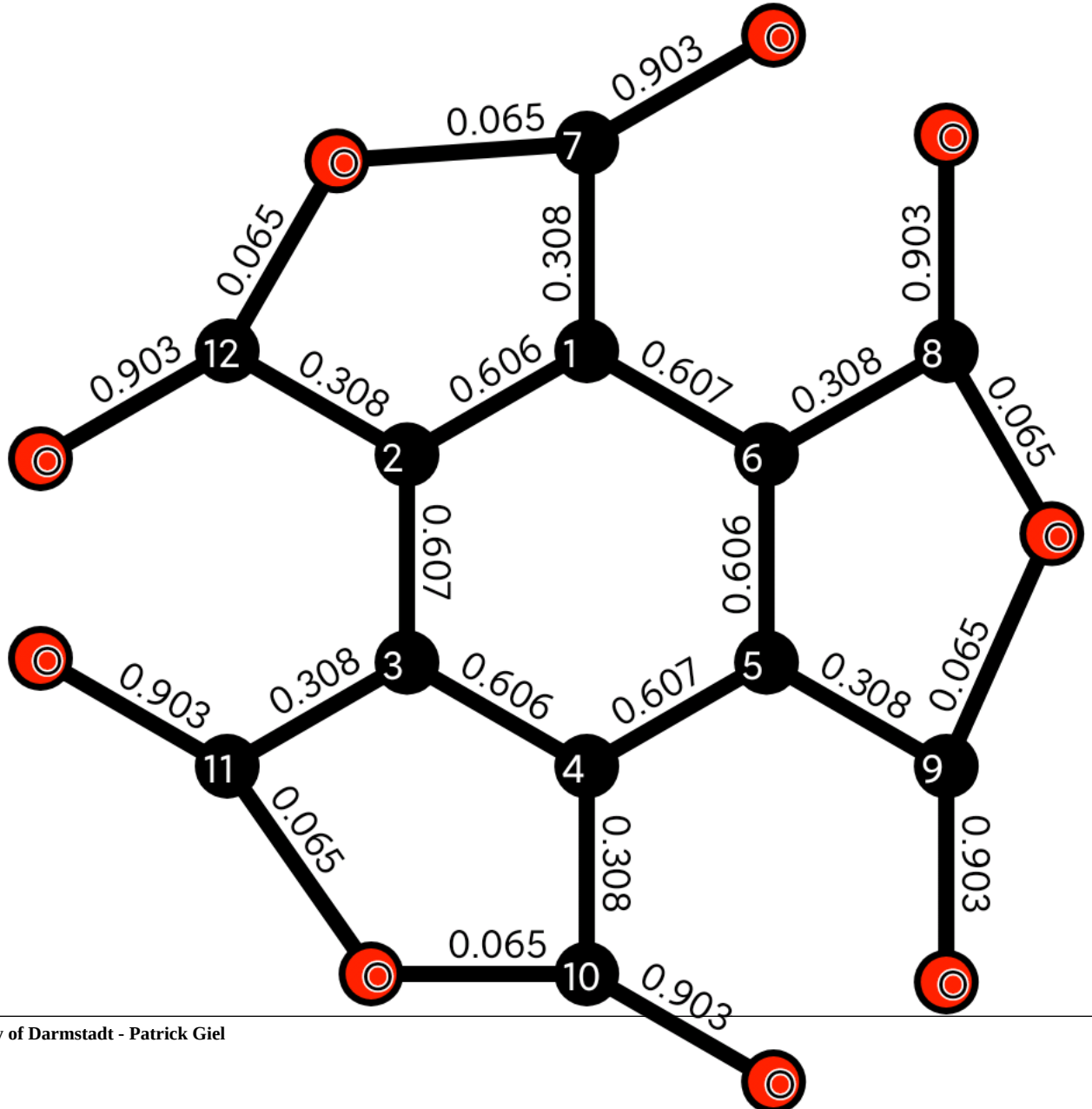
The picture export was cancelled, more than 20 pictures are not possible.

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	20	21
1	0.95																				
2	0.606	0.95																			
3	0.009	0.607	0.95																		
4	-0.279	0.009	0.606	0.95																	
5	0.009	-0.279	0.009	0.607	0.95																
6	0.607	0.009	-0.279	0.009	0.606	0.95															
7	0.308	0.076	-0.026	-0.056	-0.026	0.077	0.742														
8	0.077	-0.026	-0.056	-0.026	0.076	0.308	-0.005	0.742													
9	-0.026	-0.056	-0.026	0.077	0.308	0.076	-0.006	-0.006	0.742												
10	-0.056	-0.026	0.076	0.308	0.077	-0.026	-0.004	-0.006	-0.005	0.742											
11	-0.026	0.077	0.308	0.076	-0.026	-0.056	-0.006	-0.004	-0.006	-0.006	0.742										
12	0.076	0.308	0.077	-0.026	-0.056	-0.026	-0.006	-0.006	-0.004	-0.006	-0.005	0.742									
13	-0.009	0.007	0.007	-0.009	-0.016	-0.016	0.0	0.065	0.065	0.0	0.002	0.002	1.993								
14	0.007	-0.009	-0.016	-0.016	-0.009	0.007	0.002	0.002	0.0	0.065	0.065	0.0	0.0	1.993							
15	-0.016	-0.016	-0.009	0.007	0.007	-0.009	0.065	0.0	0.002	0.002	0.0	0.065	0.0	0.0	1.993						
16	-0.026	-0.169	0.004	0.115	0.002	-0.17	0.903	-0.027	0.008	0.022	0.008	-0.029	0.003	-0.003	-0.046	1.312					
17	-0.169	-0.026	-0.17	0.002	0.115	0.004	-0.029	0.008	0.022	0.008	-0.027	0.903	-0.003	0.003	-0.046	0.069	1.312				
18	0.002	-0.17	-0.026	-0.169	0.004	0.115	0.008	0.022	0.008	-0.029	0.903	-0.027	-0.003	-0.046	0.003	-0.003	0.065	1.312			
19	0.115	0.004	-0.169	-0.026	-0.17	0.002	0.022	0.008	-0.027	0.903	-0.029	0.008	0.003	-0.046	-0.003	-0.05	-0.003	0.069	1.312		
20	0.004	0.115	0.002	-0.17	-0.026	-0.169	0.008	-0.029	0.903	-0.027	0.008	0.022	-0.046	0.003	-0.003	-0.003	-0.05	-0.003	0.065	1.312	
21	-0.17	0.002	0.115	0.004	-0.169	-0.026	-0.027	0.903	-0.029	0.008	0.022	0.008	-0.046	-0.003	0.003	0.065	-0.003	-0.05	-0.003	0.069	1.312

3.2. Presentation of bond order:


0.903
0.065
7
0.065
0.308
0.903
0.903
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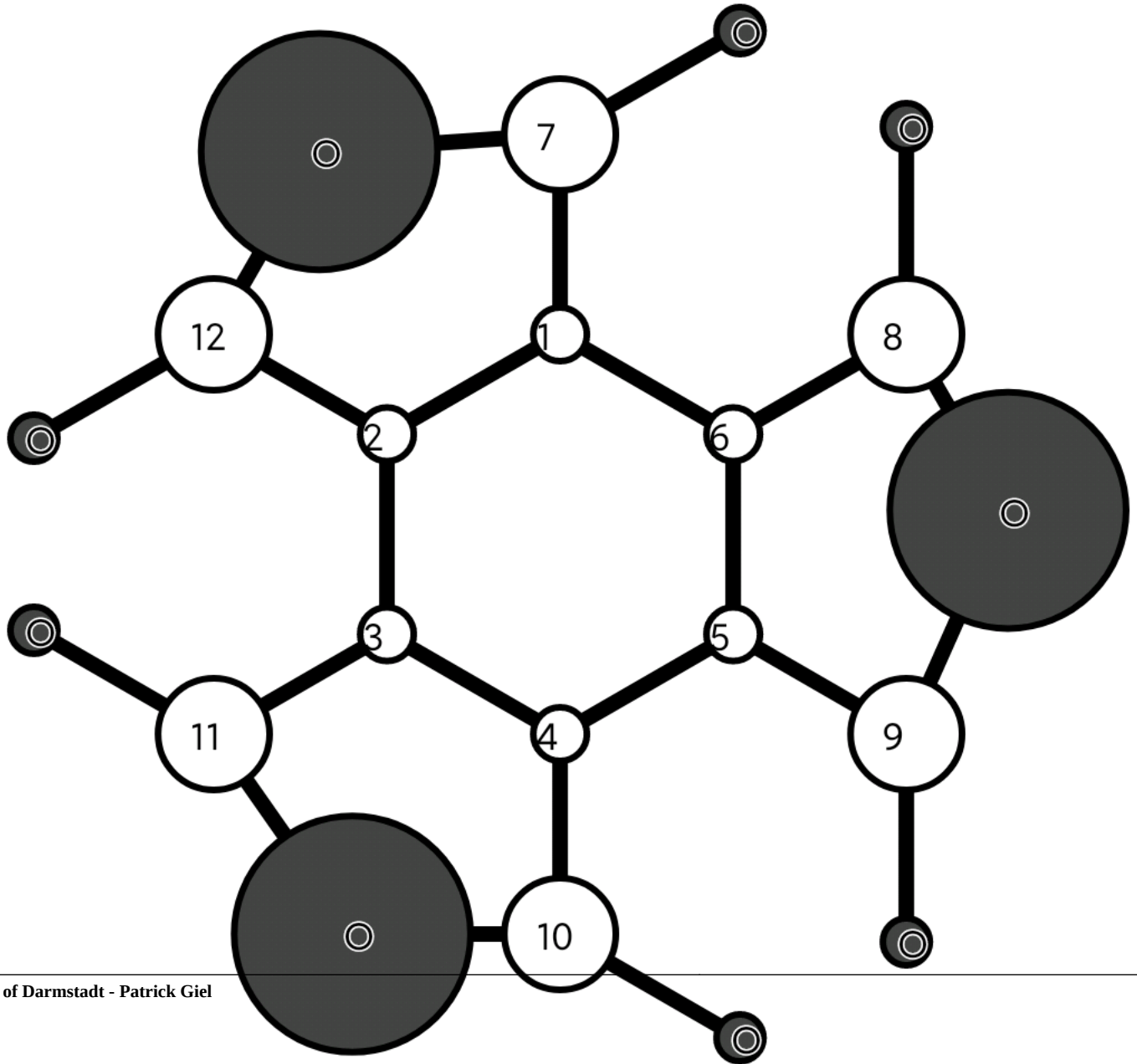
0.308
0.606
1
0.607
0.308
8
0.065
2
0.607
0.606
6
3
0.903
0.308
0.606
0.607
5
0.308
0.065
11
4
9
0.065
0.308
0.903
0.065
10
0.903

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	20	21
1	0.193																				
2		0.193																			
3			0.193																		
4				0.193																	
5					0.193																
6						0.193															
7							0.401														
8								0.401													
9									0.401												
10										0.401											
11											0.401										
12												0.401									
13													-0.85								
14														-0.85							
15															-0.85						
16																-0.169					
17																	-0.169				
18																		-0.169			
19																			-0.169		
20																				-0.169	
21																					-0.169

4.2. Presentation of molecule: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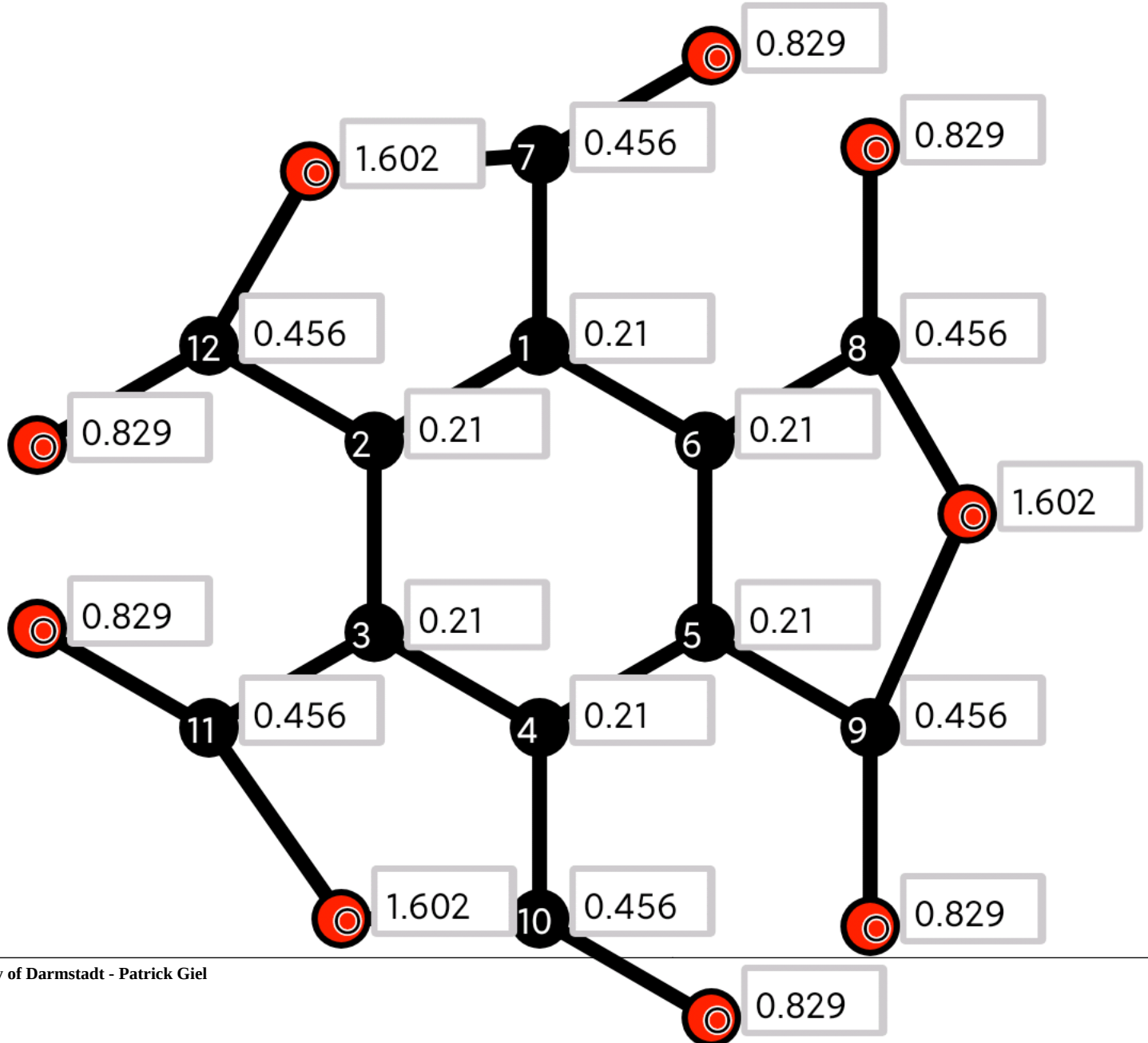
5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
0.21	0.21	0.21	0.21	0.21	0.21	0.456	0.456	0.456	0.456	0.456	0.456	1.602	1.602	1.602	0.829	0.829	0.829	0.829	0.829	0.829

5.2. Presentation of molecule:

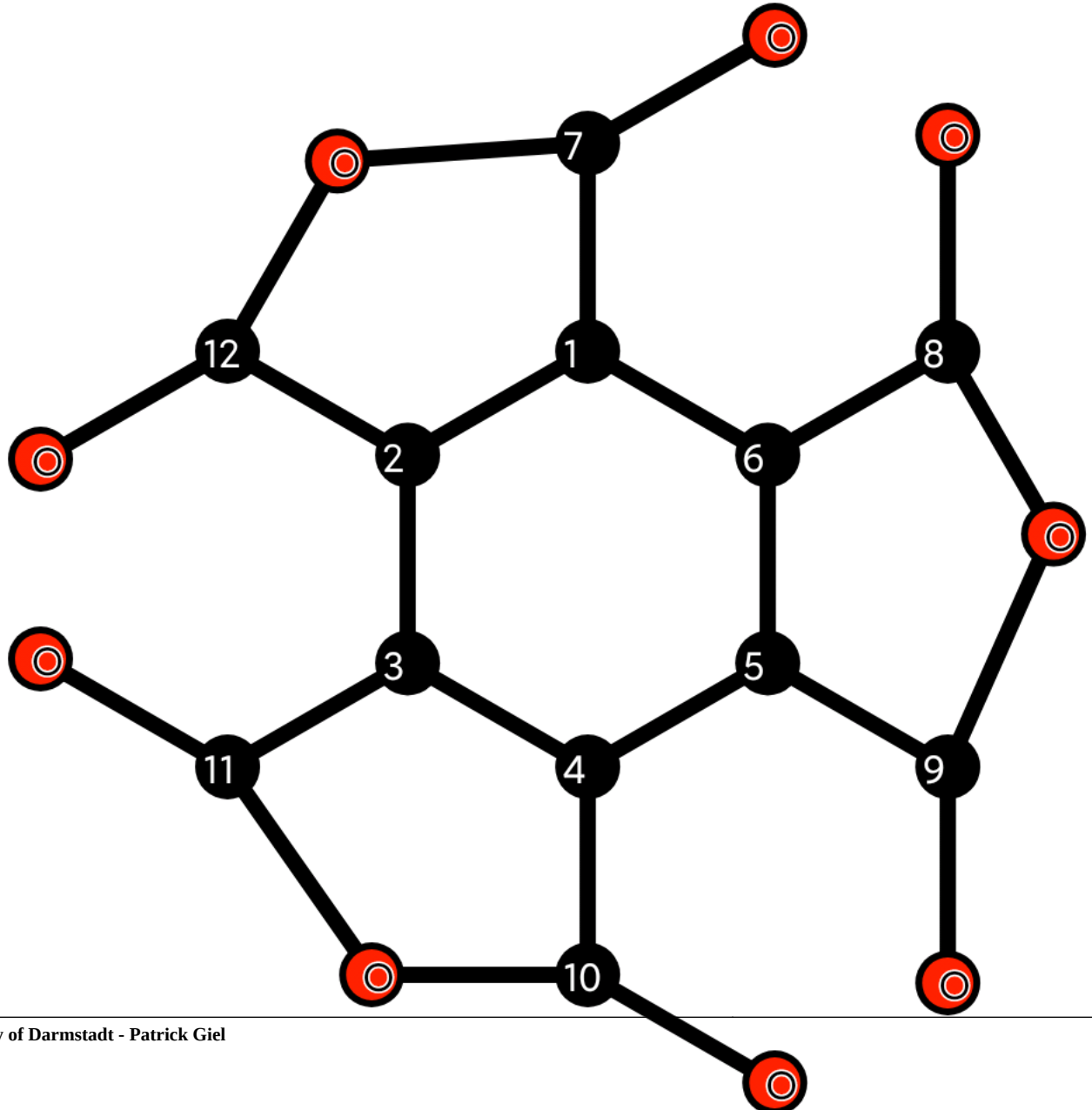

0.829
1.602
7
0.456
0.829
12
0.456
1
0.21
8
0.456
0.829
2
0.21
6
0.21
1.602
0.829
3
0.21
5
0.21
11
0.456
4
0.21
9
0.456
1.602
10
0.456
0.829
0.829

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	20	21
1	0.386																				
2	-0.131	0.386																			
3	0.008	-0.132	0.386																		
4	-0.081	0.008	-0.131	0.386																	
5	0.008	-0.081	0.008	-0.132	0.386																
6	-0.132	0.008	-0.081	0.008	-0.131	0.386															
7	-0.011	-0.002	0.0	-0.003	0.0	-0.002	0.215														
8	-0.002	0.0	-0.003	0.0	-0.002	-0.011	0.0	0.215													
9	0.0	-0.003	0.0	-0.002	-0.011	-0.002	0.0	0.0	0.215												
10	-0.003	0.0	-0.002	-0.011	-0.002	0.0	0.0	0.0	0.0	0.215											
11	0.0	-0.002	-0.011	-0.002	0.0	-0.003	0.0	0.0	0.0	0.0	0.215										
12	-0.002	-0.011	-0.002	0.0	-0.003	0.0	0.0	0.0	0.0	0.0	0.0	0.215									
13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.001	-0.001	0.0	0.0	0.0	0.004								
14	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.001	-0.001	0.0	0.0	0.004							
15	0.0	0.0	0.0	0.0	0.0	0.0	-0.001	0.0	0.0	0.0	0.0	-0.001	0.0	0.0	0.004						
16	0.023	-0.024	0.001	-0.017	0.001	-0.024	-0.195	-0.001	0.0	-0.001	0.0	-0.001	0.0	0.0	-0.001	0.25					
17	-0.024	0.023	-0.024	0.001	-0.017	0.001	-0.001	0.0	-0.001	0.0	-0.001	-0.195	0.0	0.0	-0.001	-0.005	0.25				
18	0.001	-0.024	0.023	-0.024	0.001	-0.017	0.0	-0.001	0.0	-0.001	-0.195	-0.001	0.0	-0.001	0.0	0.0	-0.005	0.25			
19	-0.017	0.001	-0.024	0.023	-0.024	0.001	-0.001	0.0	-0.001	-0.195	-0.001	0.0	0.0	-0.001	0.0	-0.004	0.0	-0.005	0.25		
20	0.001	-0.017	0.001	-0.024	0.023	-0.024	0.0	-0.001	-0.195	-0.001	0.0	-0.001	-0.001	0.0	0.0	0.0	-0.004	0.0	-0.005	0.25	
21	-0.024	0.001	-0.017	0.001	-0.024	0.023	-0.001	-0.195	-0.001	0.0	-0.001	0.0	-0.001	0.0	0.0	-0.005	0.0	-0.004	0.0	-0.005	0.25

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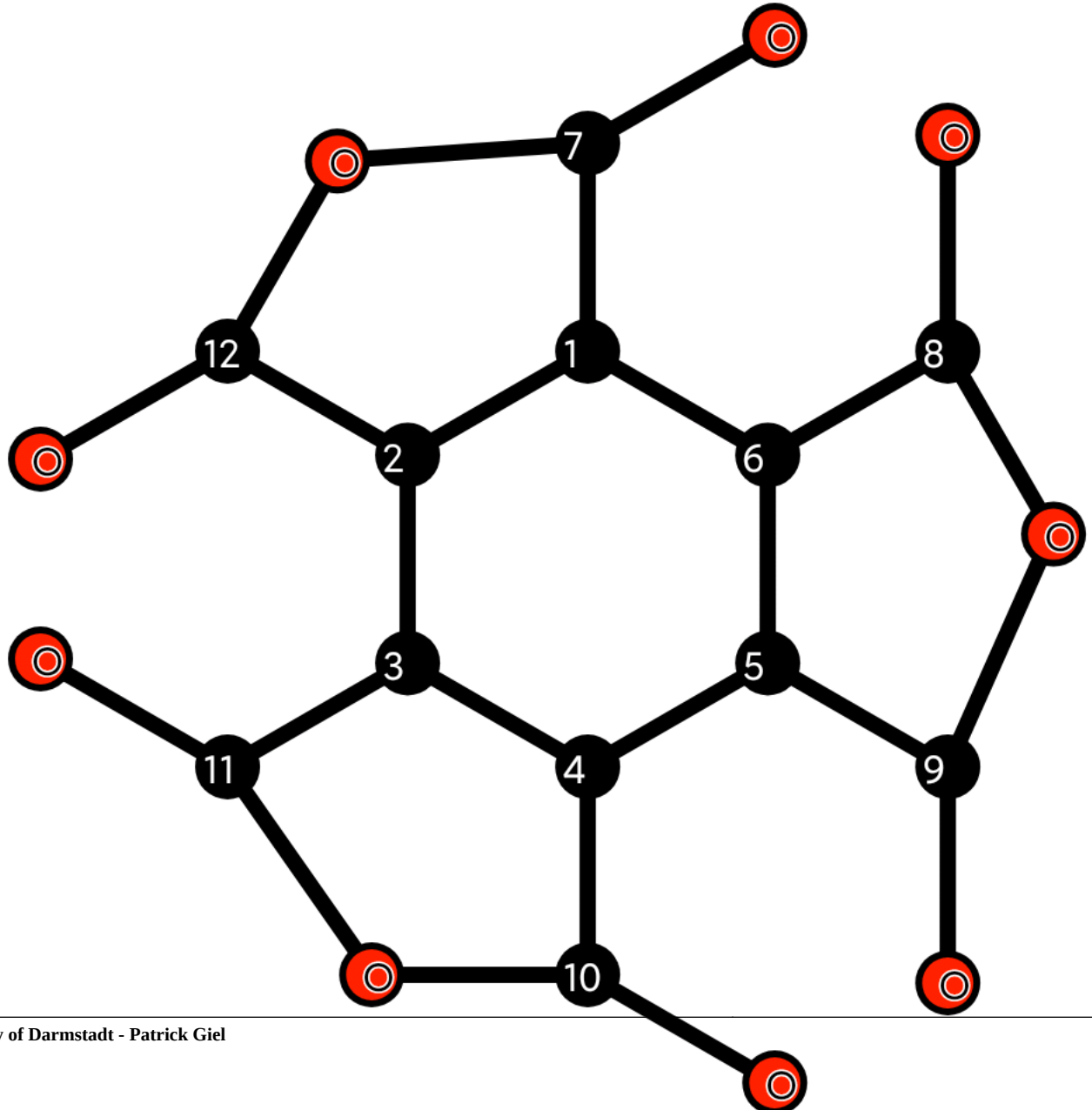
7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
1 2	0.011	0.011	-0.002	0.001	0.001	-0.002	-0.007	0.002	-0.001	-0.001	0.002	-0.007	0.0	0.0	0.0	-0.003	-0.003	0.001	-0.001	-0.001	0.001
1 6	0.011	-0.002	0.001	0.001	-0.002	0.011	-0.007	-0.007	0.002	-0.001	-0.001	0.002	0.0	0.0	0.0	-0.003	0.001	0.0	0.0	0.001	-0.003
1 7	0.031	-0.026	0.001	-0.018	0.002	-0.026	0.031	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.019	-0.005	0.0	-0.004	0.0	-0.005
2 3	-0.002	0.011	0.011	-0.002	0.001	0.001	0.002	-0.001	-0.001	0.002	-0.007	-0.007	0.0	0.0	0.0	0.001	-0.003	-0.003	0.001	0.0	0.0
2 12	-0.026	0.031	-0.026	0.002	-0.018	0.001	0.0	0.0	0.0	0.0	0.0	0.031	0.0	0.0	0.0	-0.005	0.019	-0.005	0.0	-0.004	0.0
3 4	0.001	-0.002	0.011	0.011	-0.002	0.001	-0.001	-0.001	0.002	-0.007	-0.007	0.002	0.0	0.0	0.0	-0.001	0.001	-0.003	-0.003	0.001	-0.001
3 11	0.002	-0.026	0.031	-0.026	0.001	-0.018	0.0	0.0	0.0	0.0	0.031	0.0	0.0	0.0	0.0	0.0	-0.005	0.019	-0.005	0.0	-0.004
4 5	0.001	0.001	-0.002	0.011	0.011	-0.002	-0.001	0.002	-0.007	-0.007	0.002	-0.001	0.0	0.0	0.0	0.0	0.0	0.001	-0.003	-0.003	0.001
4 10	-0.018	0.001	-0.026	0.031	-0.026	0.002	0.0	0.0	0.0	0.031	0.0	0.0	0.0	0.0	0.0	-0.004	0.0	-0.005	0.019	-0.005	0.0
5 6	-0.002	0.001	0.001	-0.002	0.011	0.011	0.002	-0.007	-0.007	0.002	-0.001	-0.001	0.0	0.0	0.0	0.001	-0.001	-0.001	0.001	-0.003	-0.003
5 9	0.001	-0.018	0.002	-0.026	0.031	-0.026	0.0	0.0	0.031	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.004	0.0	-0.005	0.019	-0.005
6 8	-0.026	0.002	-0.018	0.001	-0.026	0.031	0.0	0.031	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.005	0.0	-0.004	0.0	-0.005	0.019
7 15	0.001	0.001	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.018	0.016	-0.001	0.0	0.0	0.0	0.0
7 16	-0.008	0.011	0.0	0.008	-0.001	0.011	0.051	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.001	-0.079	0.002	0.0	0.002	0.0	0.002
8 13	0.0	0.0	0.0	0.0	0.001	0.001	0.0	0.0	0.0	0.0	0.0	0.0	-0.018	0.0	0.0	0.0	0.0	0.0	0.0	-0.001	0.016
8 21	0.011	-0.001	0.008	0.0	0.011	-0.008	0.0	0.051	0.0	0.0	0.0	0.0	0.001	0.0	0.0	0.002	0.0	0.002	0.0	0.002	-0.079
9 13	0.0	0.0	0.0	0.0	0.001	0.001	0.0	0.0	0.0	0.0	0.0	0.0	-0.018	0.0	0.0	0.0	0.0	0.0	0.0	0.016	-0.001
9 20	0.0	0.008	-0.001	0.011	-0.008	0.011	0.0	0.0	0.051	0.0	0.0	0.0	0.001	0.0	0.0	0.0	0.002	0.0	0.002	-0.079	0.002
10 14	0.0	0.0	0.001	0.001	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.018	0.0	0.0	0.0	-0.001	0.016	0.0	0.0
10 19	0.008	0.0	0.011	-0.008	0.011	-0.001	0.0	0.0	0.0	0.051	0.0	0.0	0.0	0.001	0.0	0.002	0.0	0.002	-0.079	0.002	0.0
11 14	0.0	0.0	0.001	0.001	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.018	0.0	0.0	0.0	0.016	-0.001	0.0	0.0
11 18	-0.001	0.011	-0.008	0.011	0.0	0.008	0.0	0.0	0.0	0.0	0.051	0.0	0.0	0.001	0.0	0.0	0.002	-0.079	0.002	0.0	0.002
12 15	0.001	0.001	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.018	-0.001	0.016	0.0	0.0	0.0	0.0
12 17	0.011	-0.008	0.011	-0.001	0.008	0.0	0.0	0.0	0.0	0.0	0.0	0.051	0.0	0.0	0.001	0.002	-0.079	0.002	0.0	0.002	0.0

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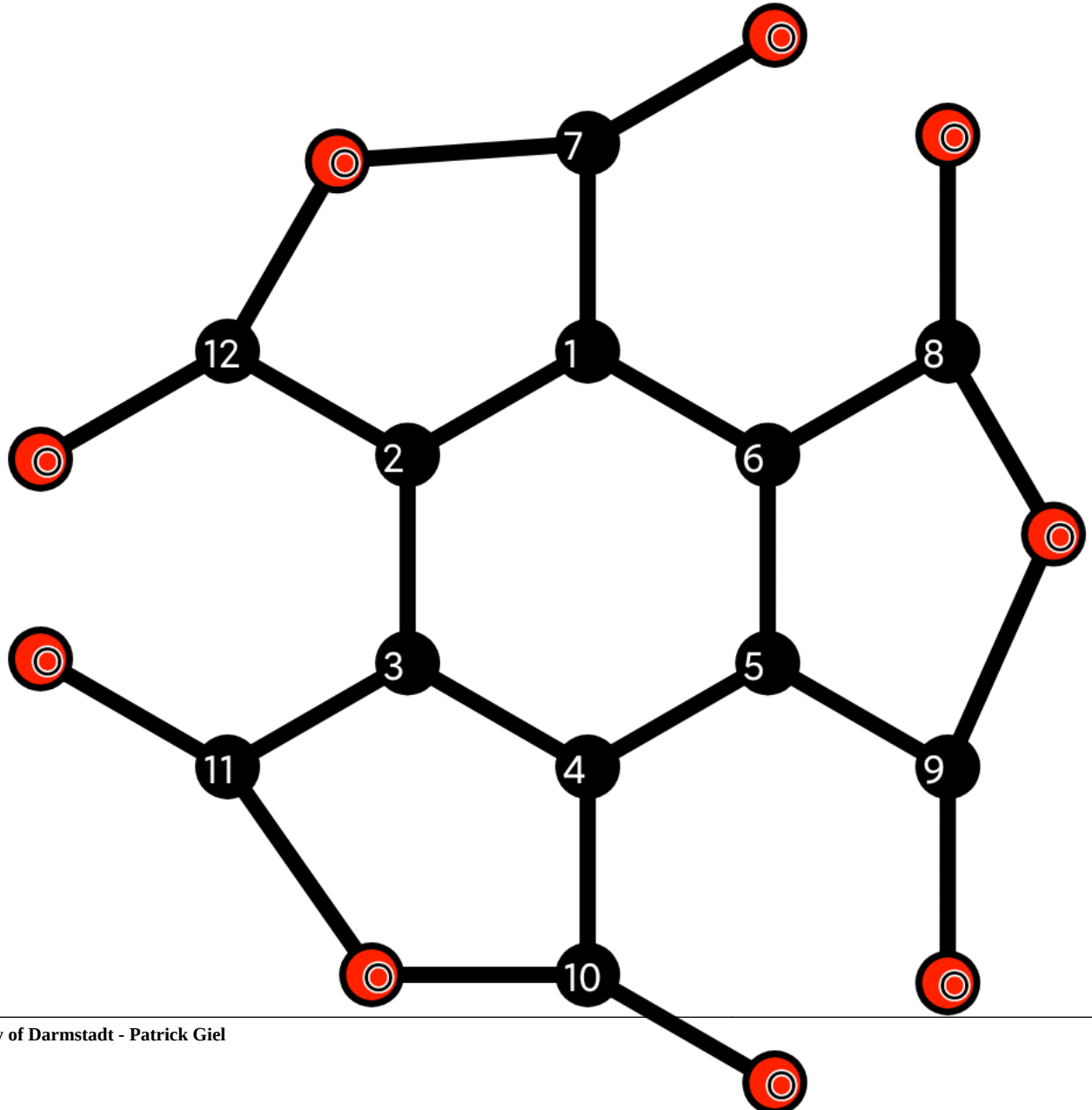
8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	1 7	2 3	2 12	3 4	3 11	4 5	4 10	5 6	5 9	6 8	7 15	7 16	8 13	8 21	9 13	9 20	10 14	10 19	11 14	11 18	12 15	12 17
1 2	0.254																							
1 6	-0.174	0.254																						
1 7	-0.057	-0.057	0.287																					
2 3	-0.174	0.106	0.01	0.254																				
2 12	-0.057	0.01	-0.004	-0.057	0.287																			
3 4	0.106	-0.073	-0.005	-0.174	0.01	0.254																		
3 11	0.01	-0.005	0.0	-0.057	-0.004	-0.057	0.287																	
4 5	-0.073	0.106	-0.005	0.106	-0.005	-0.174	0.01	0.254																
4 10	-0.005	-0.005	-0.006	0.01	0.0	-0.057	-0.004	-0.057	0.287															
5 6	0.106	-0.174	0.01	-0.073	-0.005	0.106	-0.005	-0.174	0.01	0.254														
5 9	-0.005	0.01	0.0	-0.005	-0.006	0.01	0.0	-0.057	-0.004	-0.057	0.287													
6 8	0.01	-0.057	-0.004	-0.005	0.0	-0.005	-0.006	0.01	0.0	-0.057	-0.004	0.287												
7 15	0.002	0.002	-0.008	0.0	-0.001	0.0	0.0	0.001	0.0	-0.001	0.0	0.0	0.347											
7 16	0.019	0.019	-0.097	-0.004	0.002	0.003	0.0	0.002	0.003	-0.004	0.0	0.002	-0.022	0.078										
8 13	-0.001	0.002	0.0	0.001	0.0	0.0	0.0	0.0	0.0	0.002	-0.001	-0.008	0.0	0.0	0.347									
8 21	-0.004	0.019	0.002	0.002	0.0	0.003	0.003	-0.004	0.0	0.019	0.002	-0.097	0.0	-0.001	-0.022	0.078								
9 13	0.0	0.0	0.0	0.001	0.0	-0.001	0.0	0.002	0.0	0.002	-0.008	-0.001	0.0	0.0	-0.007	0.001	0.347							
9 20	0.003	-0.004	0.0	0.002	0.003	-0.004	0.0	0.019	0.002	0.019	-0.097	0.002	0.0	0.0	0.001	-0.001	-0.022	0.078						
10 14	0.0	0.001	0.0	0.0	0.0	0.002	-0.001	0.002	-0.008	-0.001	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.347					
10 19	0.003	0.002	0.003	-0.004	0.0	0.019	0.002	0.019	-0.097	-0.004	0.002	0.0	0.0	-0.001	0.0	0.0	0.0	-0.001	-0.022	0.078				
11 14	-0.001	0.001	0.0	0.002	0.0	0.002	-0.008	0.0	-0.001	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.007	0.001	0.347			
11 18	-0.004	0.002	0.0	0.019	0.002	0.019	-0.097	-0.004	0.002	0.003	0.0	0.003	0.0	0.0	0.0	-0.001	0.0	0.0	0.001	-0.001	-0.022	0.078		
12 15	0.002	0.0	-0.001	0.002	-0.008	-0.001	0.0	0.001	0.0	0.0	0.0	0.0	-0.007	0.001	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.347	
12 17	0.019	-0.004	0.002	0.019	-0.097	-0.004	0.002	0.002	0.0	0.003	0.003	0.0	0.001	-0.001	0.0	0.0	0.0	-0.001	0.0	0.0	0.0	-0.001	-0.022	0.078

8.2. Presentation of molecule: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