Print calculated values

Report generated by:root, 17.02.2020 - 16:59:27

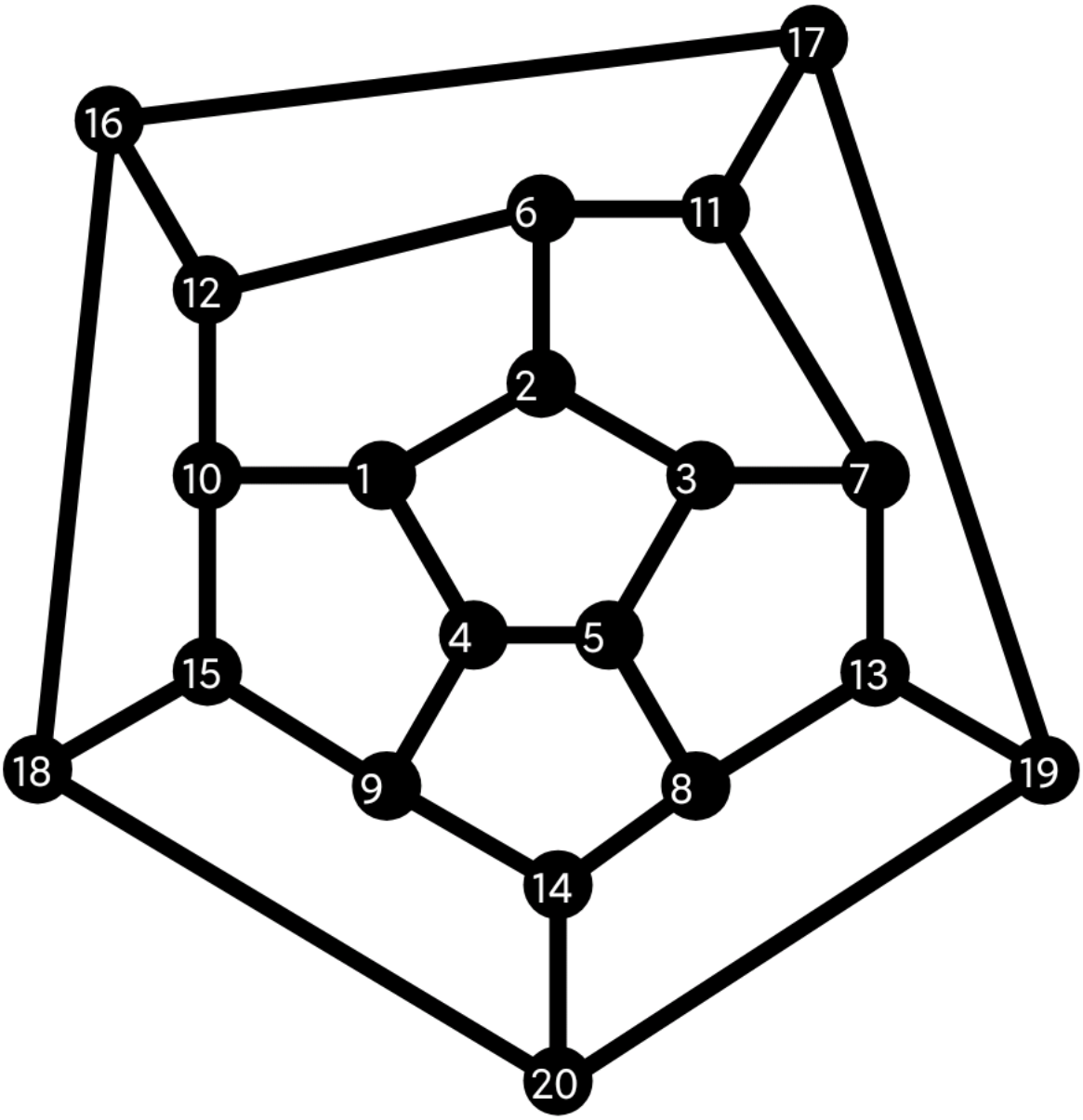
The following determinant is calculated:

-x	1.0	0.0	1.0	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	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	0.0	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	0.0
1.0	0.0	0.0	-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	1.0	-x	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	0.0	0.0	0.0	-x	0.0	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	1.0	0.0	0.0	0.0	-x	0.0	0.0	0.0	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	1.0	0.0	0.0	-x	0.0	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	1.0	0.0	0.0	0.0	0.0	-x	0.0	0.0	0.0	0.0	1.0	1.0	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	-x	0.0	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	1.0	1.0	0.0	0.0	0.0	-x	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	1.0	0.0	0.0	0.0	1.0	0.0	-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	1.0	1.0	0.0	0.0	0.0	0.0	-x	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	1.0	1.0	0.0	0.0	0.0	0.0	-x	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	1.0	1.0	0.0	0.0	0.0	0.0	-x	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	0.0	0.0	0.0	-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	1.0	0.0	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	0.0	0.0	1.0	1.0	0.0	-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	1.0	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	1.0	0.0	0.0	0.0	1.0	1.0	-x

It is about this molecule:

HMO-Energies

x1 = 3.0; x2 = 2.236; x3 = 2.236; x4 = 2.236; x5 = 1.0; x6 = 1.0; x7 = 1.0; x8 = 1.0;
x9 = 1.0; x10 = 0.0; x11 = 0.0; x12 = 0.0; x13 = 0.0; x14 = -2.0; x15 = -2.0; x16 = -2.0;
x17 = -2.0; x18 = -2.236; x19 = -2.236; x20 = -2.236;


17
16
6
11
12
2
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1
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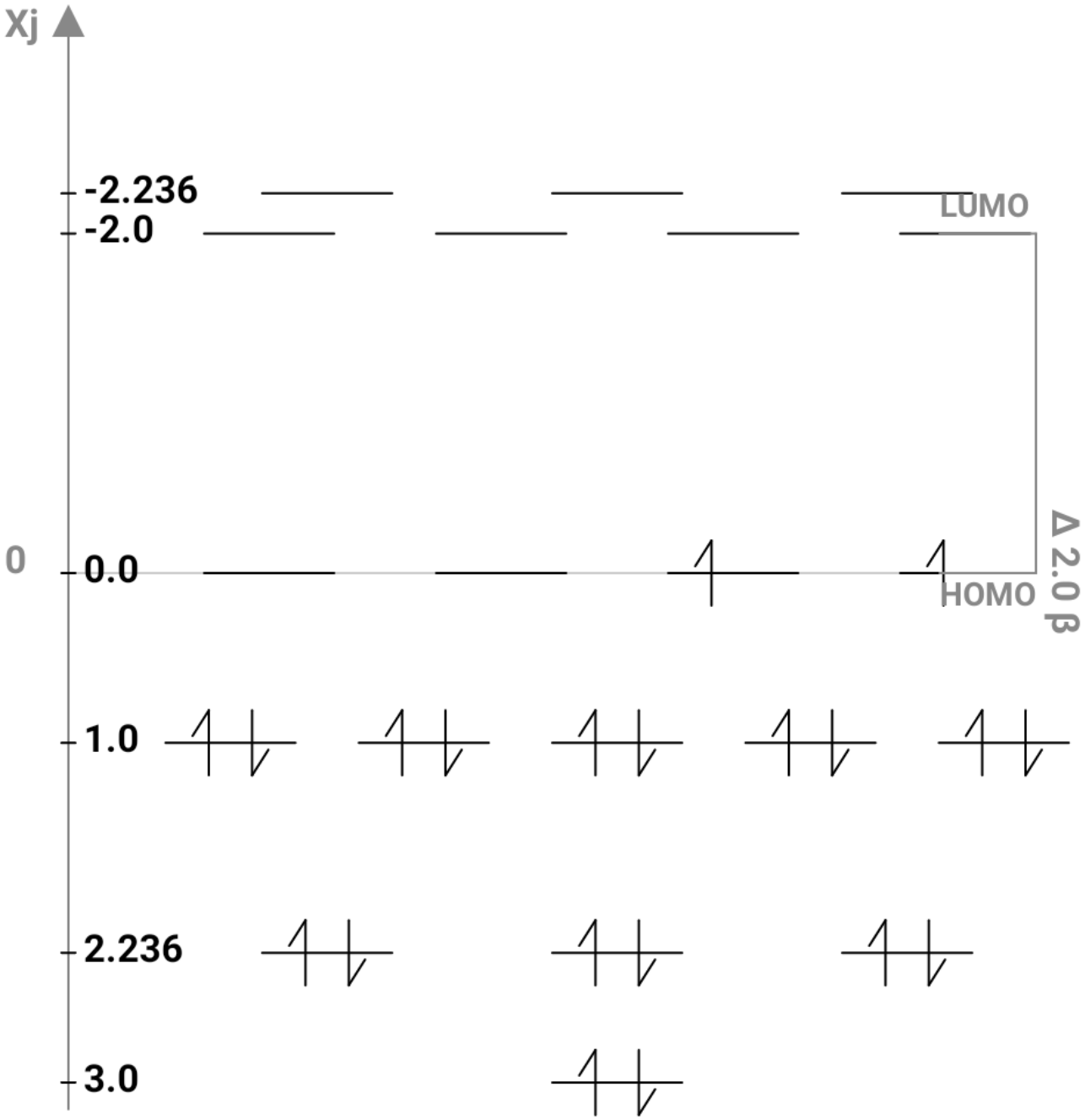
20

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 20α + 29.416β -

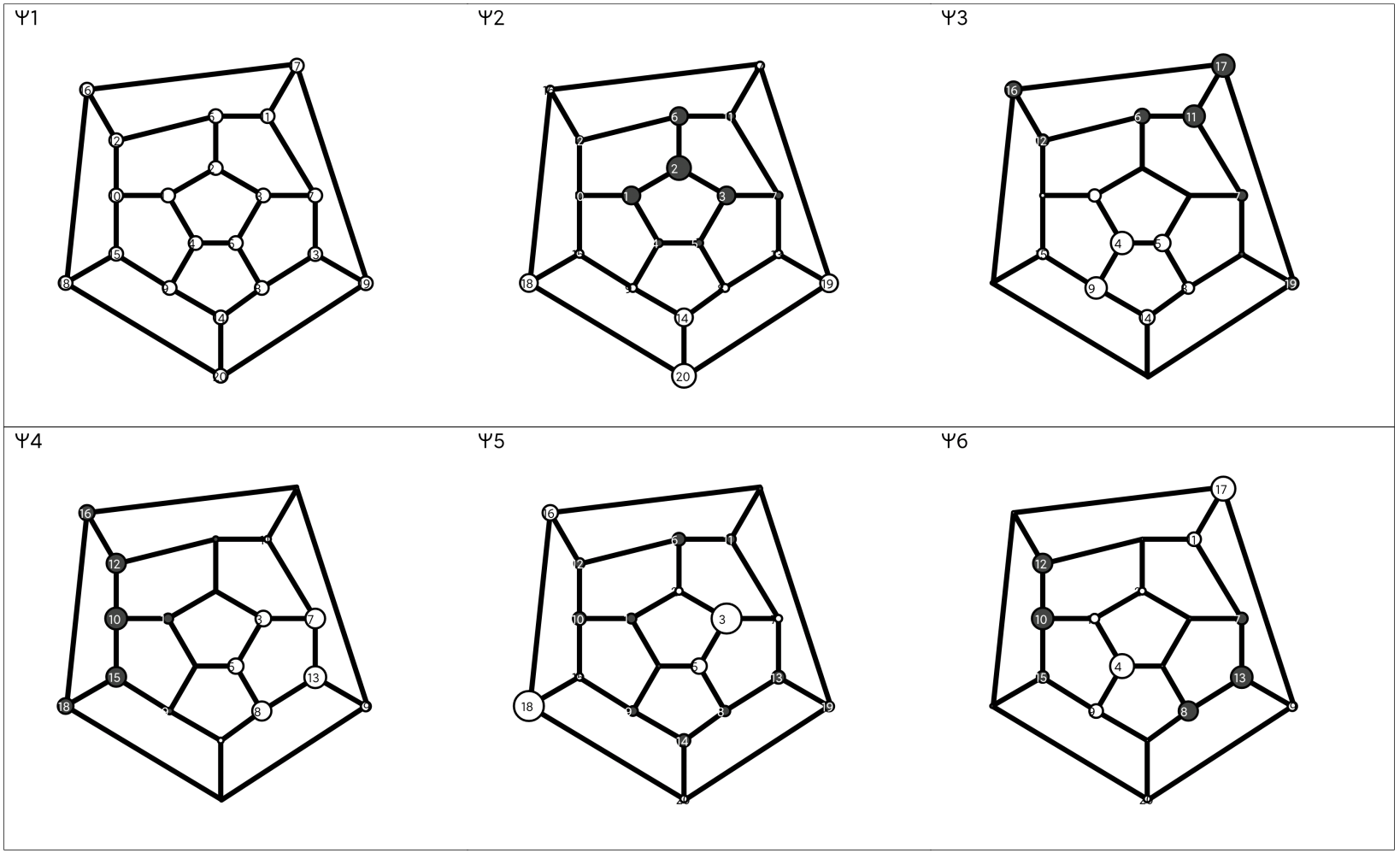
this corresponds to one πelectron: 1.471β

2. Hueckel-coefficient

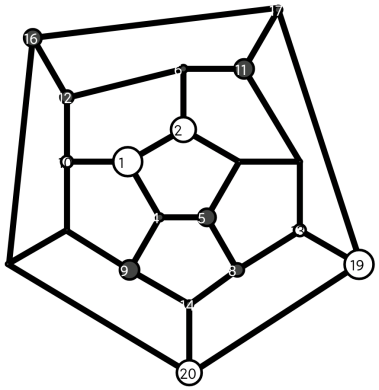
2.1. Calculated values:

	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
	x1= 3.0	x2= 2.236	x3= 2.236	x4= 2.236	x5= 1.0	x6= 1.0	x7= 1.0	x8= 1.0	x9= 1.0	x10= 0.0	x11= 0.0	x12= 0.0	x13= 0.0	x14= -2.0	x15= -2.0	x16= -2.0	x17= -2.0	x18= -2.236	x19= -2.236	x20= -2.236
1	0.224	-0.289	0.2	-0.163	-0.162	0.152	0.403	0.153	-0.123	-0.026	0.094	0.304	-0.313	0.285	-0.27	-0.214	-0.013	0.306	-0.237	0.001
2	0.224	-0.387	0.0	0.0	0.119	0.113	0.345	-0.319	0.04	-0.445	-0.001	-0.047	-0.009	-0.446	0.028	-0.007	0.0	-0.386	-0.027	0.014
3	0.224	-0.289	0.041	0.255	0.488	-0.062	0.048	-0.041	0.067	-0.021	-0.038	0.122	0.428	0.318	0.284	-0.095	0.095	0.271	0.138	-0.239
4	0.224	-0.129	0.365	-0.009	-0.069	0.39	-0.107	0.238	-0.157	0.242	-0.288	-0.111	-0.215	-0.057	0.322	0.158	-0.261	-0.156	0.268	-0.231
5	0.224	-0.129	0.267	0.25	0.25	0.016	-0.242	0.054	-0.355	0.25	0.232	-0.267	0.109	-0.1	-0.364	0.159	0.179	-0.1	-0.339	0.157
6	0.224	-0.289	-0.241	-0.092	-0.207	0.023	-0.105	-0.432	0.097	0.047	-0.057	-0.426	-0.115	0.289	-0.07	0.323	-0.082	0.286	0.159	0.207
7	0.224	-0.129	-0.175	0.32	0.118	-0.191	-0.056	0.225	0.382	0.194	-0.231	0.314	-0.1	-0.09	-0.232	0.039	-0.37	-0.12	0.057	0.364
8	0.224	0.129	0.19	0.312	-0.168	-0.312	-0.183	-0.144	-0.265	-0.221	0.325	-0.011	-0.213	-0.061	0.123	-0.38	-0.192	0.109	0.352	0.118
9	0.224	0.129	0.349	-0.106	-0.158	0.222	-0.268	0.032	0.321	-0.224	-0.327	-0.036	0.204	-0.071	-0.01	-0.26	0.357	0.144	-0.023	0.359
10	0.224	-0.129	0.083	-0.356	-0.211	-0.352	0.164	0.234	-0.007	0.203	0.289	0.158	0.224	-0.067	0.189	0.277	0.288	-0.142	0.289	0.215
11	0.224	-0.129	-0.349	0.106	-0.158	0.222	-0.268	0.032	0.321	0.224	0.327	0.036	-0.204	-0.071	-0.01	-0.26	0.357	-0.144	0.023	-0.359
12	0.224	-0.129	-0.19	-0.312	-0.168	-0.312	-0.183	-0.144	-0.265	0.221	-0.325	0.011	0.213	-0.061	0.123	-0.38	-0.192	-0.109	-0.352	-0.118
13	0.224	0.129	-0.083	0.356	-0.211	-0.352	0.164	0.234	-0.007	-0.203	-0.289	-0.158	-0.224	-0.067	0.189	0.277	0.288	0.142	-0.289	-0.215
14	0.224	0.289	0.241	0.092	-0.207	0.023	-0.105	-0.432	0.097	-0.047	0.057	0.426	0.115	0.289	-0.07	0.323	-0.082	-0.286	-0.159	-0.207
15	0.224	0.129	0.175	-0.32	0.118	-0.191	-0.056	0.225	0.382	-0.194	0.231	-0.314	0.1	-0.09	-0.232	0.039	-0.37	0.12	-0.057	-0.364
16	0.224	0.129	-0.267	-0.25	0.25	0.016	-0.242	0.054	-0.355	-0.25	-0.232	0.267	-0.109	-0.1	-0.364	0.159	0.179	0.1	0.339	-0.157
17	0.224	0.129	-0.365	0.009	-0.069	0.39	-0.107	0.238	-0.157	-0.242	0.288	0.111	0.215	-0.057	0.322	0.158	-0.261	0.156	-0.268	0.231
18	0.224	0.289	-0.041	-0.255	0.488	-0.062	0.048	-0.041	0.067	0.021	0.038	-0.122	-0.428	0.318	0.284	-0.095	0.095	-0.271	-0.138	0.239
19	0.224	0.289	-0.2	0.163	-0.162	0.152	0.403	0.153	-0.123	0.026	-0.094	-0.304	0.313	0.285	-0.27	-0.214	-0.013	-0.306	0.237	-0.001
20	0.224	0.387	0.0	0.0	0.119	0.113	0.345	-0.319	0.04	0.445	0.001	0.047	0.009	-0.446	0.028	-0.007	0.0	0.386	0.027	-0.014

2.2. Molecule orbital presentation:


Ψ1
Ψ2
Ψ3
Ψ4
Ψ5
Ψ6

Ψ7



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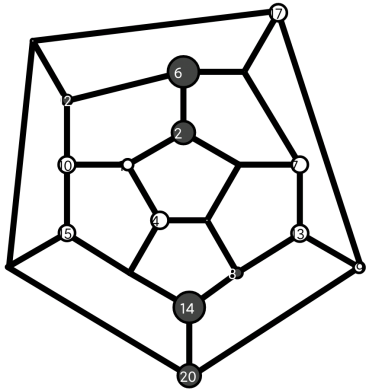

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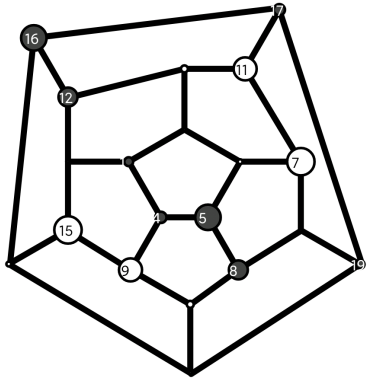

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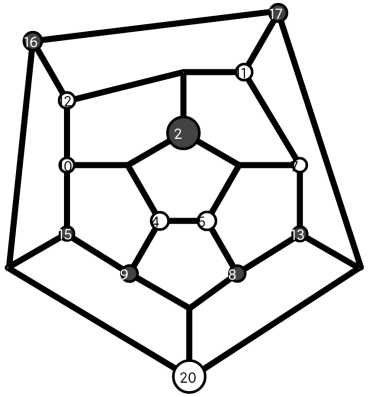

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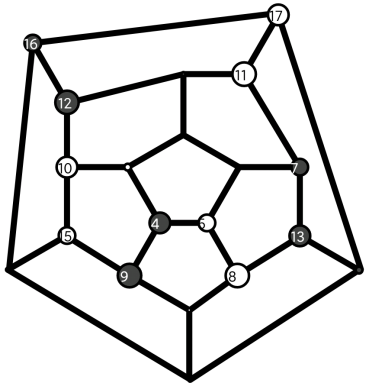

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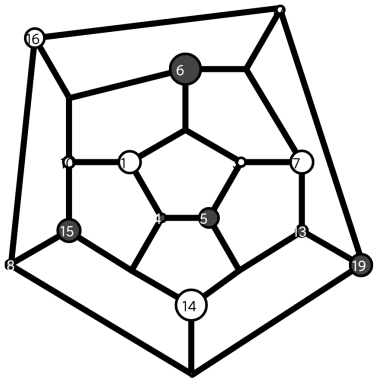

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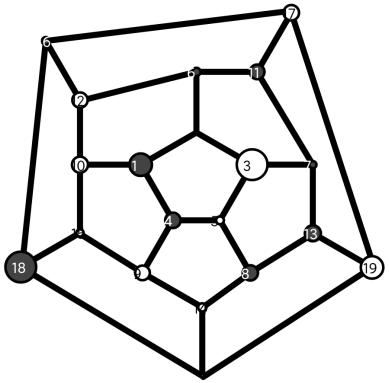

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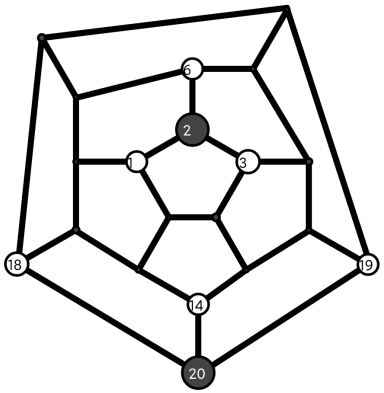

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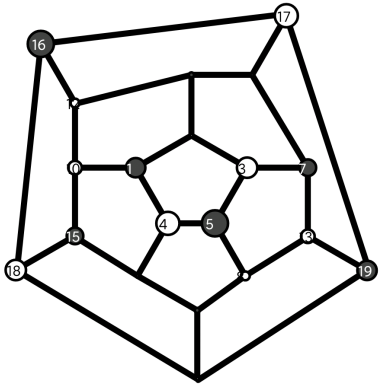

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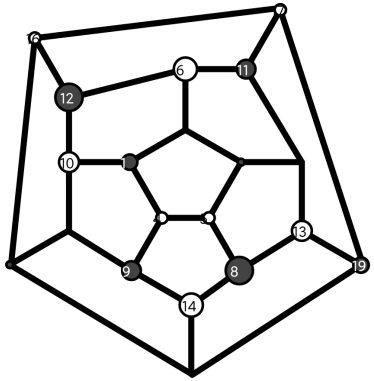

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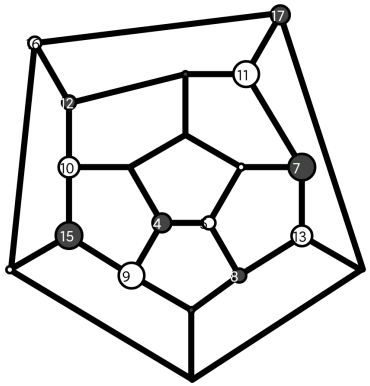

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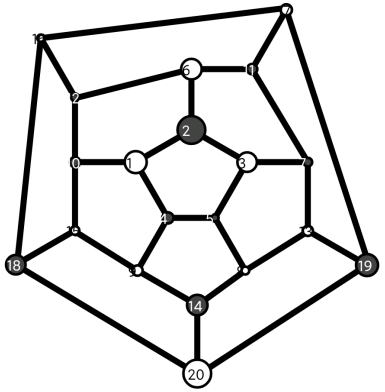

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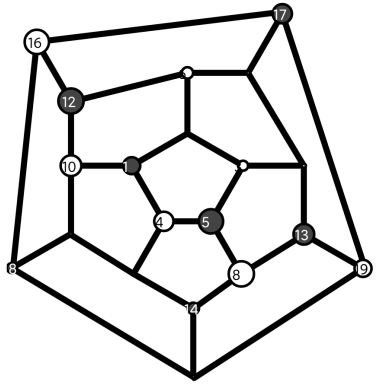

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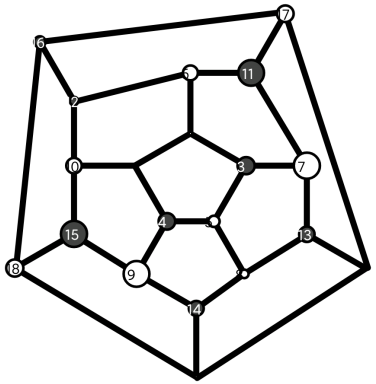


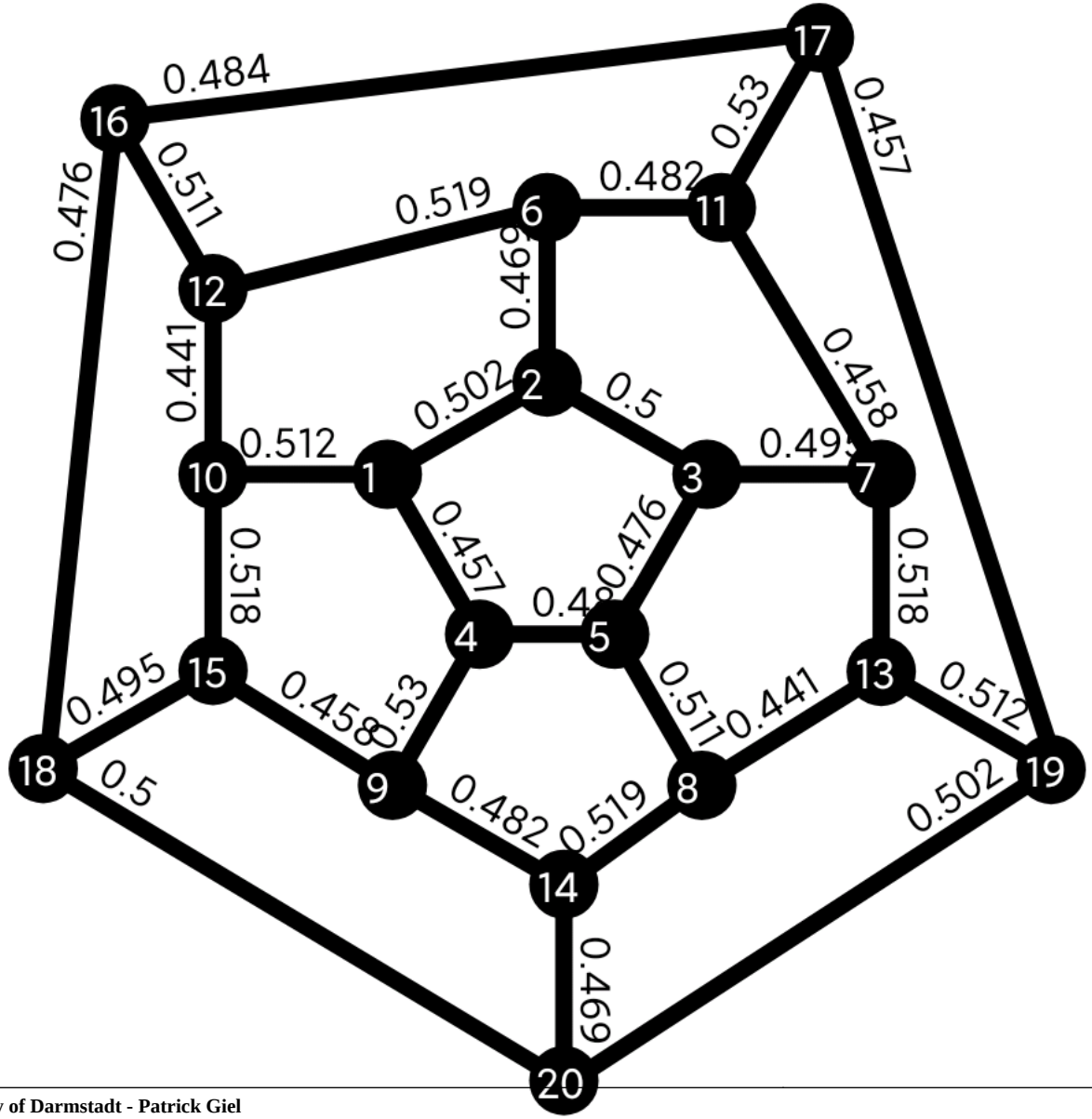
The picture export was cancelled, more than 20 pictures are not possible.

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
1	0.91																			
2	0.502	1.098																		
3	0.03	0.5	0.902																	
4	0.457	-0.074	0.039	1.041																
5	0.049	-0.078	0.476	0.484	1.017															
6	0.027	0.469	0.034	-0.139	-0.168	0.905														
7	-0.194	-0.053	0.495	-0.053	0.028	0.056	0.991													
8	-0.13	-0.069	0.026	-0.114	0.511	0.014	-0.085	1.055												
9	0.008	-0.067	-0.15	0.53	-0.099	0.051	0.075	-0.024	1.057											
10	0.512	-0.057	-0.182	-0.001	-0.049	0.027	0.016	0.092	-0.107	1.025										
11	-0.142	-0.067	0.016	0.003	-0.035	0.482	0.458	-0.11	0.143	-0.027	1.057									
12	-0.003	-0.064	-0.159	-0.02	0.023	0.519	-0.049	0.145	-0.11	0.441	-0.024	1.055								
13	0.021	-0.076	0.048	-0.133	-0.085	-0.16	0.518	0.441	-0.027	0.175	-0.107	0.092	1.025							
14	-0.16	0.064	-0.168	0.006	0.035	0.295	-0.189	0.519	0.482	-0.16	0.051	0.014	0.027	0.905						
15	0.06	-0.081	0.038	-0.08	-0.162	-0.189	0.209	-0.049	0.458	0.518	0.075	-0.085	0.016	0.056	0.991					
16	-0.182	-0.055	0.057	0.049	0.183	0.035	-0.162	0.023	-0.035	-0.085	-0.099	0.511	-0.049	-0.168	0.028	1.017				
17	0.077	-0.06	-0.172	0.159	0.049	0.006	-0.08	-0.02	0.003	-0.133	0.53	-0.114	-0.001	-0.139	-0.053	0.484	1.041			
18	-0.164	0.034	0.298	-0.172	0.057	-0.168	0.038	-0.159	0.016	0.048	-0.15	0.026	-0.182	0.034	0.495	0.476	0.039	0.902		
19	0.29	0.031	-0.164	0.077	-0.182	-0.16	0.06	-0.003	-0.142	0.021	0.008	-0.13	0.512	0.027	-0.194	0.049	0.457	0.03	0.91	
20	0.031	0.102	0.034	-0.06	-0.055	0.064	-0.081	-0.064	-0.067	-0.076	-0.067	-0.069	-0.057	0.469	-0.053	-0.078	-0.074	0.5	0.502	1.098

3.2. Presentation of bond order:

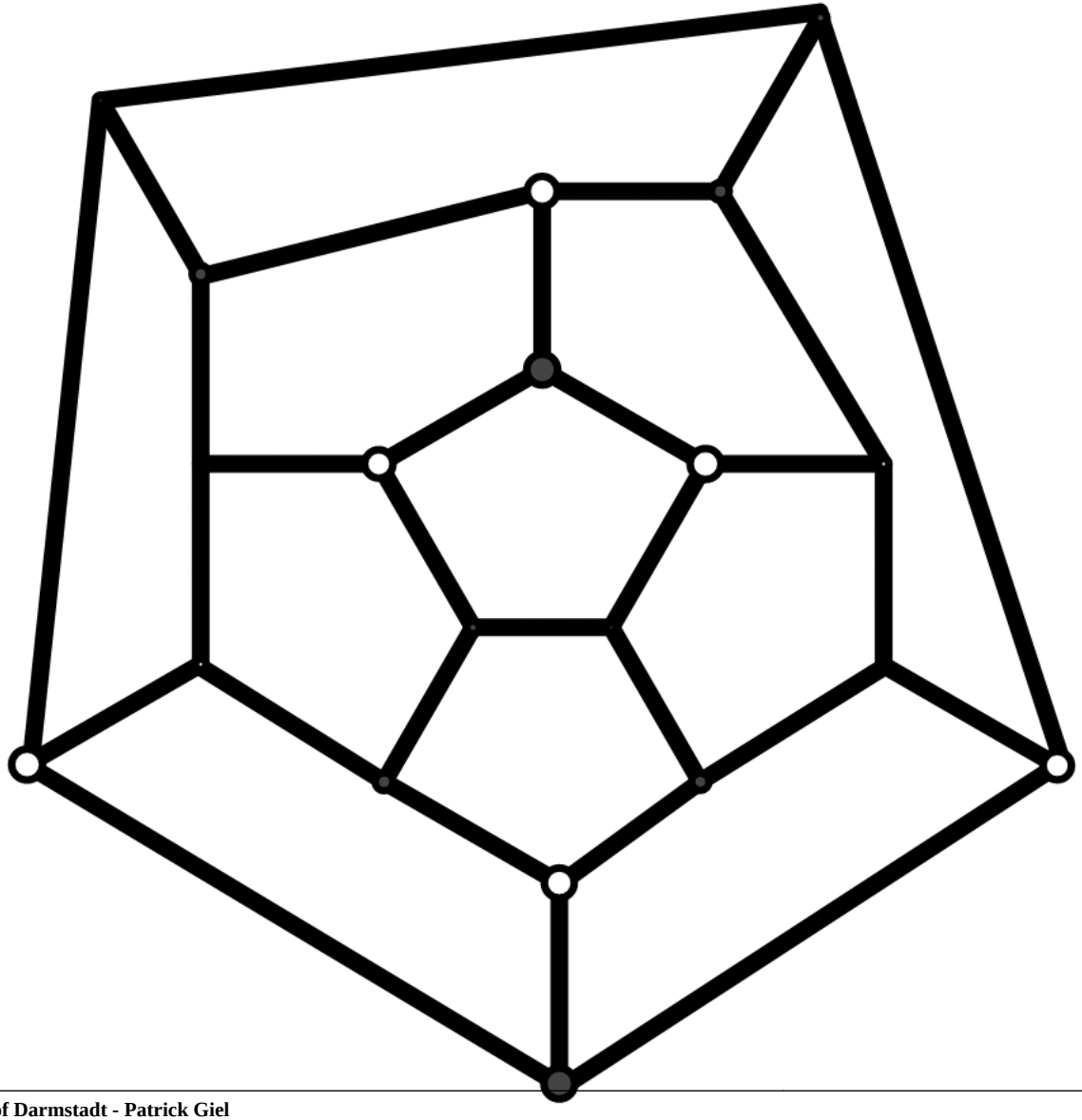

17
0.484
16
0.53
0.457
0.476
0.511
0.519
0.482
6
11
0.469
12
0.458
0.441
0.502
2
0.5
0.512
0.49
10
1
3
7
0.457
0.476
0.518
0.518
0.4
4
5
15
0.495
0.458
0.53
0.511
0.441
13
0.512
18
0.5
9
0.482
0.519
8
19
0.502
14
0.469
20

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
1	0.09																			
2		-0.098																		
3			0.098																	
4				-0.041																
5					-0.017															
6						0.095														
7							0.009													
8								-0.055												
9									-0.057											
10										-0.025										
11											-0.057									
12												-0.055								
13													-0.025							
14														0.095						
15															0.009					
16																-0.017				
17																	-0.041			
18																		0.098		
19																			0.09	
20																				-0.098

4.2. Presentation of molecule:

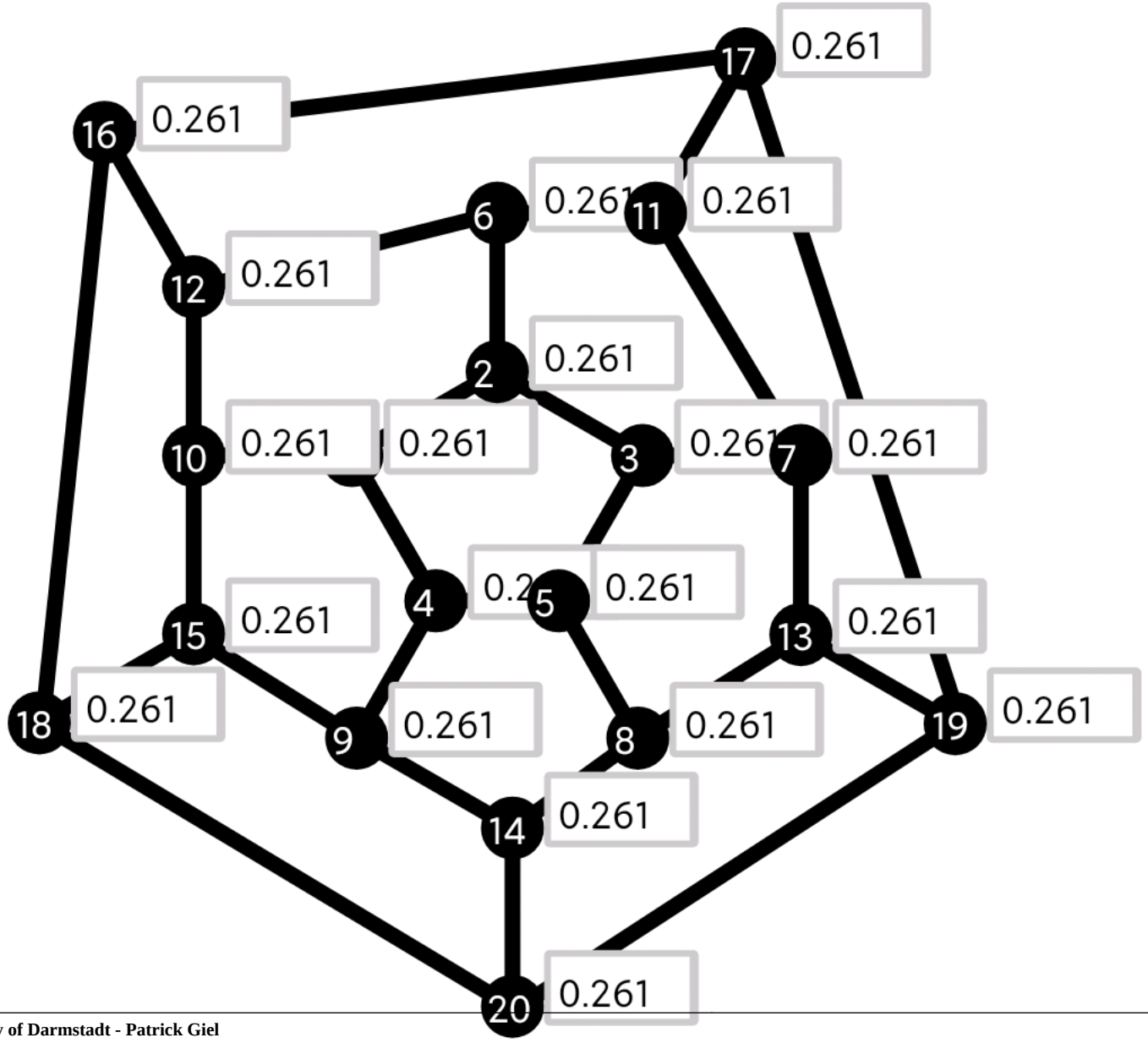


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
0.261	0.261	0.261	0.261	0.261	0.261	0.261	0.261	0.261	0.261	0.261	0.261	0.261	0.261	0.261	0.261	0.261	0.261	0.261	0.261

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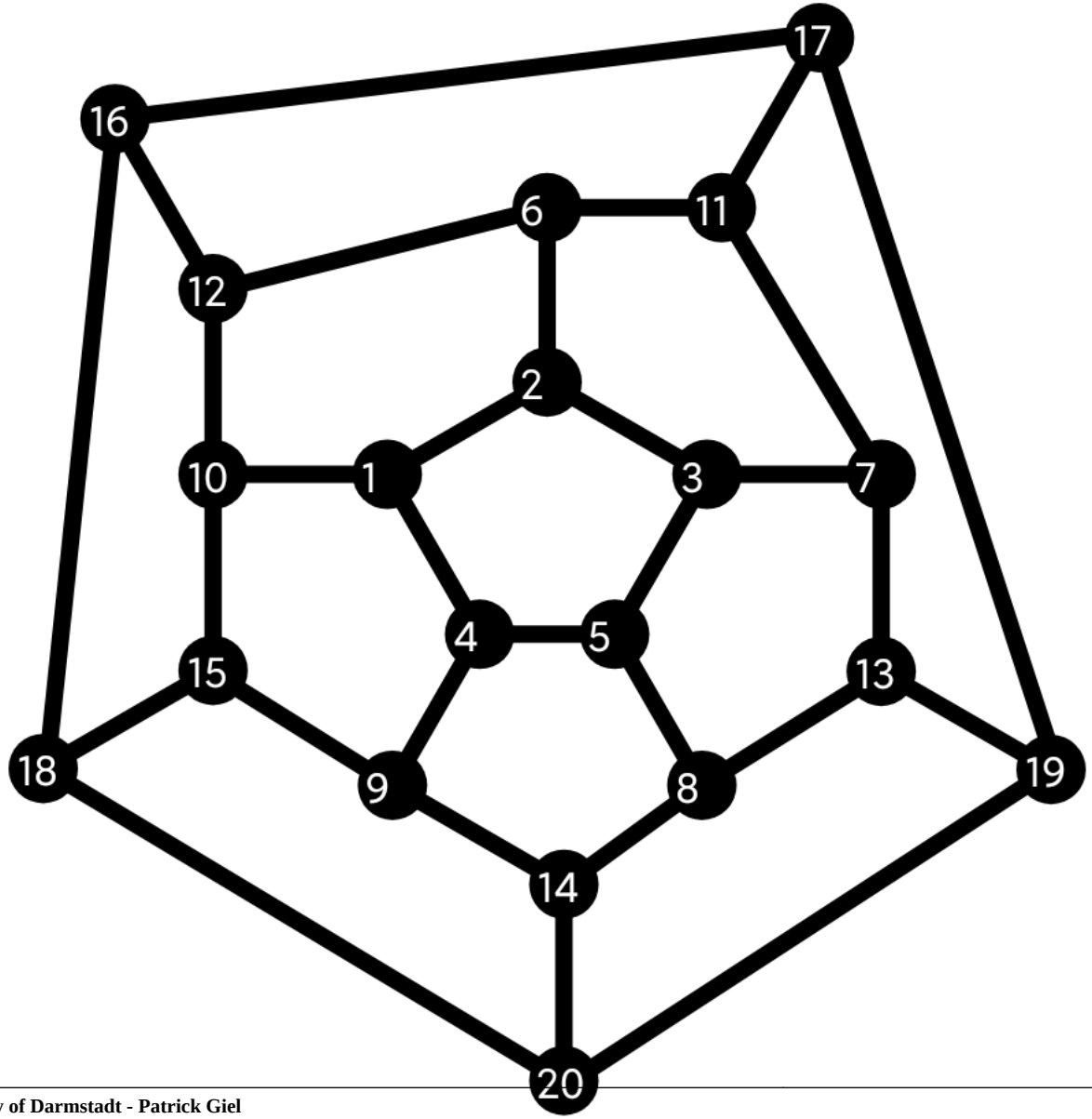
6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0.439																			
2	-0.067	0.376																		
3	0.015	-0.066	0.442																	
4	-0.043	-0.002	0.017	0.395																
5	0.018	-0.003	-0.054	-0.058	0.403															
6	0.015	-0.05	0.016	-0.029	-0.034	0.44														
7	-0.039	0.002	-0.064	-0.015	0.015	0.02	0.412													
8	-0.028	-0.018	0.015	-0.009	-0.072	0.002	-0.004	0.391												
9	0.012	-0.017	-0.031	-0.082	-0.006	-0.003	-0.006	0.006	0.39											
10	-0.073	0.001	-0.037	0.01	-0.014	0.015	0.002	-0.008	-0.007	0.401										
11	-0.03	-0.001	0.013	0.004	-0.012	-0.057	-0.044	-0.025	-0.093	-0.011	0.39									
12	0.01	0.0	-0.033	-0.01	0.001	-0.077	-0.014	-0.094	-0.025	-0.035	0.006	0.391								
13	0.001	-0.019	0.018	-0.028	-0.004	-0.033	-0.076	-0.035	-0.011	-0.104	-0.007	-0.008	0.401							
14	-0.033	-0.004	-0.034	0.011	0.016	-0.143	-0.038	-0.077	-0.057	-0.033	-0.003	0.002	0.015	0.44						
15	0.02	-0.02	-0.001	-0.003	-0.033	-0.038	-0.115	-0.014	-0.044	-0.076	-0.006	-0.004	0.002	0.02	0.412					
16	-0.037	-0.015	-0.003	-0.002	-0.106	0.016	-0.033	0.001	-0.012	-0.004	-0.006	-0.072	-0.014	-0.034	0.015	0.403				
17	-0.006	-0.016	-0.035	-0.098	-0.002	0.011	-0.003	-0.01	0.004	-0.028	-0.082	-0.009	0.01	-0.029	-0.015	-0.058	0.395			
18	-0.034	0.0	-0.145	-0.035	-0.003	-0.034	-0.001	-0.033	0.013	0.018	-0.031	0.015	-0.037	0.016	-0.064	-0.054	0.017	0.442		
19	-0.142	0.0	-0.034	-0.006	-0.037	-0.033	0.02	0.01	-0.03	0.001	0.012	-0.028	-0.073	0.015	-0.039	0.018	-0.043	0.015	0.439	
20	0.0	-0.079	0.0	-0.016	-0.015	-0.004	-0.02	0.0	-0.001	-0.019	-0.017	-0.018	0.001	-0.05	0.002	-0.003	-0.002	-0.066	-0.067	0.376

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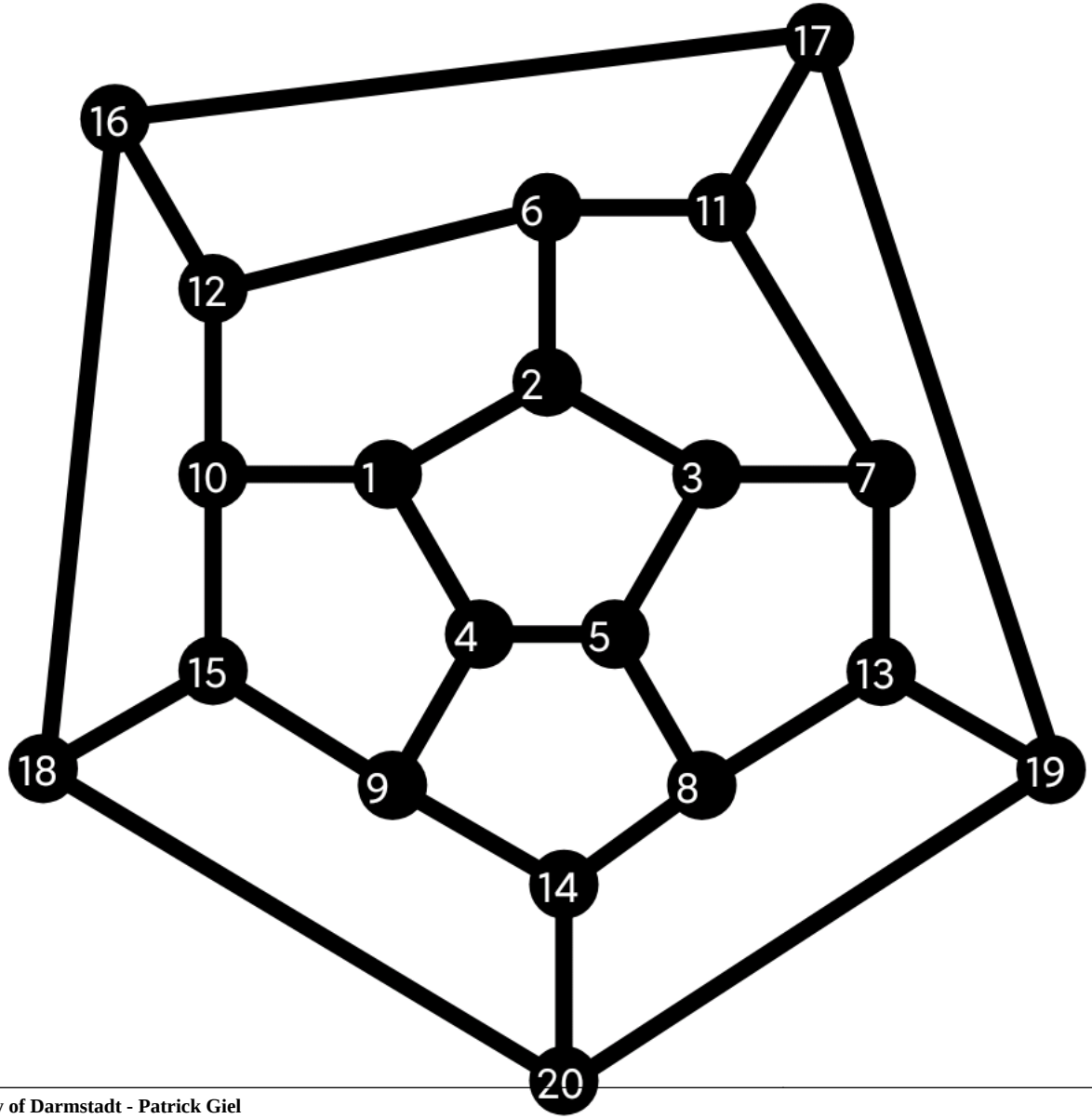
7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1 2	0.038	-0.012	-0.015	0.009	0.008	-0.017	-0.005	-0.023	0.011	0.009	-0.002	0.005	0.004	0.013	0.014	-0.026	0.007	0.011	-0.019	-0.007
1 4	0.046	0.013	0.016	0.01	-0.022	0.006	-0.027	-0.005	-0.007	-0.006	0.007	0.014	0.007	0.003	0.009	0.013	-0.018	-0.034	-0.027	0.003
1 10	0.036	0.008	0.003	-0.011	0.015	0.015	0.011	0.013	0.002	0.006	-0.02	-0.011	-0.01	-0.033	-0.022	-0.007	0.012	0.006	-0.018	0.004
2 3	-0.015	-0.012	0.04	0.007	0.012	-0.019	0.006	0.012	-0.024	-0.004	0.006	-0.003	0.013	0.013	0.005	0.005	-0.026	-0.02	0.01	-0.007
2 6	-0.014	-0.007	-0.016	-0.002	-0.005	0.045	0.011	0.003	0.005	0.008	0.009	0.011	-0.026	-0.025	-0.029	0.014	0.011	0.011	0.01	-0.012
3 5	0.017	0.014	0.044	-0.019	0.014	0.004	-0.015	-0.013	-0.005	-0.026	0.014	0.009	0.007	0.004	0.011	-0.017	0.012	-0.024	-0.035	0.003
3 7	0.002	0.007	0.041	0.014	-0.017	0.018	0.017	0.005	0.013	0.01	-0.015	-0.024	-0.019	-0.036	-0.015	0.012	-0.006	-0.021	0.007	0.005
4 5	-0.024	-0.002	-0.02	0.006	0.012	-0.032	0.013	0.024	0.022	0.011	-0.001	0.0	-0.003	0.014	-0.005	-0.015	-0.014	0.013	0.015	-0.016
4 9	-0.013	0.004	0.006	-0.002	0.018	0.01	0.007	-0.001	-0.006	0.001	-0.005	-0.017	-0.02	-0.01	0.011	0.003	-0.006	0.002	0.013	0.005
5 8	0.009	0.003	-0.016	0.022	0.008	0.009	0.006	-0.002	0.0	0.008	-0.018	-0.008	0.01	-0.015	-0.024	-0.011	0.002	0.012	0.0	0.006
6 11	0.006	0.008	0.015	0.006	-0.023	0.042	-0.026	0.005	-0.013	0.015	0.002	0.001	-0.007	-0.023	0.016	0.005	-0.006	-0.033	0.003	0.007
6 12	0.012	0.007	0.005	-0.02	0.01	0.036	0.016	-0.007	0.008	-0.019	-0.002	-0.004	0.015	-0.017	-0.007	-0.016	0.001	0.004	-0.03	0.007
7 11	-0.034	0.0	-0.012	0.001	0.015	-0.024	0.024	-0.001	-0.017	0.0	0.006	0.009	0.023	0.014	-0.021	-0.006	0.017	0.01	0.016	-0.019
7 13	0.011	0.005	-0.021	-0.022	0.006	0.007	0.014	0.01	0.005	-0.009	0.018	0.008	0.005	0.002	-0.011	-0.024	0.004	0.012	-0.022	0.004
8 13	0.007	-0.018	0.017	-0.005	0.016	0.009	0.017	0.01	0.011	-0.022	-0.003	-0.02	0.017	-0.013	0.001	0.002	0.014	-0.035	-0.005	0.0
8 14	-0.03	0.007	0.004	0.001	-0.016	-0.017	-0.007	-0.004	-0.002	0.015	0.008	-0.007	-0.019	0.036	0.016	0.01	-0.02	0.005	0.012	0.007
9 14	0.003	0.007	-0.033	-0.006	0.005	-0.023	0.016	0.001	0.002	-0.007	-0.013	0.005	0.015	0.042	-0.026	-0.023	0.006	0.015	0.006	0.008
9 15	0.016	-0.019	0.01	0.017	-0.006	0.014	-0.021	0.009	0.006	0.023	-0.017	-0.001	0.0	-0.024	0.024	0.015	0.001	-0.012	-0.034	0.0
10 12	-0.005	0.0	-0.035	0.014	0.002	-0.013	0.001	-0.02	-0.003	0.017	0.011	0.01	-0.022	0.009	0.017	0.016	-0.005	0.017	0.007	-0.018
10 15	-0.022	0.004	0.012	0.004	-0.024	0.002	-0.011	0.008	0.018	0.005	0.005	0.01	-0.009	0.007	0.014	0.006	-0.022	-0.021	0.011	0.005
11 17	0.013	0.005	0.002	-0.006	0.003	-0.01	0.011	-0.017	-0.005	-0.02	-0.006	-0.001	0.001	0.01	0.007	0.018	-0.002	0.006	-0.013	0.004
12 16	0.0	0.006	0.012	0.002	-0.011	-0.015	-0.024	-0.008	-0.018	0.01	0.0	-0.002	0.008	0.009	0.006	0.008	0.022	-0.016	0.009	0.003
13 19	-0.018	0.004	0.006	0.012	-0.007	-0.033	-0.022	-0.011	-0.02	-0.01	0.002	0.013	0.006	0.015	0.011	0.015	-0.011	0.003	0.036	0.008
14 20	0.01	-0.012	0.011	0.011	0.014	-0.025	-0.029	0.011	0.009	-0.026	0.005	0.003	0.008	0.045	0.011	-0.005	-0.002	-0.016	-0.014	-0.007
15 18	0.007	0.005	-0.021	-0.006	0.012	-0.036	-0.015	-0.024	-0.015	-0.019	0.013	0.005	0.01	0.018	0.017	-0.017	0.014	0.041	0.002	0.007
16 17	0.015	-0.016	0.013	-0.014	-0.015	0.014	-0.005	0.0	-0.001	-0.003	0.022	0.024	0.011	-0.032	0.013	0.012	0.006	-0.02	-0.024	-0.002
16 18	-0.035	0.003	-0.024	0.012	-0.017	0.004	0.011	0.009	0.014	0.007	-0.005	-0.013	-0.026	0.004	-0.015	0.014	-0.019	0.044	0.017	0.014
17 19	-0.027	0.003	-0.034	-0.018	0.013	0.003	0.009	0.014	0.007	0.007	-0.007	-0.005	-0.006	0.006	-0.027	-0.022	0.01	0.016	0.046	0.013
18 20	0.01	-0.007	-0.02	-0.026	0.005	0.013	0.005	-0.003	0.006	0.013	-0.024	0.012	-0.004	-0.019	0.006	0.012	0.007	0.04	-0.015	-0.012
19 20	-0.019	-0.007	0.011	0.007	-0.026	0.013	0.014	0.005	-0.002	0.004	0.011	-0.023	0.009	-0.017	-0.005	0.008	0.009	-0.015	0.038	-0.012

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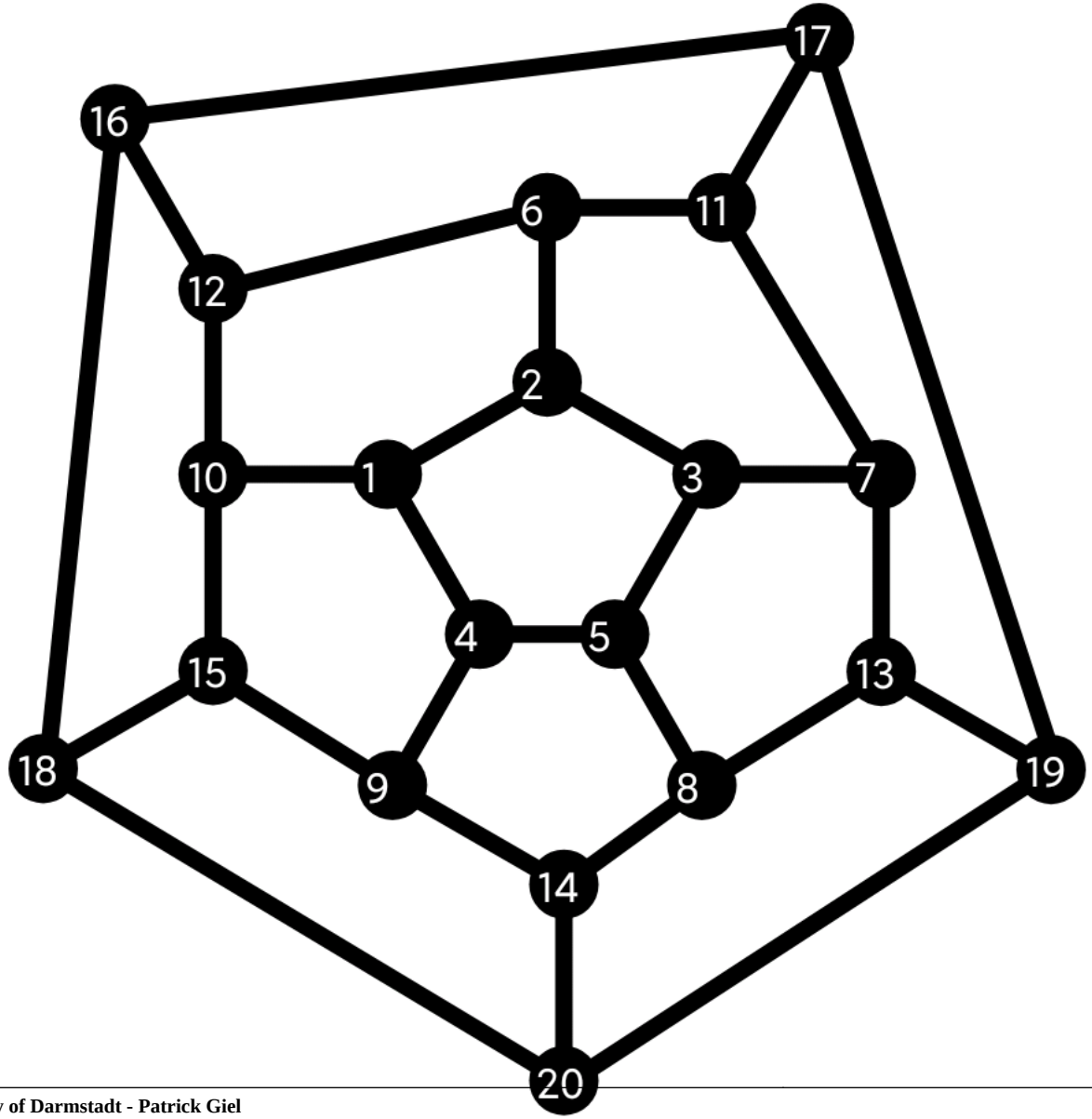
8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 4	1 10	2 3	2 6	3 5	3 7	4 5	4 9	5 8	6 11	6 12	7 11	7 13	8 13	8 14	9 14	9 15	10 12	10 15	11 17	12 16	13 19	14 20	15 18	16 17	16 18	17 19	18 20	19 20
1 2	0.34																													
1 4	-0.104	0.374																												
1 10	-0.122	-0.119	0.347																											
2 3	-0.118	-0.011	0.055	0.343																										
2 6	-0.109	0.042	-0.006	-0.11	0.358																									
3 5	-0.014	0.001	0.018	-0.109	0.05	0.369																								
3 7	0.059	0.016	-0.047	-0.118	-0.013	-0.125	0.363																							
4 5	0.018	-0.109	0.022	0.018	-0.007	-0.115	0.027	0.341																						
4 9	0.018	-0.115	0.029	0.01	-0.023	0.043	-0.029	-0.104	0.31																					
5 8	0.012	0.037	-0.026	0.021	-0.029	-0.12	0.028	-0.098	-0.01	0.325																				
6 11	0.041	-0.04	0.021	-0.007	-0.104	0.018	-0.004	-0.013	0.053	-0.029	0.358																			
6 12	-0.002	0.02	-0.007	0.046	-0.114	-0.043	0.021	-0.014	-0.025	0.06	-0.125	0.339																		
7 11	-0.007	-0.013	-0.017	0.017	0.015	0.022	-0.111	-0.024	0.038	0.014	-0.109	0.023	0.357																	
7 13	-0.033	-0.031	0.066	0.028	0.011	0.032	-0.132	0.011	-0.001	-0.023	0.044	-0.029	-0.097	0.33																
8 13	-0.02	-0.028	0.051	0.025	-0.022	-0.014	-0.005	0.029	0.006	-0.089	-0.03	0.054	0.024	-0.093	0.361															
8 14	-0.015	-0.002	-0.015	-0.032	0.053	0.06	-0.004	-0.004	0.03	-0.129	0.06	-0.116	-0.03	0.05	-0.109	0.339														
9 14	-0.03	0.055	-0.004	-0.014	0.05	-0.001	-0.02	-0.011	-0.12	0.032	-0.121	0.06	0.057	-0.029	0.018	-0.125	0.358													
9 15	0.024	-0.016	-0.002	-0.021	-0.021	-0.032	0.057	0.04	-0.099	0.003	0.057	-0.03	-0.11	0.038	-0.019	0.023	-0.109	0.357												
10 12	0.016	0.015	-0.105	-0.008	0.017	-0.013	-0.017	-0.019	0.011	0.035	0.018	-0.109	-0.019	0.037	-0.107	0.054	-0.03	0.024	0.361											
10 15	0.032	0.03	-0.136	-0.03	0.006	-0.032	0.066	0.007	-0.016	0.001	-0.029	0.05	0.038	-0.107	0.037	-0.029	0.044	-0.097	-0.093	0.33										
11 17	-0.021	0.053	-0.024	0.007	0.018	-0.03	0.046	0.037	-0.092	-0.003	-0.12	0.03	-0.099	-0.016	0.011	-0.025	0.053	0.038	0.006	-0.001	0.31									
12 16	0.006	-0.028	0.045	-0.024	0.023	0.058	-0.028	0.036	-0.003	-0.099	0.032	-0.129	0.003	0.001	0.035	0.06	-0.029	0.014	-0.089	-0.023	-0.01	0.325								

	1 2	**1 4**	**1 10**	**2 3**	**2 6**	**3 5**	**3 7**	**4 5**	**4 9**	**5 8**	**6 11**	**6 12**	**7 11**	**7 13**	**8 13**	**8 14**	**9 14**	**9 15**	**10 12**	**10 15**	**11 17**	**12 16**	**13 19**	**14 20**	**15 18**	**16 17**	**16 18**	**17 19**	**18 20**	**19 20**
13 19	0.055	0.062	-0.121	-0.036	-0.016	-0.001	0.063	-0.03	-0.024	0.045	-0.004	-0.015	-0.002	-0.136	-0.105	-0.007	0.021	-0.017	0.051	0.066	0.029	-0.026	0.347							
14 20	0.051	-0.031	-0.016	0.052	-0.116	-0.033	-0.015	0.025	0.018	0.023	0.05	0.053	-0.021	0.006	0.017	-0.114	-0.104	0.015	-0.022	0.011	-0.023	-0.029	-0.006	0.358						
15 18	-0.037	0.001	0.063	0.055	-0.015	0.067	-0.131	-0.033	0.046	-0.028	-0.02	-0.004	0.057	0.066	-0.017	0.021	-0.004	-0.111	-0.005	-0.132	-0.029	0.028	-0.047	-0.013	0.363					
16 17	-0.02	0.057	-0.03	-0.02	0.025	0.059	-0.033	-0.105	0.037	0.036	-0.011	-0.004	0.04	0.007	-0.019	-0.014	-0.013	-0.024	0.029	0.011	-0.104	-0.098	0.022	-0.007	0.027	0.341				
16 18	-0.013	-0.024	-0.001	0.05	-0.033	-0.129	0.067	0.059	-0.03	0.058	-0.001	0.06	-0.032	-0.032	-0.013	-0.043	0.018	0.022	-0.014	0.032	0.043	-0.12	0.018	0.05	-0.125	-0.115	0.369			
17 19	0.049	-0.126	0.062	-0.014	-0.031	-0.024	0.001	0.057	0.053	-0.028	0.055	-0.002	-0.016	0.03	0.015	0.02	-0.04	-0.013	-0.028	-0.031	-0.115	0.037	-0.119	0.042	0.016	-0.109	0.001	0.374		
18 20	0.053	-0.014	-0.036	-0.112	0.052	0.05	0.055	-0.02	0.007	-0.024	-0.014	-0.032	-0.021	-0.03	-0.008	0.046	-0.007	0.017	0.025	0.028	0.01	0.021	0.055	-0.11	-0.118	0.018	-0.109	-0.011	0.343	
19 20	-0.111	0.049	0.055	0.053	0.051	-0.013	-0.037	-0.02	-0.021	0.006	-0.03	-0.015	0.024	0.032	0.016	-0.002	0.041	-0.007	-0.02	-0.033	0.018	0.012	-0.122	-0.109	0.059	0.018	-0.014	-0.104	-0.118	0.34

8.2. Presentation of molecule: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