Print calculated values

Report generated by:root, 18.02.2020 - 22:00:47

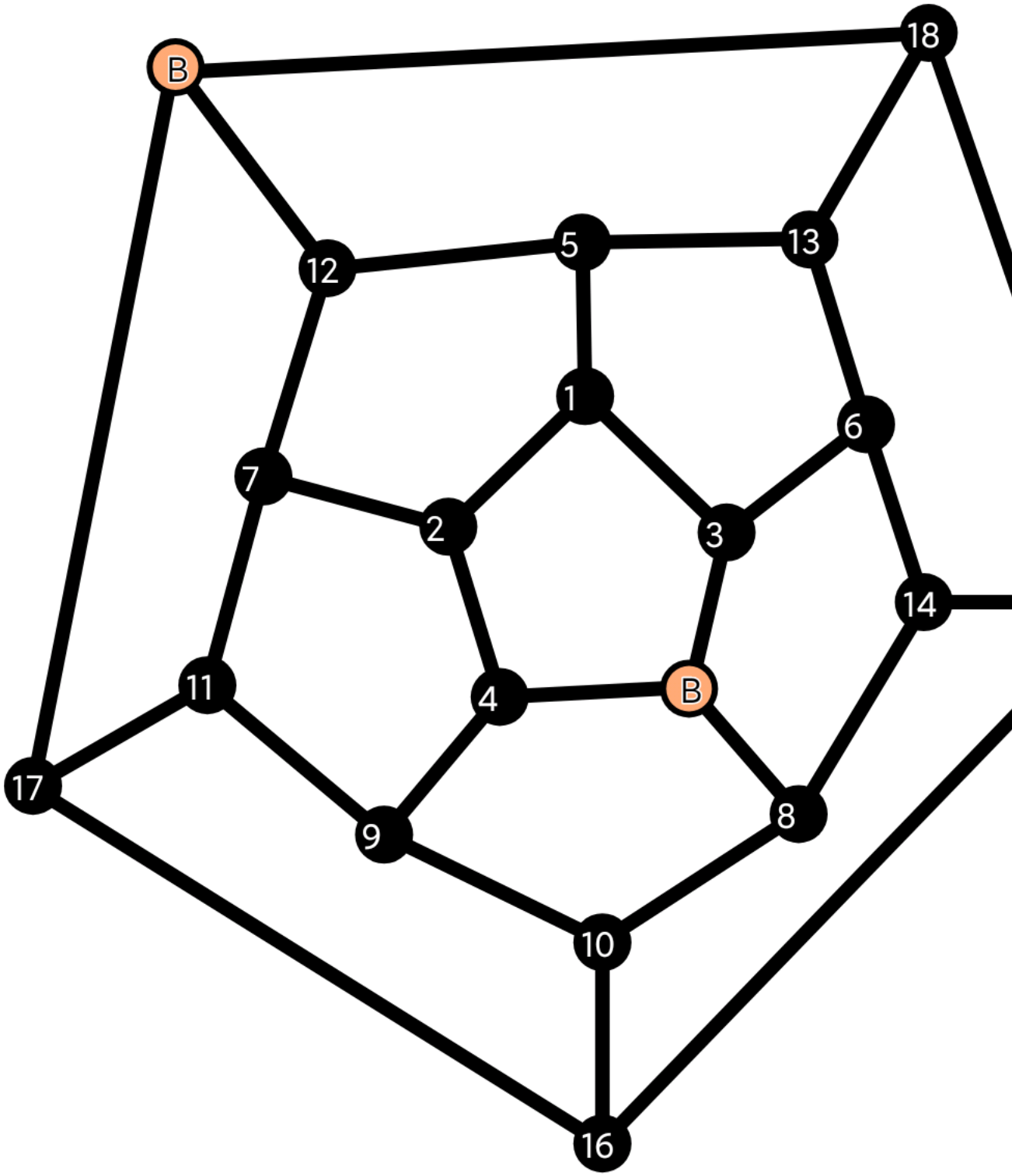
The following determinant is calculated:

-x	1.0	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	0.0	0.0
1.0	-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	0.0	0.0	0.0
1.0	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	0.7	0.0
0.0	1.0	0.0	-x	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	0.7	0.0
1.0	0.0	0.0	0.0	-x	0.0	0.0	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	-x	0.0	0.0	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	1.0	0.0	0.0	0.0	0.0	-x	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	0.0	0.0	-x	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.7	0.0
0.0	0.0	0.0	1.0	0.0	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	0.0	0.0	0.0	0.0	1.0	1.0	-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	0.0	0.0	1.0	0.0	1.0	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	1.0	0.0	1.0	0.0	0.0	0.0	0.0	-x	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.7
0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	-x	0.0	0.0	0.0	0.0	1.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	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	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	1.0	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	1.0	0.0	0.0	0.0	0.0	1.0	-x	0.0	0.0	0.7
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	1.0	0.0	0.0	-x	0.0	0.7
0.0	0.0	0.7	0.7	0.0	0.0	0.0	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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	0.7	0.0	0.0	0.0	0.0	0.7	0.7	0.0	-x+-1.0

It is about this molecule:

HMO-Energies

x1 = 2.821; x2 = 2.236; x3 = 2.236; x4 = 1.711; x5 = 1.0; x6 = 1.0; x7 = 1.0; x8 = 1.0;
x9 = 0.168; x10 = 0.0; x11 = 0.0; x12 = 0.0; x13 = -0.538; x14 = -1.989; x15 = -2.0; x16 = -2.0;
x17 = -2.0; x18 = -2.173; x19 = -2.236; x20 = -2.236;


B
18
12
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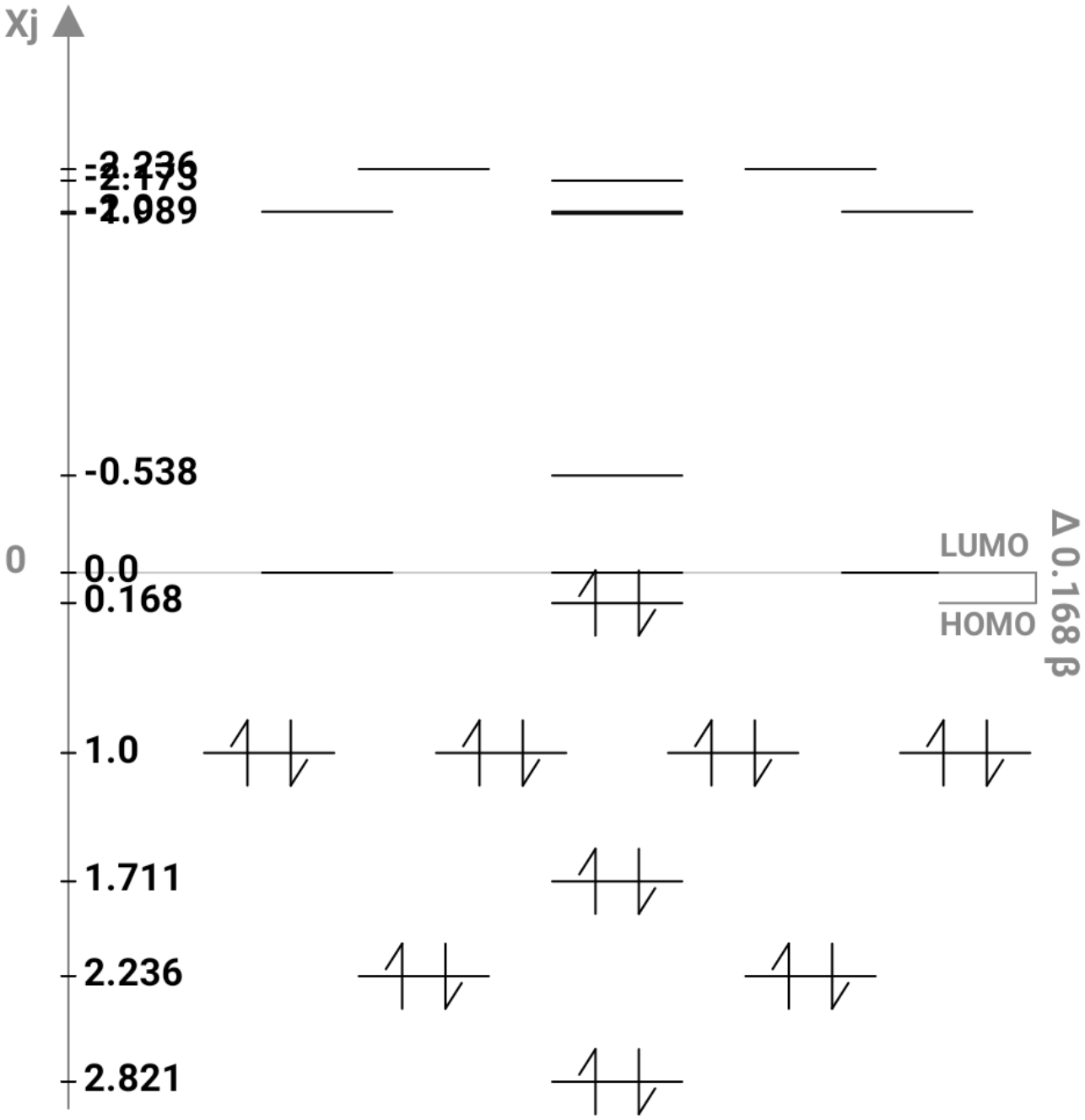
16

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 20α + 26.344β -

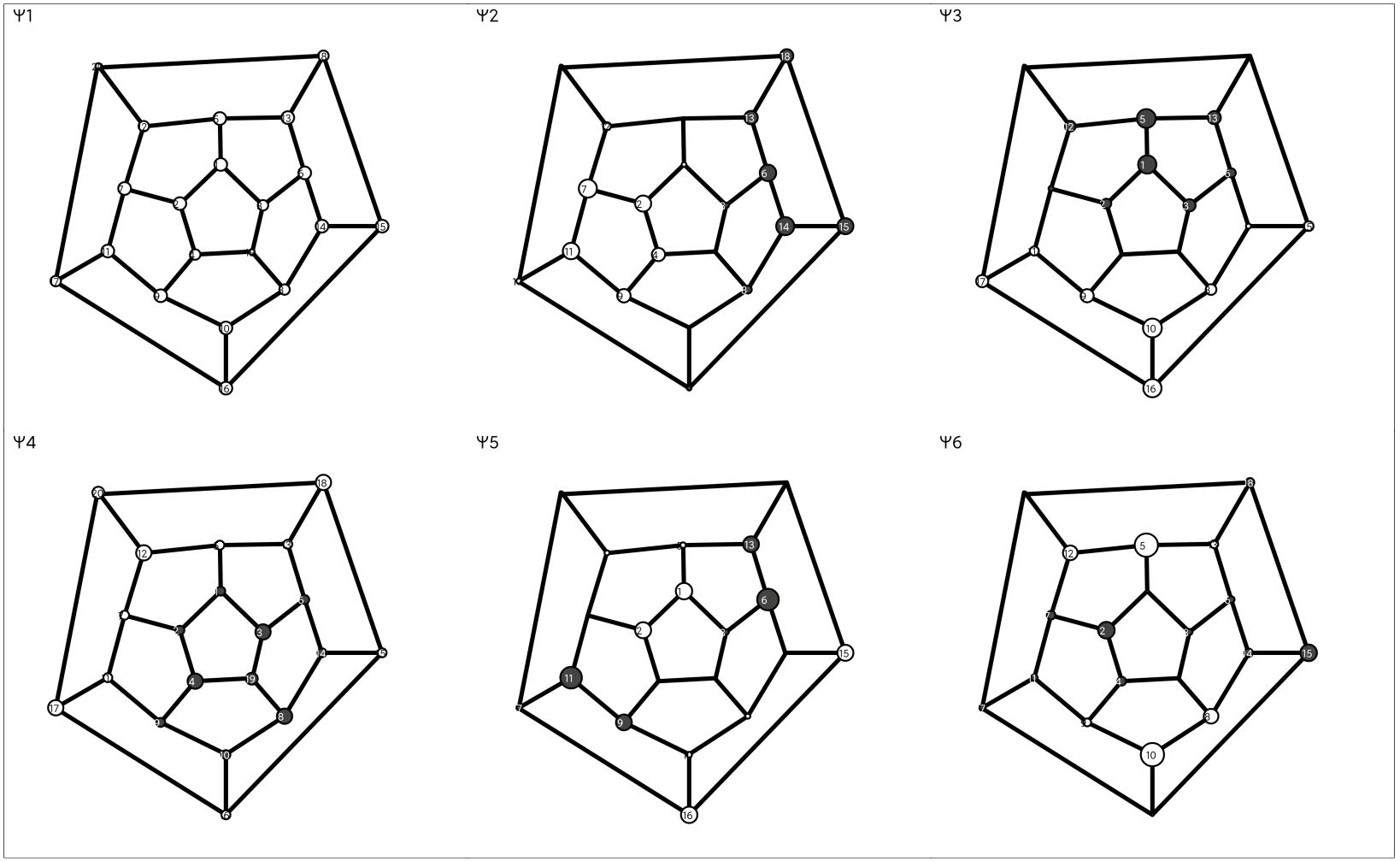
this corresponds to one πelectron: 1.464β

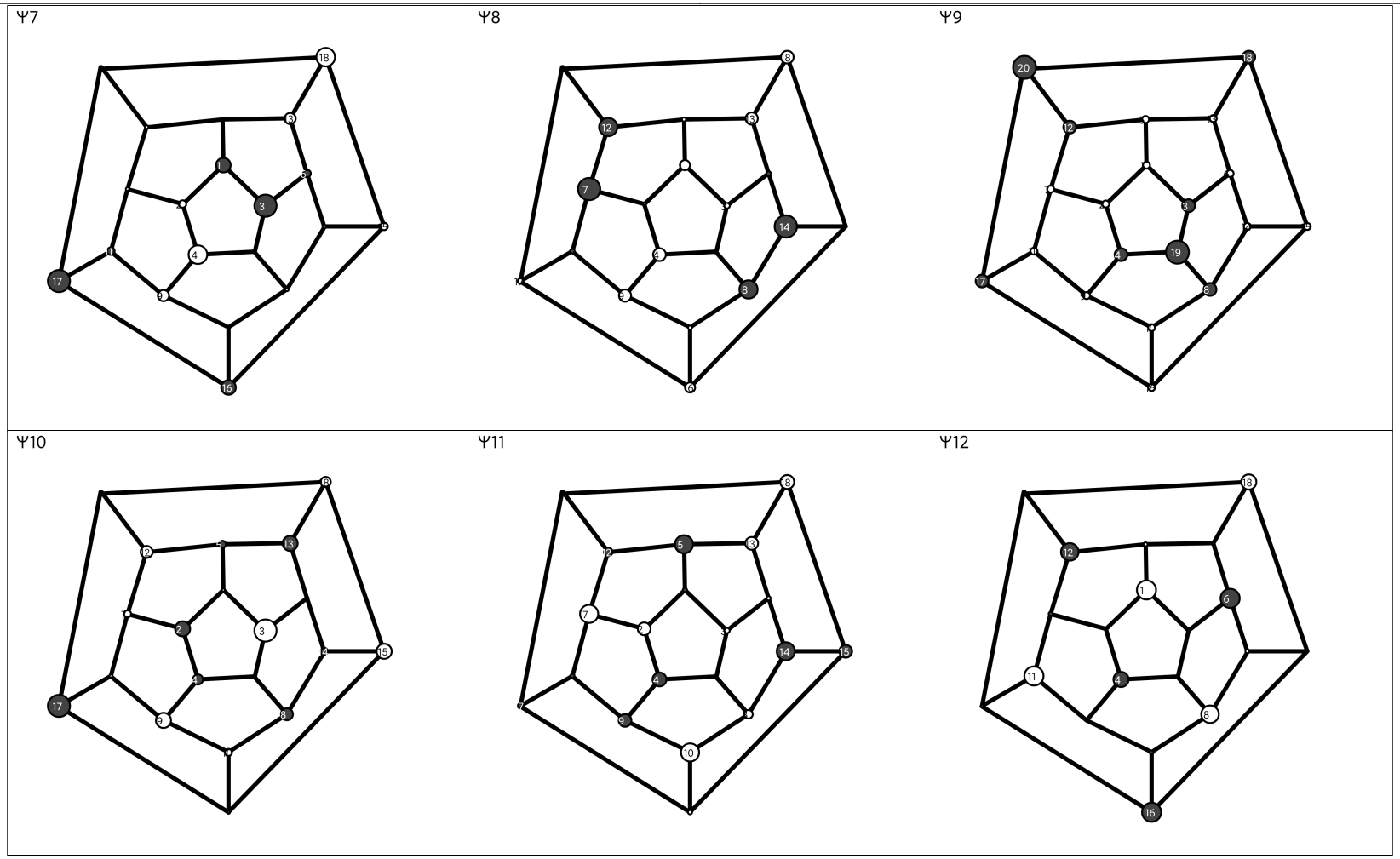
2. Hueckel-coefficient

2.1. Calculated values:

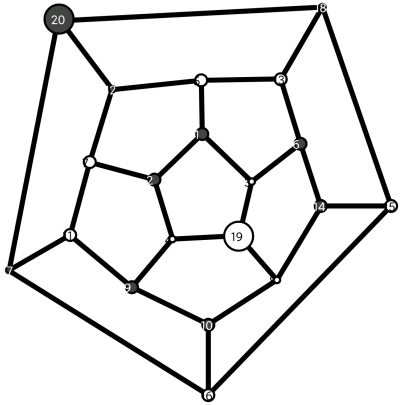
	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11	Psi 12	Psi 13	Psi 14	Psi 15	Psi 16	Psi 17	Psi 18	Psi 19	Psi 20
	x1= 2.821	x2= 2.236	x3= 2.236	x4= 1.711	x5= 1.0	x6= 1.0	x7= 1.0	x8= 1.0	x9= 0.168	x10= 0.0	x11= 0.0	x12= 0.0	x13= -0.538	x14= -1.989	x15= -2.0	x16= -2.0	x17= -2.0	x18= -2.173	x19= -2.236	x20= -2.236
1	0.247	0.09	-0.354	-0.174	0.319	0.014	-0.285	0.198	0.136	0.061	-0.083	0.373	-0.197	0.063	0.312	0.227	0.213	0.119	0.338	0.139
2	0.247	0.312	-0.189	-0.174	0.311	-0.323	0.145	0.01	0.136	-0.295	0.249	-0.031	-0.197	0.063	-0.192	-0.394	0.05	0.119	-0.288	-0.224
3	0.202	-0.103	-0.237	-0.297	-0.101	-0.115	-0.433	0.108	-0.25	0.432	0.104	-0.047	0.106	-0.252	-0.329	0.013	-0.053	-0.259	-0.129	-0.224
4	0.202	0.257	0.03	-0.297	0.004	-0.17	0.363	0.248	-0.25	-0.198	-0.271	-0.296	0.106	-0.252	0.209	0.154	-0.209	-0.259	0.258	0.0
5	0.247	-0.008	-0.365	0.174	0.108	0.452	0.003	0.079	0.136	-0.138	-0.354	0.078	0.197	0.063	-0.104	-0.073	-0.422	-0.119	-0.338	0.138
6	0.247	-0.32	-0.176	-0.174	-0.419	-0.129	-0.147	-0.09	0.136	-0.061	0.083	-0.373	-0.197	0.063	0.345	-0.253	-0.107	0.119	-0.05	0.362
7	0.247	0.352	-0.099	0.174	-0.011	-0.167	0.067	-0.436	0.136	0.138	0.354	-0.078	0.197	0.063	-0.136	0.406	-0.103	-0.119	0.049	0.362
8	0.202	-0.154	0.207	-0.297	0.097	0.285	0.07	-0.356	-0.25	-0.234	0.167	0.343	0.106	-0.252	0.12	-0.167	0.263	-0.259	-0.129	0.223
9	0.247	0.261	0.255	-0.174	-0.307	0.154	0.218	0.238	0.136	0.295	-0.249	0.031	-0.197	0.063	-0.225	0.086	0.369	0.119	-0.289	0.223
10	0.247	0.008	0.365	-0.174	0.108	0.452	0.003	0.079	0.136	0.138	0.354	-0.078	-0.197	0.063	-0.104	-0.073	-0.422	0.119	0.338	-0.138
11	0.247	0.32	0.176	0.174	-0.419	-0.129	-0.147	-0.09	0.136	0.061	-0.083	0.373	0.197	0.063	0.345	-0.253	-0.107	-0.119	0.05	-0.362
12	0.202	0.154	-0.207	0.297	0.097	0.285	0.07	-0.356	-0.25	0.234	-0.167	-0.343	-0.106	-0.252	0.12	-0.167	0.263	0.259	0.129	-0.223
13	0.247	-0.261	-0.255	0.174	-0.307	0.154	0.218	0.238	0.136	-0.295	0.249	-0.031	0.197	0.063	-0.225	0.086	0.369	-0.119	0.289	-0.223
14	0.247	-0.352	0.099	-0.174	-0.011	-0.167	0.067	-0.436	0.136	-0.138	-0.354	0.078	-0.197	0.063	-0.136	0.406	-0.103	0.119	-0.049	-0.362
15	0.247	-0.312	0.189	0.174	0.311	-0.323	0.145	0.01	0.136	0.295	-0.249	0.031	0.197	0.063	-0.192	-0.394	0.05	-0.119	0.288	0.224
16	0.247	-0.09	0.354	0.174	0.319	0.014	-0.285	0.198	0.136	-0.061	0.083	-0.373	0.197	0.063	0.312	0.227	0.213	-0.119	-0.338	-0.139
17	0.202	0.103	0.237	0.297	-0.101	-0.115	-0.433	0.108	-0.25	-0.432	-0.104	0.047	-0.106	-0.252	-0.329	0.013	-0.053	0.259	0.129	0.224
18	0.202	-0.257	-0.03	0.297	0.004	-0.17	0.363	0.248	-0.25	0.198	0.271	0.296	-0.106	-0.252	0.209	0.154	-0.209	0.259	-0.258	0.0
19	0.111	0.0	0.0	-0.23	0.0	0.0	0.0	0.0	-0.449	0.0	0.0	0.0	0.482	0.535	0.0	0.0	0.0	0.463	0.0	0.0
20	0.111	0.0	0.0	0.23	0.0	0.0	0.0	0.0	-0.449	0.0	0.0	0.0	-0.482	0.535	0.0	0.0	0.0	-0.463	0.0	0.0

2.2. Molecule orbital presentation:

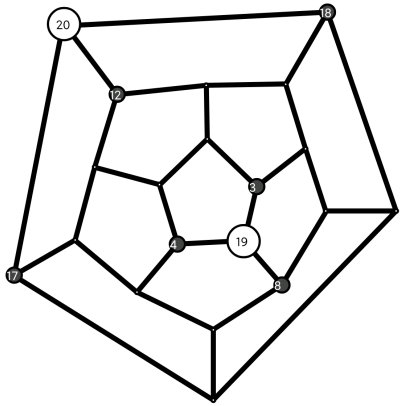

Ψ1
Ψ2
Ψ3
Ψ4
Ψ5
Ψ6


Ψ7
Ψ8
Ψ9
Ψ10
Ψ11
Ψ12

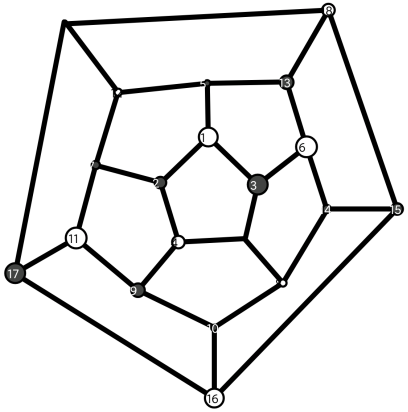
Ψ13



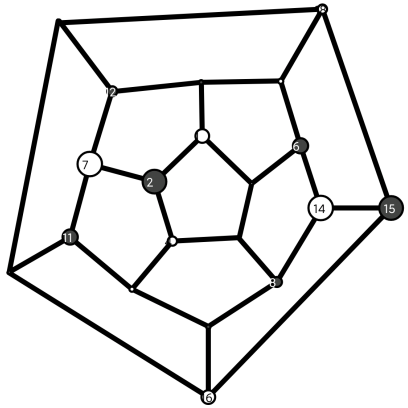
Ψ14



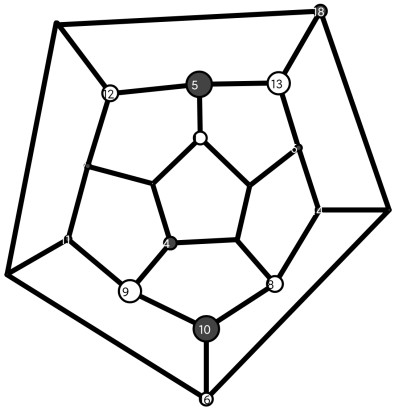
Ψ15



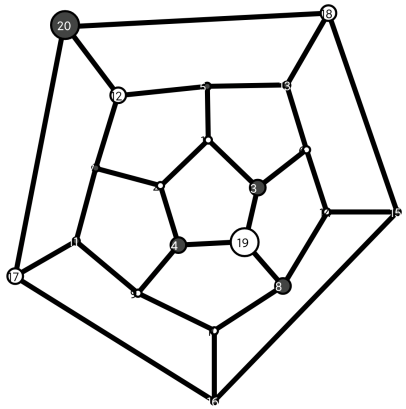
Ψ16

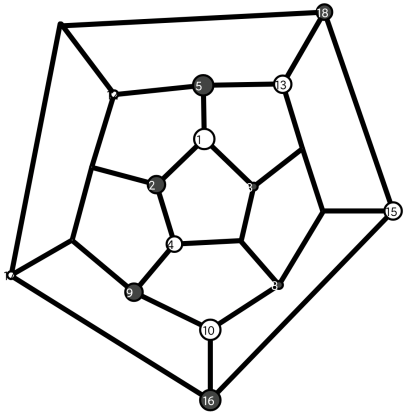
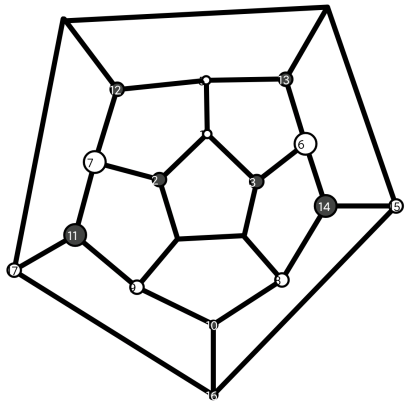


Ψ17



Ψ18



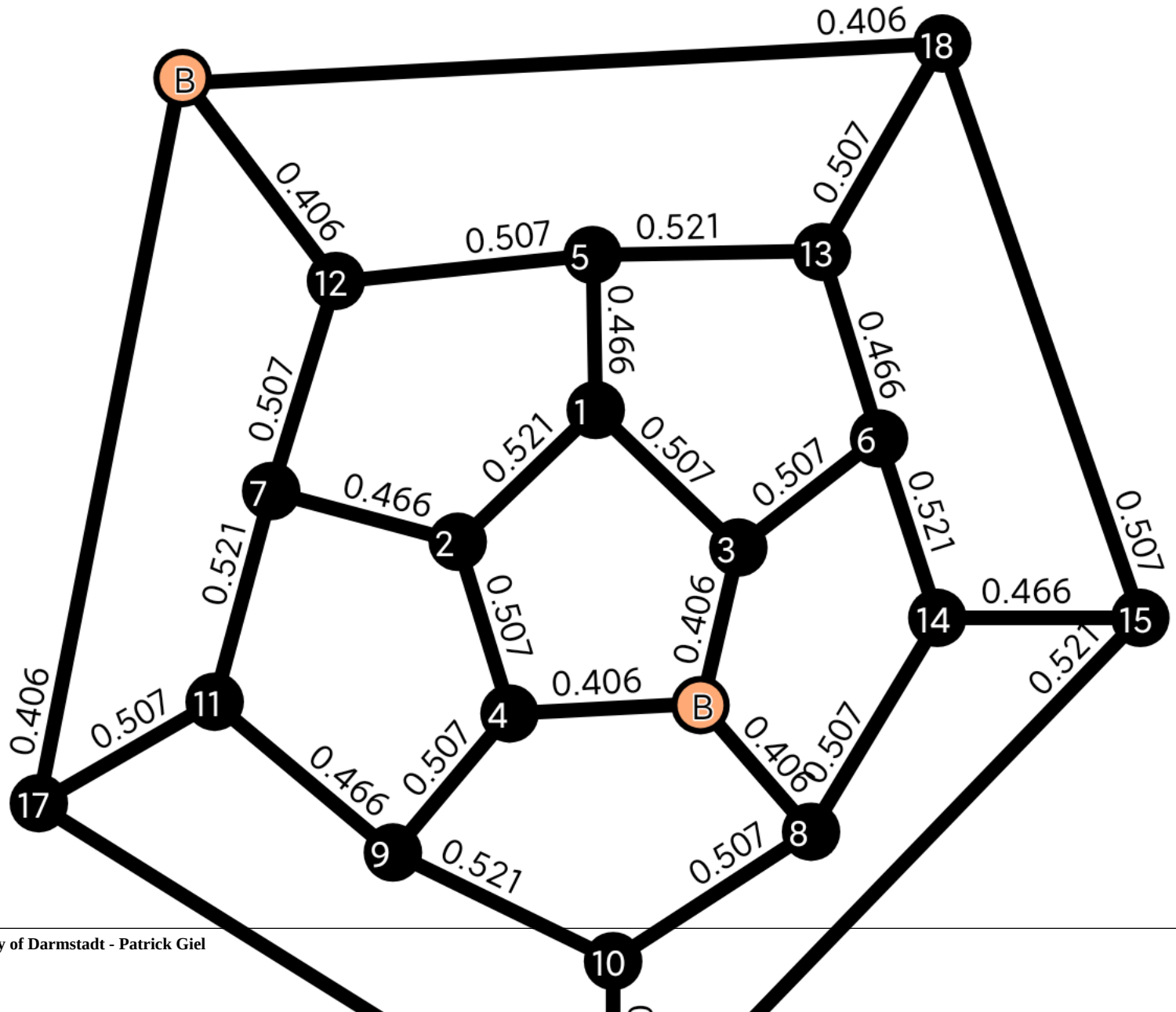
Ψ19	Ψ20	
		**The picture export was cancelled, more than 20 pictures are not possible.**

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
1	0.93																			
2	0.521	0.93																		
3	0.507	0.05	0.961																	
4	0.05	0.507	0.095	0.961																
5	0.466	0.009	-0.008	-0.208	0.93															
6	0.064	-0.136	0.507	-0.15	0.009	0.93														
7	0.009	0.466	-0.208	-0.008	0.064	0.019	0.93													
8	-0.15	-0.15	0.095	0.095	0.001	0.05	0.001	0.961												
9	-0.136	0.064	-0.15	0.507	0.019	0.073	0.009	0.05	0.93											
10	0.073	-0.136	-0.15	0.05	0.276	-0.136	-0.191	0.507	0.521	0.93										
11	-0.191	0.009	0.001	-0.008	-0.136	0.276	0.521	-0.208	0.466	0.009	0.93									
12	-0.008	-0.008	-0.126	-0.126	0.507	-0.208	0.507	0.341	-0.208	0.001	0.05	0.961								
13	0.009	-0.191	-0.008	0.001	0.521	0.466	-0.136	-0.208	0.276	0.019	0.073	0.05	0.93							
14	-0.136	0.073	0.05	-0.15	-0.191	0.521	0.276	0.507	-0.136	0.064	0.019	0.001	0.009	0.93						
15	0.019	0.276	-0.208	0.001	-0.136	0.009	0.073	-0.008	-0.191	0.009	-0.136	-0.15	0.064	0.466	0.93					
16	0.276	0.019	0.001	-0.208	0.073	-0.191	-0.136	-0.008	0.009	0.466	0.064	-0.15	-0.136	0.009	0.521	0.93				
17	0.001	-0.208	0.341	-0.126	-0.15	0.001	0.05	-0.126	-0.008	-0.008	0.507	0.095	-0.15	-0.208	0.05	0.507	0.961			
18	-0.208	0.001	-0.126	0.341	0.05	-0.008	-0.15	-0.126	0.001	-0.208	-0.15	0.095	0.507	-0.008	0.507	0.05	0.095	0.961		
19	0.013	0.013	0.406	0.406	-0.148	0.013	-0.148	0.406	0.013	0.013	-0.148	0.132	-0.148	0.013	-0.148	-0.148	0.132	0.132	0.534	
20	-0.148	-0.148	0.132	0.132	0.013	-0.148	0.013	0.132	-0.148	-0.148	0.013	0.406	0.013	-0.148	0.013	0.013	0.406	0.406	0.322	0.534

3.2. Presentation of bond order:


B
18
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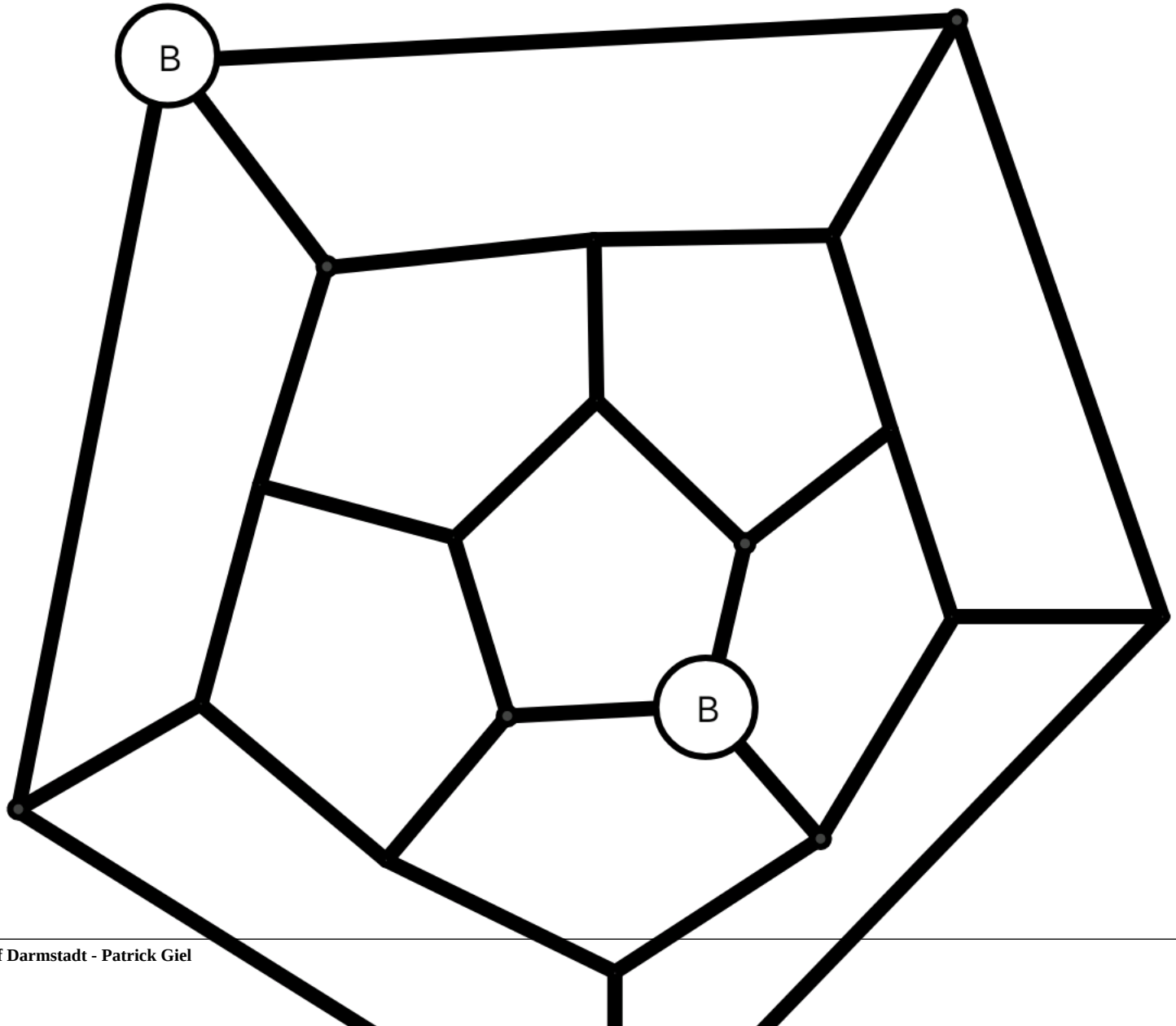
14
15
11
4
B
17
9
8
10
0.406
0.406
0.507
0.521
0.507
0.466
0.507
0.521
0.507
0.466
0.521
0.507
0.507
0.521
0.466
0.406
0.406
0.507
0.466
0.507
0.406
0.507
0.521
0.507
0.521

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	-0.03																			
2		-0.03																		
3			-0.061																	
4				-0.061																
5					-0.03															
6						-0.03														
7							-0.03													
8								-0.061												
9									-0.03											
10										-0.03										
11											-0.03									
12												-0.061								
13													-0.03							
14														-0.03						
15															-0.03					
16																-0.03				
17																	-0.061			
18																		-0.061		
19																			0.366	
20																				0.366

4.2. Presentation of molecule:

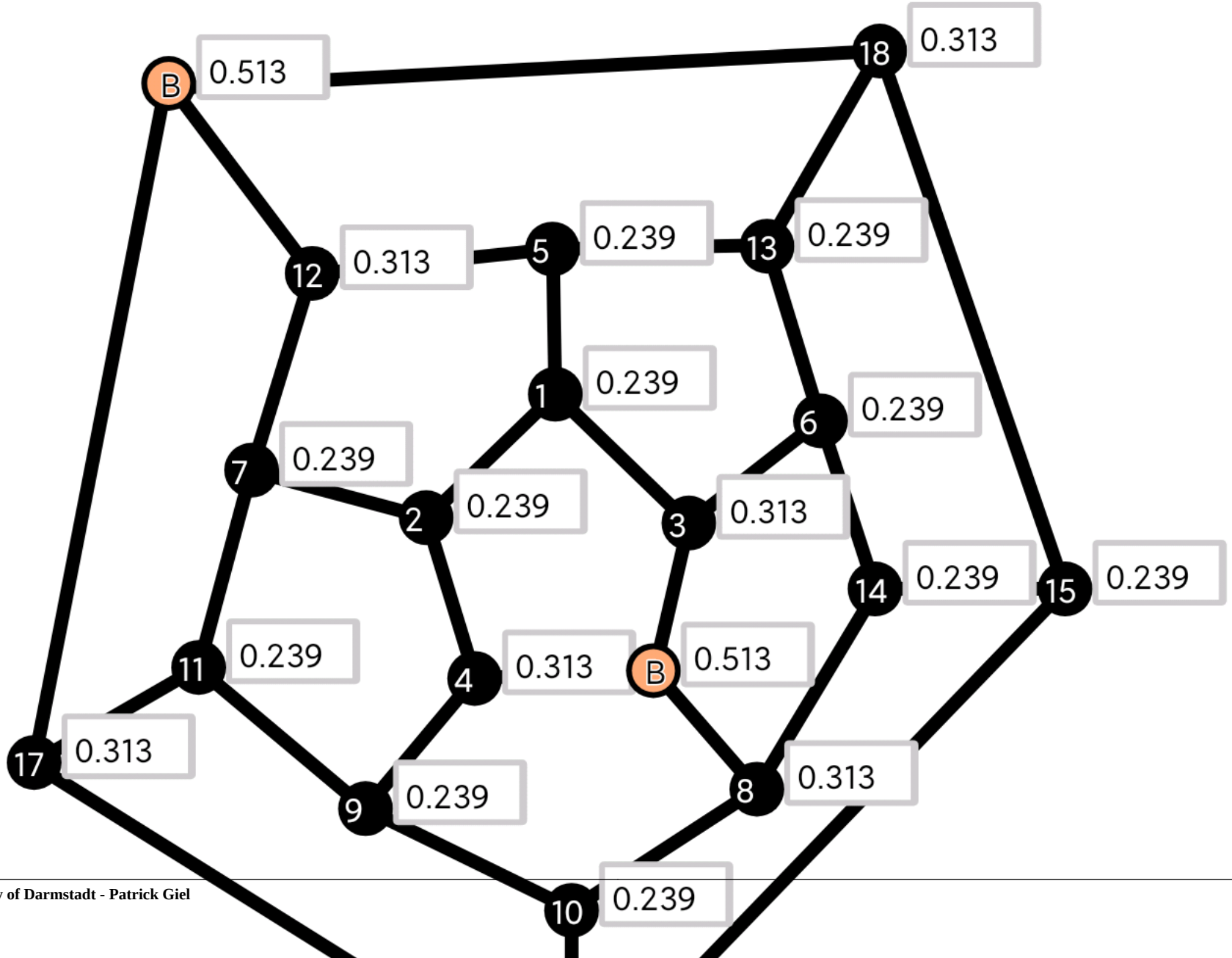

B
B

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
0.239	0.239	0.313	0.313	0.239	0.239	0.239	0.313	0.239	0.239	0.239	0.313	0.239	0.239	0.239	0.239	0.313	0.313	0.513	0.513

5.2. Presentation of molecule:

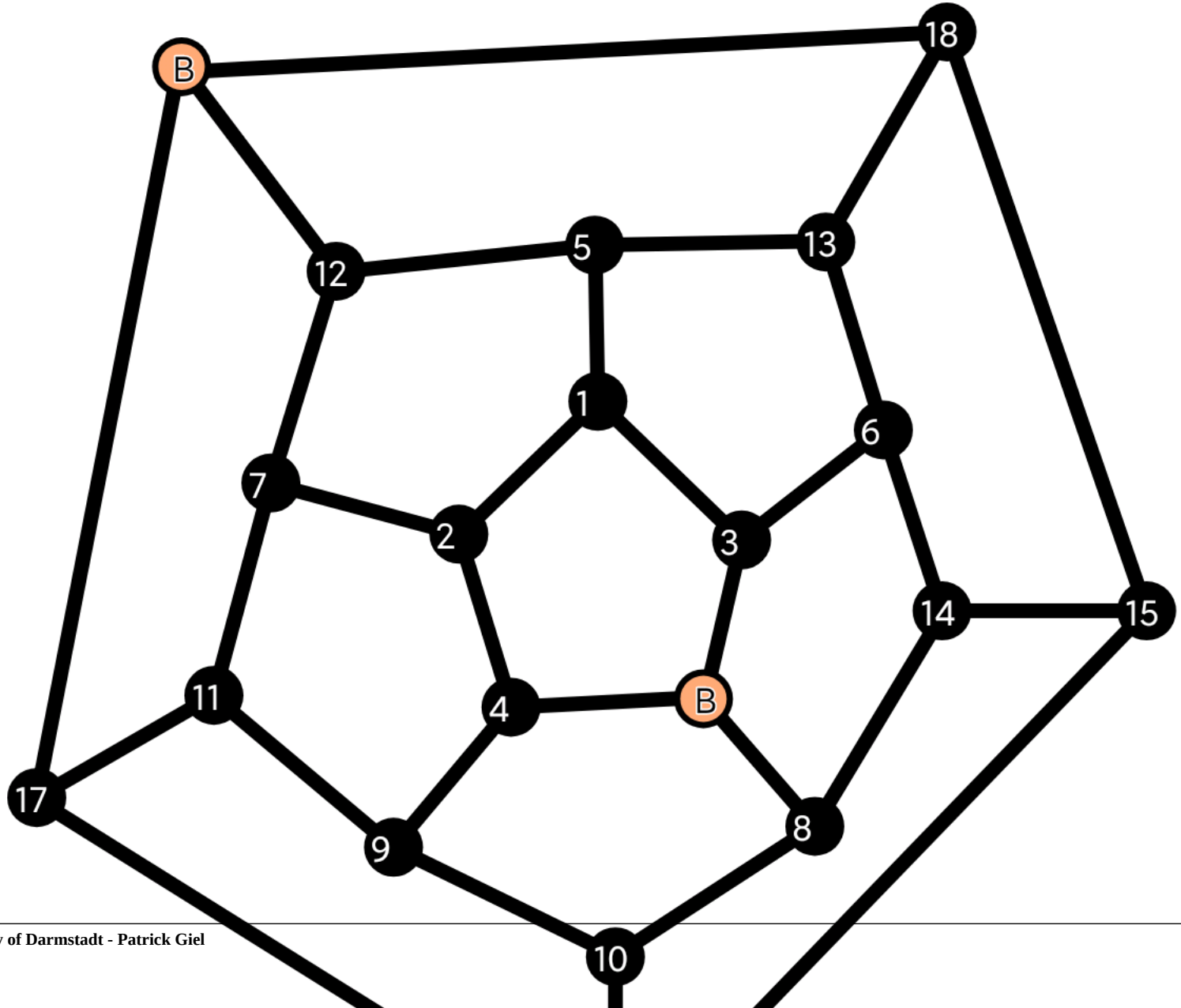

B
0.513
18
0.313
12
0.313
5
0.239
13
0.239
1
0.239
6
0.239
7
0.239
2
0.239
3
0.313
14
0.239
15
0.239
11
0.239
4
0.313
B
0.513
17
0.313
9
0.239
8
0.313
10
0.239

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	0.479																			
2	-0.098	0.479																		
3	-0.065	0.083	0.746																	
4	0.083	-0.065	-0.119	0.746																
5	-0.031	-0.007	0.082	-0.117	0.479															
6	-0.032	-0.003	-0.065	-0.093	-0.007	0.479														
7	-0.007	-0.031	-0.117	0.082	-0.032	0.019	0.479													
8	-0.093	-0.093	-0.119	-0.119	-0.001	0.083	-0.001	0.746												
9	-0.003	-0.032	-0.093	-0.065	0.019	-0.025	-0.007	0.083	0.479											
10	-0.025	-0.003	-0.093	0.083	-0.172	-0.003	0.003	-0.065	-0.098	0.479										
11	0.003	-0.007	-0.001	0.082	-0.003	-0.172	-0.098	-0.117	-0.031	-0.007	0.479									
12	0.082	0.082	0.097	0.097	-0.065	-0.117	-0.065	-0.414	-0.117	-0.001	0.083	0.746								
13	-0.007	0.003	0.082	-0.001	-0.098	-0.031	-0.003	-0.117	-0.172	0.019	-0.025	0.083	0.479							
14	-0.003	-0.025	0.083	-0.093	0.003	-0.098	-0.172	-0.065	-0.003	-0.032	0.019	-0.001	-0.007	0.479						
15	0.019	-0.172	-0.117	-0.001	-0.003	-0.007	-0.025	0.082	0.003	-0.007	-0.003	-0.093	-0.032	-0.031	0.479					
16	-0.172	0.019	-0.001	-0.117	-0.025	0.003	-0.003	0.082	-0.007	-0.031	-0.032	-0.093	-0.003	-0.007	-0.098	0.479				
17	-0.001	-0.117	-0.414	0.097	-0.093	-0.001	0.083	0.097	0.082	0.082	-0.065	-0.119	-0.093	-0.117	0.083	-0.065	0.746			
18	-0.117	-0.001	0.097	-0.414	0.083	0.082	-0.093	0.097	-0.001	-0.117	-0.093	-0.119	-0.065	0.082	-0.065	0.083	-0.119	0.746		
19	0.019	0.019	-0.034	-0.034	-0.034	0.019	-0.034	-0.034	0.019	0.019	-0.034	-0.032	-0.034	0.019	-0.034	-0.034	-0.032	-0.032	0.505	
20	-0.034	-0.034	-0.032	-0.032	0.019	-0.034	0.019	-0.032	-0.034	-0.034	0.019	-0.034	0.019	-0.034	0.019	0.019	-0.034	-0.034	-0.218	0.505

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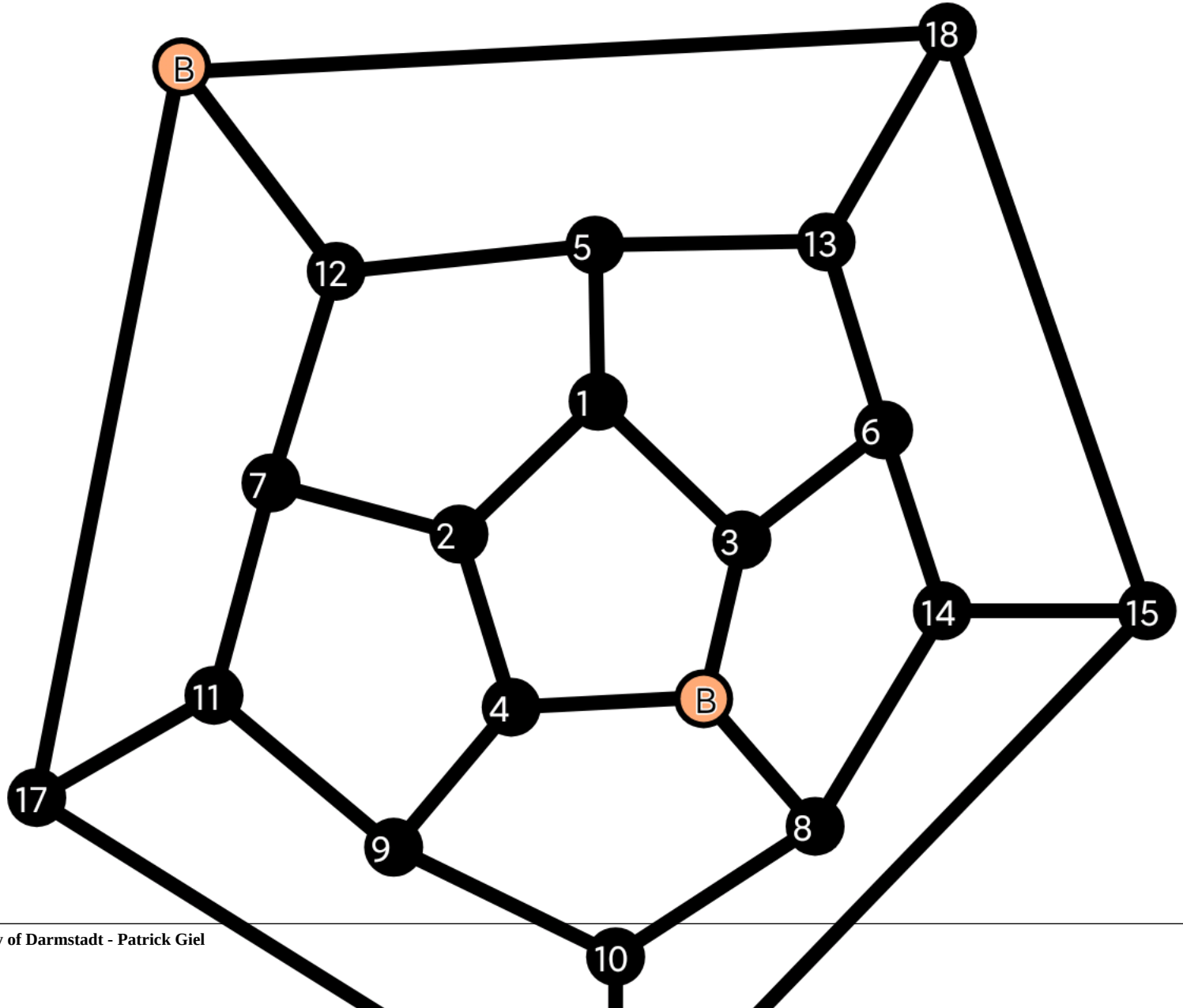
7. Bond-Atom-Polarizability

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	0.043	0.043	0.015	0.015	-0.013	-0.004	-0.013	-0.093	-0.004	0.016	0.012	0.082	0.012	0.016	-0.025	-0.025	-0.03	-0.03	0.019	-0.034
1 3	-0.025	-0.022	-0.045	-0.022	-0.041	0.02	0.035	0.106	-0.027	0.049	-0.041	-0.094	0.017	-0.028	0.009	0.044	0.058	-0.003	-0.025	0.036
1 5	0.078	-0.024	0.026	0.009	0.078	-0.018	-0.018	-0.028	0.02	-0.067	0.002	0.026	-0.024	0.002	0.02	-0.067	-0.028	0.009	0.001	0.001
2 4	-0.022	-0.025	-0.022	-0.045	0.035	-0.027	-0.041	0.106	0.02	-0.028	0.017	-0.094	-0.041	0.049	0.044	0.009	-0.003	0.058	-0.025	0.036
2 7	-0.024	0.078	0.009	0.026	-0.018	0.02	0.078	-0.028	-0.018	0.002	-0.024	0.026	0.002	-0.067	-0.067	0.02	0.009	-0.028	0.001	0.001
3 6	0.02	-0.028	-0.045	0.106	0.017	-0.025	0.009	-0.022	0.049	-0.027	0.044	-0.003	-0.041	-0.022	0.035	-0.041	0.058	-0.094	-0.025	0.036
3 19	0.002	0.074	0.292	-0.135	0.055	0.002	-0.096	-0.135	-0.054	-0.054	-0.004	0.123	0.055	0.074	-0.096	-0.004	-0.275	0.123	0.142	-0.087
4 9	-0.028	0.02	0.106	-0.045	0.009	0.049	0.017	-0.022	-0.025	-0.022	-0.041	-0.003	0.044	-0.027	-0.041	0.035	-0.094	0.058	-0.025	0.036
4 19	0.074	0.002	-0.135	0.292	-0.096	-0.054	0.055	-0.135	0.002	0.074	0.055	0.123	-0.004	-0.054	-0.004	-0.096	0.123	-0.275	0.142	-0.087
5 12	-0.041	0.017	-0.094	-0.003	-0.025	0.035	0.02	0.058	0.009	0.044	-0.028	-0.045	-0.022	-0.041	-0.027	0.049	0.106	-0.022	0.036	-0.025
5 13	-0.013	0.012	0.082	-0.03	0.043	-0.013	-0.004	-0.03	-0.025	-0.025	0.016	0.015	0.043	0.012	-0.004	0.016	-0.093	0.015	-0.034	0.019
6 13	-0.018	0.002	0.026	-0.028	-0.024	0.078	0.02	0.009	-0.067	0.02	-0.067	0.009	0.078	-0.024	-0.018	0.002	-0.028	0.026	0.001	0.001
6 14	-0.004	0.016	0.015	-0.093	0.012	0.043	-0.025	0.015	0.016	-0.004	-0.025	-0.03	-0.013	0.043	-0.013	0.012	-0.03	0.082	0.019	-0.034
7 11	0.012	-0.013	-0.03	0.082	-0.004	-0.025	0.043	-0.03	-0.013	0.012	0.043	0.015	0.016	-0.025	0.016	-0.004	0.015	-0.093	-0.034	0.019
7 12	0.017	-0.041	-0.003	-0.094	0.02	0.009	-0.025	0.058	0.035	-0.041	-0.022	-0.045	-0.028	0.044	0.049	-0.027	-0.022	0.106	0.036	-0.025
8 10	0.049	-0.027	0.106	-0.022	0.044	-0.028	-0.041	-0.045	-0.022	-0.025	0.035	0.058	0.009	0.02	0.017	-0.041	-0.094	-0.003	-0.025	0.036
8 14	-0.027	0.049	-0.022	0.106	-0.041	-0.022	0.044	-0.045	-0.028	0.02	0.009	0.058	0.035	-0.025	-0.041	0.017	-0.003	-0.094	-0.025	0.036
8 19	-0.054	-0.054	-0.135	-0.135	-0.004	0.074	-0.004	0.292	0.074	0.002	-0.096	-0.275	-0.096	0.002	0.055	0.055	0.123	0.123	0.142	-0.087
9 10	0.016	-0.004	-0.093	0.015	-0.025	0.016	0.012	0.015	0.043	0.043	-0.013	-0.03	-0.025	-0.004	0.012	-0.013	0.082	-0.03	0.019	-0.034
9 11	0.002	-0.018	-0.028	0.026	0.02	-0.067	-0.024	0.009	0.078	-0.024	0.078	0.009	-0.067	0.02	0.002	-0.018	0.026	-0.028	0.001	0.001
10 16	-0.067	0.02	-0.028	0.009	-0.067	0.002	0.002	0.026	-0.024	0.078	-0.018	-0.028	0.02	-0.018	-0.024	0.078	0.026	0.009	0.001	0.001
11 17	-0.041	0.035	0.058	-0.094	-0.027	0.044	-0.022	-0.003	-0.041	0.017	-0.025	-0.022	0.049	0.009	-0.028	0.02	-0.045	0.106	0.036	-0.025
12 20	0.055	0.055	0.123	0.123	0.002	-0.096	0.002	-0.275	-0.096	-0.004	0.074	0.292	0.074	-0.004	-0.054	-0.054	-0.135	-0.135	-0.087	0.142
13 18	0.035	-0.041	-0.094	0.058	-0.022	-0.041	-0.027	-0.003	0.044	0.009	0.049	-0.022	-0.025	0.017	0.02	-0.028	0.106	-0.045	0.036	-0.025
14 15	0.02	-0.067	0.009	-0.028	0.002	-0.024	-0.067	0.026	0.002	-0.018	0.02	-0.028	-0.018	0.078	0.078	-0.024	0.009	0.026	0.001	0.001
15 16	-0.025	-0.025	-0.03	-0.03	0.016	0.012	0.016	0.082	0.012	-0.013	-0.004	-0.093	-0.004	-0.013	0.043	0.043	0.015	0.015	-0.034	0.019
15 18	0.009	0.044	-0.003	0.058	-0.028	0.017	0.049	-0.094	-0.041	0.035	-0.027	0.106	0.02	-0.041	-0.025	-0.022	-0.022	-0.045	0.036	-0.025
16 17	0.044	0.009	0.058	-0.003	0.049	-0.041	-0.028	-0.094	0.017	-0.041	0.02	0.106	-0.027	0.035	-0.022	-0.025	-0.045	-0.022	0.036	-0.025
17 20	-0.004	-0.096	-0.275	0.123	-0.054	-0.004	0.074	0.123	0.055	0.055	0.002	-0.135	-0.054	-0.096	0.074	0.002	0.292	-0.135	-0.087	0.142
18 20	-0.096	-0.004	0.123	-0.275	0.074	0.055	-0.054	0.123	-0.004	-0.096	-0.054	-0.135	0.002	0.055	0.002	0.074	-0.135	0.292	-0.087	0.142

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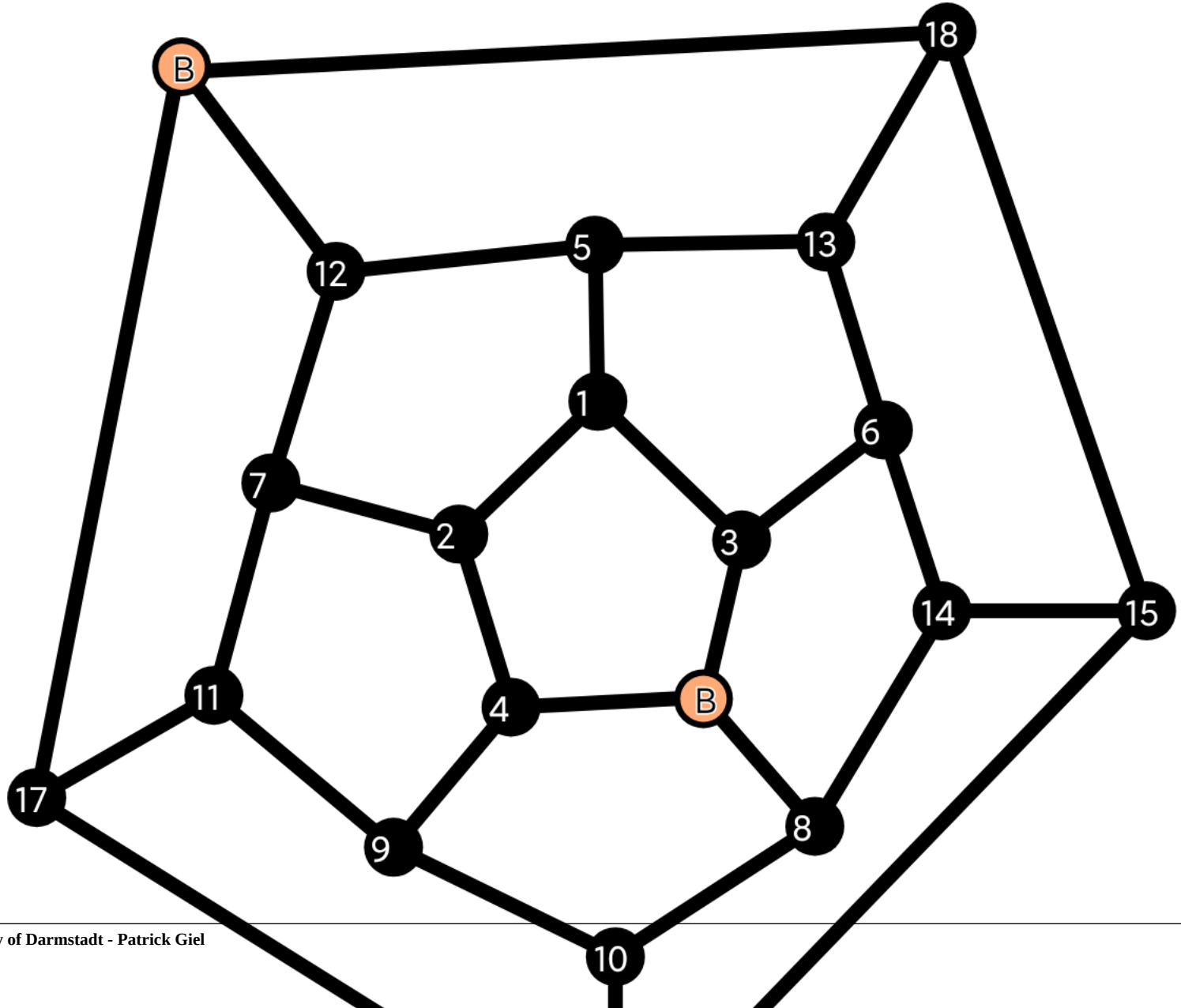
8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3	1 5	2 4	2 7	3 6	3 19	4 9	4 19	5 12	5 13	6 13	6 14	7 11	7 12	8 10	8 14	8 19	9 10	9 11	10 16	11 17	12 20	13 18	14 15	15 16	15 18	16 17	17 20	18 20
1 2	0.382																													
1 3	-0.201	0.527																												
1 5	-0.1	-0.21	0.448																											
2 4	-0.201	0.007	0.108	0.527																										
2 7	-0.1	0.108	-0.066	-0.21	0.448																									
3 6	0.062	-0.203	0.06	0.039	-0.075	0.527																								
3 19	0.075	-0.238	0.104	-0.083	0.009	-0.238	0.824																							
4 9	0.062	0.039	-0.075	-0.203	0.06	-0.148	0.198	0.527																						
4 19	0.075	-0.083	0.009	-0.238	0.104	0.198	-0.224	-0.238	0.824																					
5 12	-0.025	0.153	-0.21	-0.023	0.06	-0.023	-0.179	-0.068	0.073	0.527																				
5 13	0.069	-0.025	-0.1	-0.064	0.011	-0.025	0.11	0.133	-0.1	-0.201	0.382																			
6 13	0.011	0.06	-0.066	-0.083	0.038	-0.21	0.104	0.141	-0.085	0.108	-0.1	0.448																		
6 14	-0.046	0.062	0.011	0.022	0.032	-0.201	0.075	0.022	-0.108	-0.064	0.069	-0.1	0.382																	
7 11	0.069	-0.064	0.011	-0.025	-0.1	0.133	-0.1	-0.025	0.11	0.062	-0.046	0.032	-0.153	0.382																
7 12	-0.025	-0.023	0.06	0.153	-0.21	-0.068	0.073	-0.023	-0.179	-0.203	0.062	-0.075	0.133	-0.201	0.527															
8 10	0.022	-0.148	0.141	0.039	-0.083	0.039	0.198	0.007	-0.083	-0.272	0.133	-0.075	0.062	-0.064	0.144	0.527														
8 14	0.022	0.039	-0.083	-0.148	0.141	0.007	-0.083	0.039	0.198	0.144	-0.064	0.108	-0.201	0.133	-0.272	-0.203	0.527													
8 19	-0.108	0.198	-0.085	0.198	-0.085	-0.083	-0.224	-0.083	-0.224	0.186	-0.1	0.009	0.075	-0.1	0.186	-0.238	-0.238	0.824												
9 10	-0.046	0.022	0.032	0.062	0.011	0.022	-0.108	-0.201	0.075	0.133	-0.153	0.032	-0.046	0.069	-0.064	-0.201	0.062	0.075	0.382											
9 11	0.011	-0.083	0.038	0.06	-0.066	0.141	-0.085	-0.21	0.104	-0.075	0.032	-0.197	0.032	-0.1	0.108	0.108	-0.075	0.009	-0.1	0.448										
10 16	0.032	0.141	-0.197	-0.075	0.038	-0.083	-0.085	0.108	0.009	0.141	0.032	0.038	0.011	0.011	-0.083	-0.21	0.06	0.104	-0.1	-0.066	0.448									
11 17	-0.064	0.144	-0.083	-0.023	0.108	-0.272	0.186	0.153	-0.179	0.039	0.022	0.141	0.133	-0.201	0.007	-0.023	-0.068	0.073	-0.025	-0.21	0.06	0.527								

	1 2	**1 3**	**1 5**	**2 4**	**2 7**	**3 6**	**3 19**	**4 9**	**4 19**	**5 12**	**5 13**	**6 13**	**6 14**	**7 11**	**7 12**	**8 10**	**8 14**	**8 19**	**9 10**	**9 11**	**10 16**	**11 17**	**12 20**	**13 18**	**14 15**	**15 16**	**15 18**	**16 17**	**17 20**	**18 20**
12 20	0.11	-0.179	0.104	-0.179	0.104	0.073	0.191	0.073	0.191	-0.238	0.075	0.009	-0.1	0.075	-0.238	0.186	0.186	-0.57	-0.1	0.009	-0.085	-0.083	0.824							
13 18	-0.064	-0.023	0.108	0.144	-0.083	0.153	-0.179	-0.272	0.186	0.007	-0.201	-0.21	-0.025	0.022	0.039	-0.068	-0.023	0.073	0.133	0.141	-0.075	-0.148	-0.083	0.527						
14 15	0.032	-0.075	0.038	0.141	-0.197	0.108	0.009	-0.083	-0.085	-0.083	0.011	-0.066	-0.1	0.032	0.141	0.06	-0.21	0.104	0.011	0.038	-0.066	-0.075	-0.085	0.06	0.448					
15 16	-0.153	0.133	0.032	0.133	0.032	-0.064	-0.1	-0.064	-0.1	0.022	-0.046	0.011	0.069	-0.046	0.022	-0.025	-0.025	0.11	0.069	0.011	-0.1	0.062	-0.108	0.062	-0.1	0.382				
15 18	0.133	-0.068	-0.075	-0.272	0.141	-0.023	0.073	0.144	0.186	0.039	0.062	0.06	-0.025	0.022	-0.148	-0.023	0.153	-0.179	-0.064	-0.083	0.108	0.039	0.198	-0.203	-0.21	-0.201	0.527			
16 17	0.133	-0.272	0.141	-0.068	-0.075	0.144	0.186	-0.023	0.073	-0.148	0.022	-0.083	-0.064	0.062	0.039	0.153	-0.023	-0.179	-0.025	0.06	-0.21	-0.203	0.198	0.039	0.108	-0.201	0.007	0.527		
17 20	-0.1	0.186	-0.085	0.073	0.009	0.186	-0.57	-0.179	0.191	0.198	-0.108	-0.085	-0.1	0.075	-0.083	-0.179	0.073	0.191	0.11	0.104	0.104	-0.238	-0.224	0.198	0.009	0.075	-0.083	-0.238	0.824	
18 20	-0.1	0.073	0.009	0.186	-0.085	-0.179	0.191	0.186	-0.57	-0.083	0.075	0.104	0.11	-0.108	0.198	0.073	-0.179	0.191	-0.1	-0.085	0.009	0.198	-0.224	-0.238	0.104	0.075	-0.238	-0.083	-0.224	0.824

8.2. Presentation of molecule: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