Print calculated values

Report generated by:root, 17.02.2020 - 16:26:08

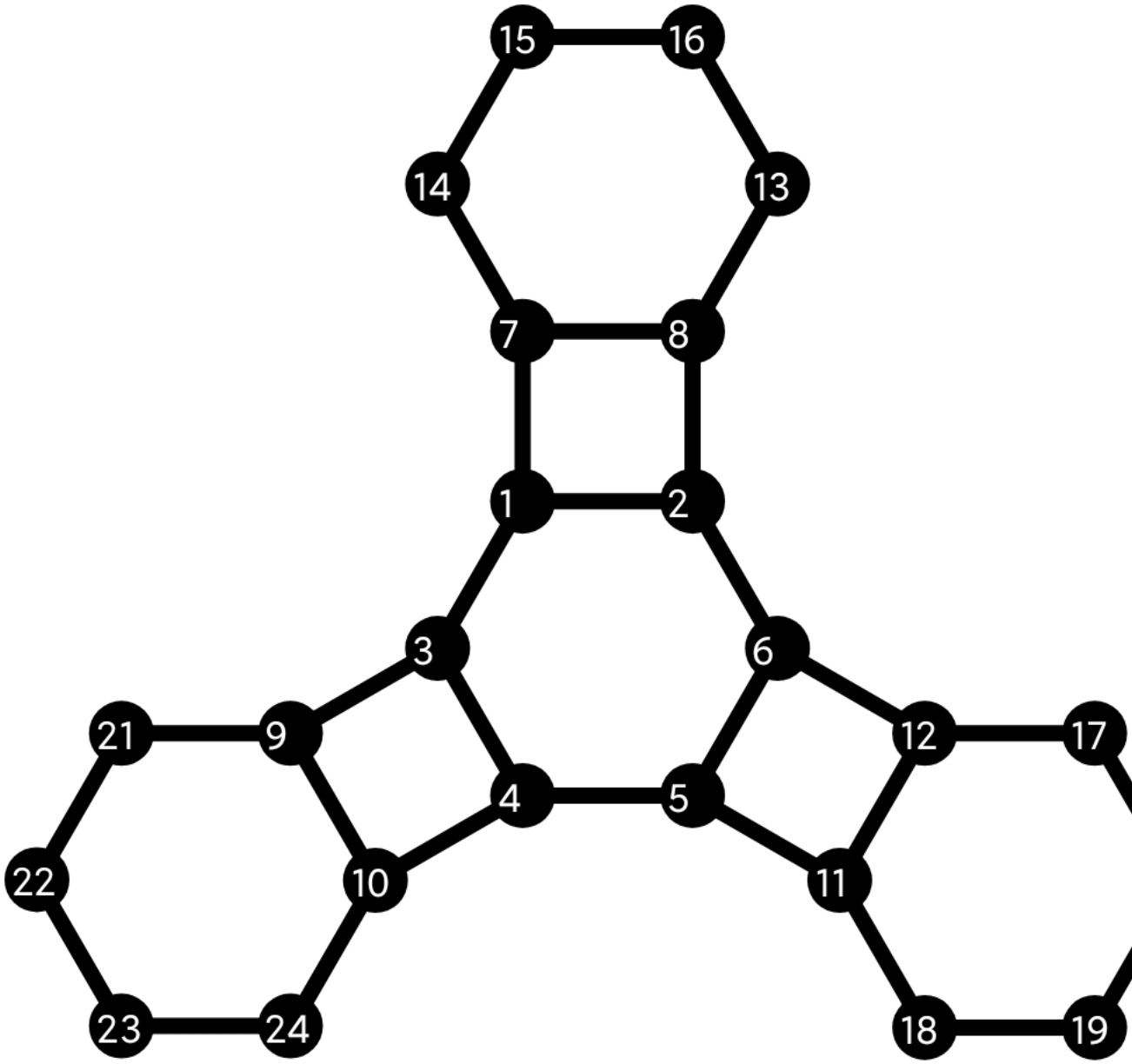
The following determinant is calculated:

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

It is about this molecule:

HMO-Energies

x1 = 2.764; x2 = 2.311; x3 = 2.311; x4 = 1.694; x5 = 1.49; x6 = 1.49; x7 = 1.113; x8 = 1.113;
x9 = 1.061; x10 = 0.604; x11 = 0.452; x12 = 0.452; x13 = -0.452; x14 = -0.452; x15 = -0.604; x16 = -1.061;
x17 = -1.113; x18 = -1.113; x19 = -1.49; x20 = -1.49; x21 = -1.694; x22 = -2.311; x23 = -2.311; x24 = -2.764;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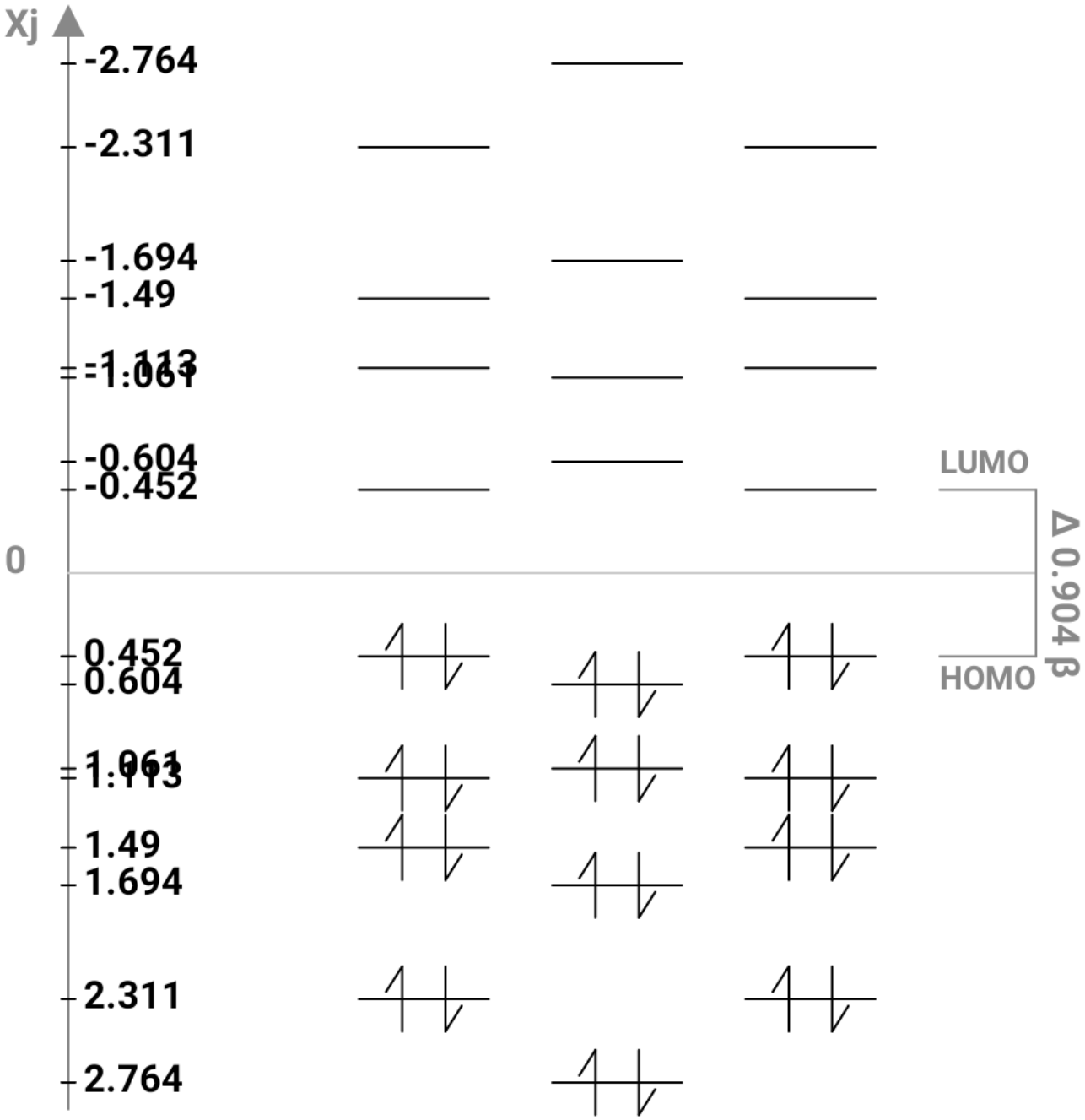
1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 24α + 33.71β -

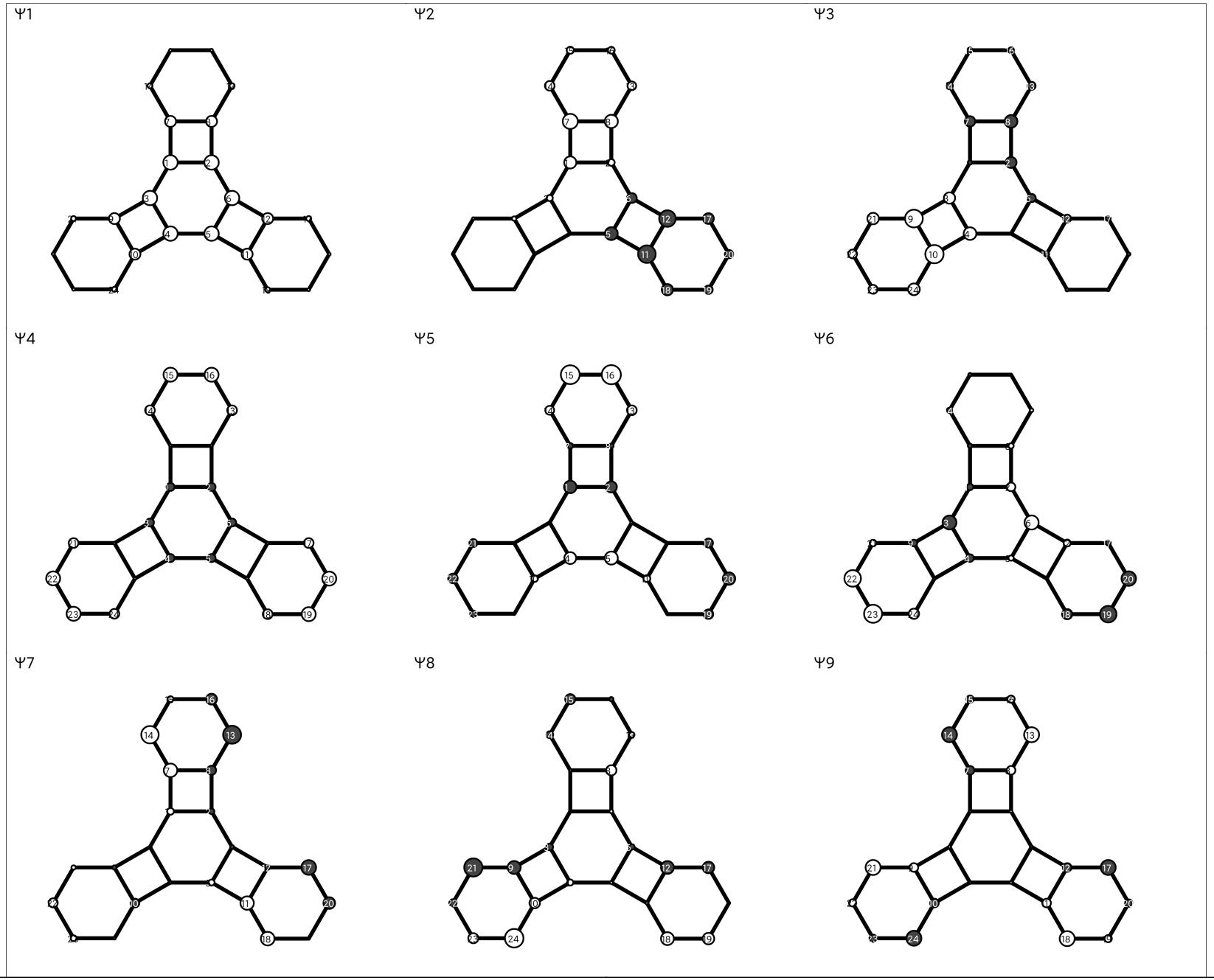
this corresponds to one πelectron: 1.405β

2. Hueckel-coefficient

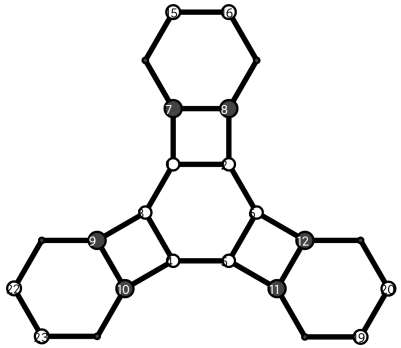
2.1. Calculated values:

	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	Psi 22	Psi 23	Psi 24
	x1= 2.764	x2= 2.311	x3= 2.311	x4= 1.694	x5= 1.49	x6= 1.49	x7= 1.113	x8= 1.113	x9= 1.061	x10= 0.604	x11= 0.452	x12= 0.452	x13= - 0.452	x14= - 0.452	x15= - 0.604	x16= - 1.061	x17= - 1.113	x18= - 1.113	x19= - 1.49	x20= - 1.49	x21= - 1.694	x22= - 2.311	x23= - 2.311	x24= - 2.764
1	0.309	0.26	-0.094	-0.172	-0.269	-0.139	0.145	-0.014	-0.061	0.194	-0.268	0.269	0.129	-0.357	0.194	-0.061	0.044	-0.138	-0.267	-0.142	0.172	0.265	0.078	0.309
2	0.309	0.144	-0.236	-0.172	-0.239	0.186	-0.122	0.079	0.061	0.194	0.297	0.237	-0.341	-0.167	-0.194	-0.061	0.103	-0.103	0.241	-0.183	-0.172	-0.158	-0.227	-0.309
3	0.309	0.133	0.243	-0.172	-0.041	-0.3	-0.008	-0.145	0.061	0.194	-0.354	0.138	0.025	0.379	-0.194	-0.061	-0.14	-0.038	0.038	0.3	-0.172	-0.118	0.25	-0.309
4	0.309	-0.049	0.272	-0.172	0.255	-0.163	-0.06	0.132	-0.061	0.194	-0.099	-0.367	-0.374	0.066	0.194	-0.061	-0.142	0.031	0.257	-0.16	0.172	-0.065	-0.269	0.309
5	0.309	-0.276	-0.006	-0.172	0.28	0.114	0.129	0.066	0.061	0.194	0.057	-0.376	0.316	-0.212	-0.194	-0.061	0.037	0.14	-0.279	-0.117	-0.172	0.275	-0.023	-0.309
6	0.309	-0.211	-0.178	-0.172	0.014	0.302	-0.084	-0.118	-0.061	0.194	0.367	0.098	0.245	0.291	0.194	-0.061	0.098	0.107	0.01	0.302	0.172	-0.2	0.191	0.309
7	0.236	0.325	-0.223	0.053	-0.12	-0.093	0.29	0.051	-0.186	-0.271	-0.064	-0.254	0.257	-0.05	0.271	0.186	-0.011	0.294	0.119	0.095	0.053	-0.337	-0.203	-0.236
8	0.236	0.283	-0.273	0.053	-0.101	0.114	-0.196	0.22	0.186	-0.271	0.035	-0.259	-0.22	0.142	-0.271	0.186	-0.256	0.146	-0.102	0.112	-0.053	0.299	0.256	0.236
9	0.236	0.095	0.382	0.053	-0.048	-0.144	-0.093	-0.28	0.186	-0.271	0.207	0.16	0.233	0.119	-0.271	0.186	0.254	0.149	-0.046	-0.145	-0.053	0.072	-0.387	0.236
10	0.236	0.031	0.392	0.053	0.141	-0.057	-0.189	0.226	-0.186	-0.271	0.252	0.071	-0.172	-0.198	0.271	0.186	0.26	-0.137	-0.141	0.055	0.053	-0.007	0.394	-0.236
11	0.236	-0.378	-0.109	0.053	0.149	0.031	0.288	0.06	0.186	-0.271	-0.242	0.099	-0.013	-0.261	-0.271	0.186	0.002	-0.294	0.148	0.032	-0.053	-0.371	0.131	0.236
12	0.236	-0.355	-0.17	0.053	-0.021	0.151	-0.101	-0.277	-0.186	-0.271	-0.188	0.183	-0.085	0.248	0.271	0.186	-0.249	-0.157	0.023	-0.15	0.053	0.344	-0.191	-0.236
13	0.108	0.186	-0.173	0.209	0.208	0.077	-0.386	0.115	0.322	-0.087	-0.217	-0.101	0.183	0.153	0.087	-0.322	0.193	-0.354	-0.208	-0.079	0.209	-0.196	-0.161	-0.108
14	0.108	0.207	-0.148	0.209	0.191	-0.113	0.374	-0.15	-0.322	-0.087	0.204	-0.125	-0.026	0.237	-0.087	-0.322	0.225	-0.334	0.192	-0.111	-0.209	0.215	0.135	0.108
15	0.061	0.153	-0.119	0.301	0.404	-0.075	0.126	-0.217	-0.156	0.219	0.156	0.197	-0.245	-0.057	-0.219	0.156	-0.239	0.078	-0.405	0.071	0.301	-0.16	-0.109	-0.061
16	0.061	0.147	-0.126	0.301	0.411	0.001	-0.234	-0.092	0.156	0.219	-0.133	0.214	0.137	-0.211	0.219	0.156	0.041	0.248	0.411	0.006	-0.301	0.154	0.117	0.061
17	0.108	-0.231	-0.105	0.209	-0.194	-0.109	-0.317	-0.249	-0.322	-0.087	-0.21	-0.114	-0.193	-0.141	-0.087	-0.322	0.177	0.362	-0.192	-0.111	-0.209	-0.225	0.119	0.108
18	0.108	-0.243	-0.075	0.209	-0.038	-0.219	0.293	0.277	0.322	-0.087	0.021	0.238	-0.224	0.082	0.087	-0.322	0.21	0.344	0.035	0.219	0.209	0.238	-0.089	-0.108
19	0.061	-0.183	-0.064	0.301	-0.205	-0.357	0.037	0.248	0.156	0.219	0.252	0.008	0.115	0.224	0.219	0.156	-0.235	-0.088	-0.201	-0.359	-0.301	-0.178	0.075	0.061
20	0.061	-0.179	-0.073	0.301	-0.268	-0.313	-0.251	0.0	-0.156	0.219	0.093	-0.234	0.172	-0.184	-0.219	0.156	0.052	-0.246	0.264	0.316	0.301	0.174	-0.084	-0.061
21	0.108	0.057	0.248	0.209	-0.171	0.142	0.093	-0.392	0.322	-0.087	0.196	-0.137	0.041	-0.235	0.087	-0.322	-0.403	0.009	0.172	-0.14	0.209	-0.042	0.251	-0.108
22	0.061	0.036	0.19	0.301	-0.207	0.356	0.197	-0.157	0.156	0.219	-0.119	-0.222	-0.252	-0.013	0.219	0.156	0.194	-0.159	-0.211	0.353	-0.301	0.024	-0.192	0.061
23	0.061	0.026	0.192	0.301	-0.137	0.388	0.125	0.218	-0.156	0.219	-0.249	0.037	0.073	0.241	-0.219	0.156	0.187	0.168	0.141	-0.386	0.301	-0.015	0.193	-0.061
24	0.108	0.025	0.253	0.209	0.003	0.222	-0.057	0.399	-0.322	-0.087	0.006	0.239	0.219	-0.096	-0.087	-0.322	-0.402	-0.027	0.0	0.222	-0.209	0.009	-0.254	0.108

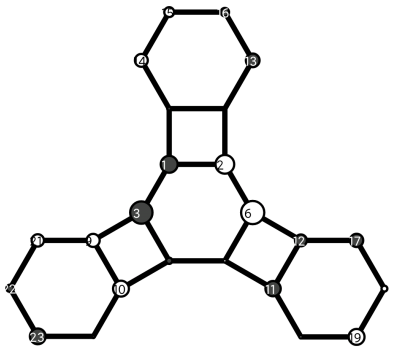
2.2. Molecule orbital presentation:


Ψ1
Ψ2
Ψ3
Ψ4
Ψ5
Ψ6
Ψ7
Ψ8
Ψ9

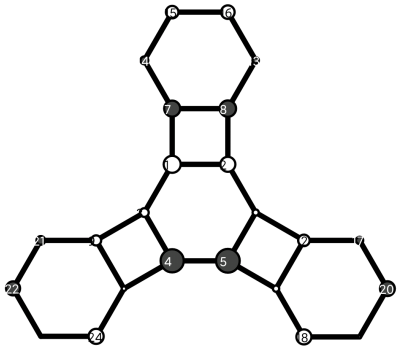
Ψ10



Ψ11



Ψ12



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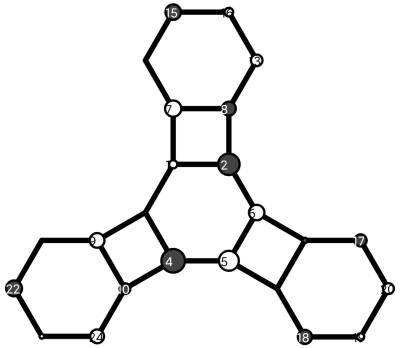

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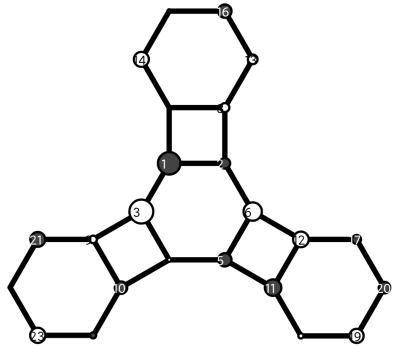

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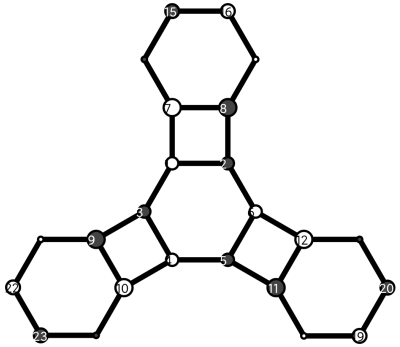
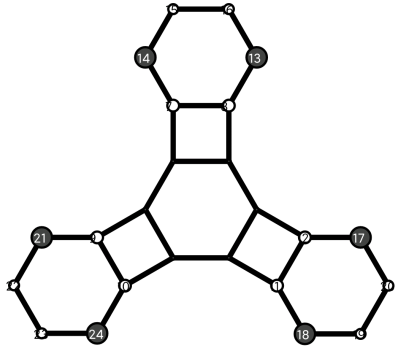


Ψ16



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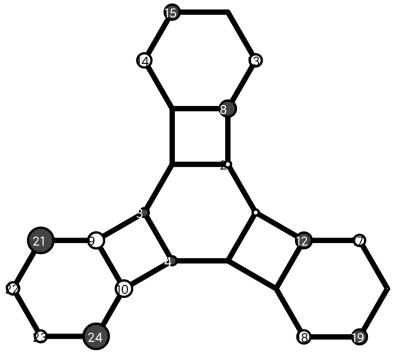

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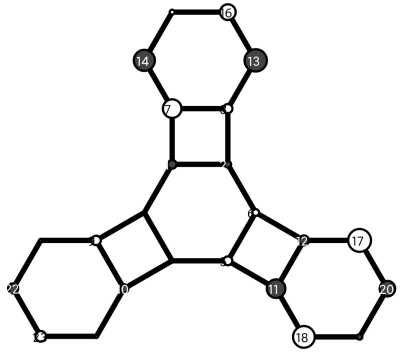

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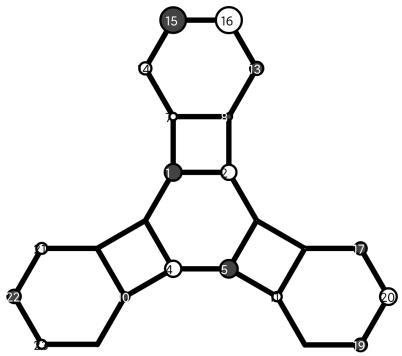
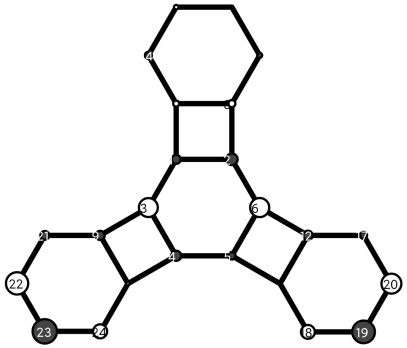


Ψ20



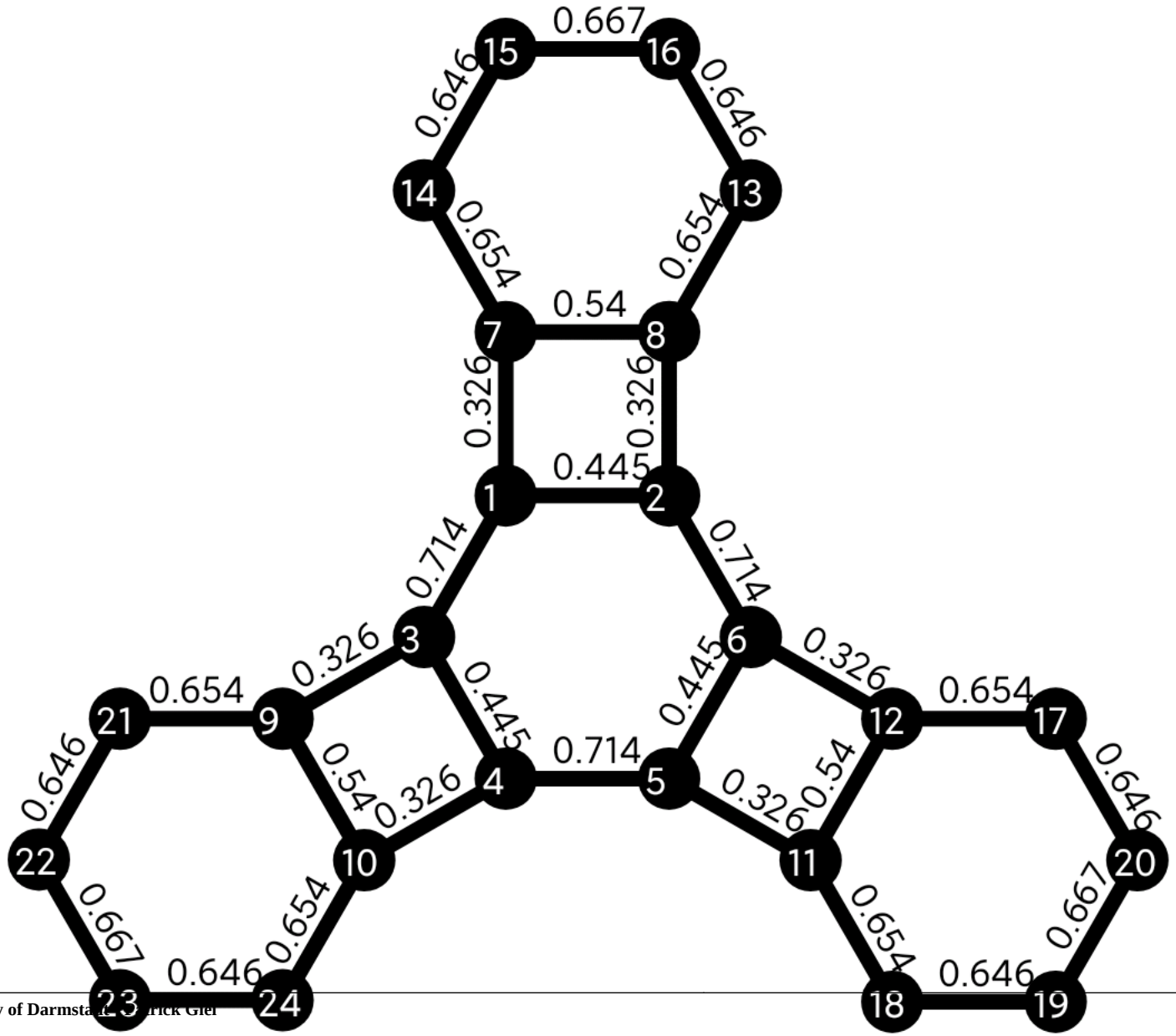
The picture export was cancelled, more than 20 pictures are not possible.

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	22	23	24
1	1.0																							
2	0.445	1.0																						
3	0.714	0.0	1.0																					
4	0.0	-0.203	0.445	1.0																				
5	-0.203	0.0	0.0	0.714	1.0																			
6	0.0	0.714	-0.203	0.0	0.445	1.0																		
7	0.326	0.0	0.0	0.039	0.0	-0.23	1.0																	
8	0.0	0.326	-0.23	0.0	0.039	0.0	0.54	1.0																
9	0.0	0.039	0.326	0.0	-0.23	0.0	-0.065	0.0	1.0															
10	-0.23	0.0	0.0	0.326	0.0	0.039	0.0	0.111	0.54	1.0														
11	0.0	-0.23	0.039	0.0	0.326	0.0	0.111	0.0	0.0	-0.065	1.0													
12	0.039	0.0	0.0	-0.23	0.0	0.326	0.0	-0.065	0.111	0.0	0.54	1.0												
13	-0.135	0.0	0.0	0.084	0.0	-0.184	0.0	0.654	-0.014	0.0	0.079	0.0	1.0											
14	0.0	-0.135	-0.184	0.0	0.084	0.0	0.654	0.0	0.0	0.079	0.0	-0.014	-0.279	1.0										
15	0.008	0.0	0.0	-0.059	0.0	0.165	0.0	-0.3	0.032	0.0	-0.08	0.0	0.0	0.646	1.0									
16	0.0	0.008	0.165	0.0	-0.059	0.0	-0.3	0.0	0.0	-0.08	0.0	0.032	0.646	0.0	0.667	1.0								
17	0.0	-0.184	0.084	0.0	-0.135	0.0	0.079	0.0	0.0	-0.014	0.0	0.654	0.072	0.0	-0.067	0.0	1.0							
18	0.084	0.0	0.0	-0.184	0.0	-0.135	0.0	-0.014	0.079	0.0	0.654	0.0	0.0	-0.04	0.0	0.026	-0.279	1.0						
19	0.0	0.165	-0.059	0.0	0.008	0.0	-0.08	0.0	0.0	0.032	0.0	-0.3	-0.067	0.0	0.066	0.0	0.0	0.646	1.0					
20	-0.059	0.0	0.0	0.165	0.0	0.008	0.0	0.032	-0.08	0.0	-0.3	0.0	0.0	0.026	0.0	-0.027	0.646	0.0	0.667	1.0				
21	-0.184	0.0	0.0	-0.135	0.0	0.084	0.0	0.079	0.654	0.0	-0.014	0.0	0.0	0.072	0.0	-0.067	-0.04	0.0	0.026	0.0	1.0			
22	0.0	-0.059	0.008	0.0	0.165	0.0	0.032	0.0	0.0	-0.3	0.0	-0.08	0.026	0.0	-0.027	0.0	0.0	-0.067	0.0	0.066	0.646	1.0		
23	0.165	0.0	0.0	0.008	0.0	-0.059	0.0	-0.08	-0.3	0.0	0.032	0.0	0.0	-0.067	0.0	0.066	0.026	0.0	-0.027	0.0	0.0	0.667	1.0	
24	0.0	0.084	-0.135	0.0	-0.184	0.0	-0.014	0.0	0.0	0.654	0.0	0.079	-0.04	0.0	0.026	0.0	0.0	0.072	0.0	-0.067	-0.279	0.0	0.646	1.0

3.2. Presentation of bond order:

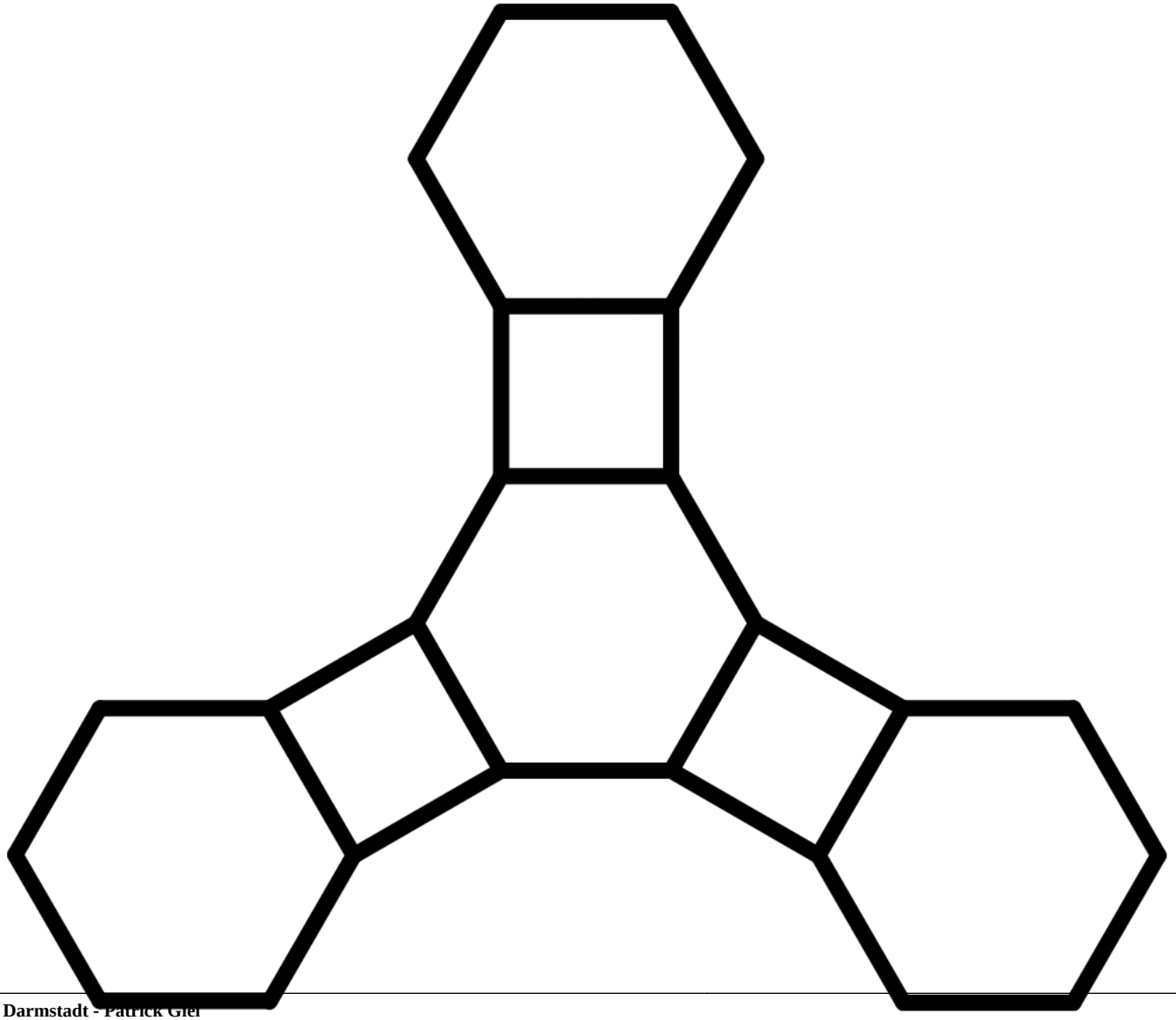

0.667
15
16
0.646
0.646
14
13
0.654
0.654
0.54
7
8
0.326
0.326
0.445
1
2
0.714
0.714
3
6
0.326
0.326
0.654
0.654
21
9
12
17
0.646
0.646
0.54
0.445
0.445
0.714
4
5
0.326
0.54
0.326
22
10
11
20
0.667
0.654
0.654
0.667
0.646
0.646
23
24
18
19

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	22	23	24
1	0.0																							
2		0.0																						
3			0.0																					
4				0.0																				
5					0.0																			
6						0.0																		
7							0.0																	
8								0.0																
9									0.0															
10										0.0														
11											0.0													
12												0.0												
13													0.0											
14														0.0										
15															0.0									
16																0.0								
17																	0.0							
18																		0.0						
19																			0.0					
20																				0.0				
21																					0.0			
22																						0.0		
23																							0.0	
24																								0.0

4.2. Presentation of molecule:

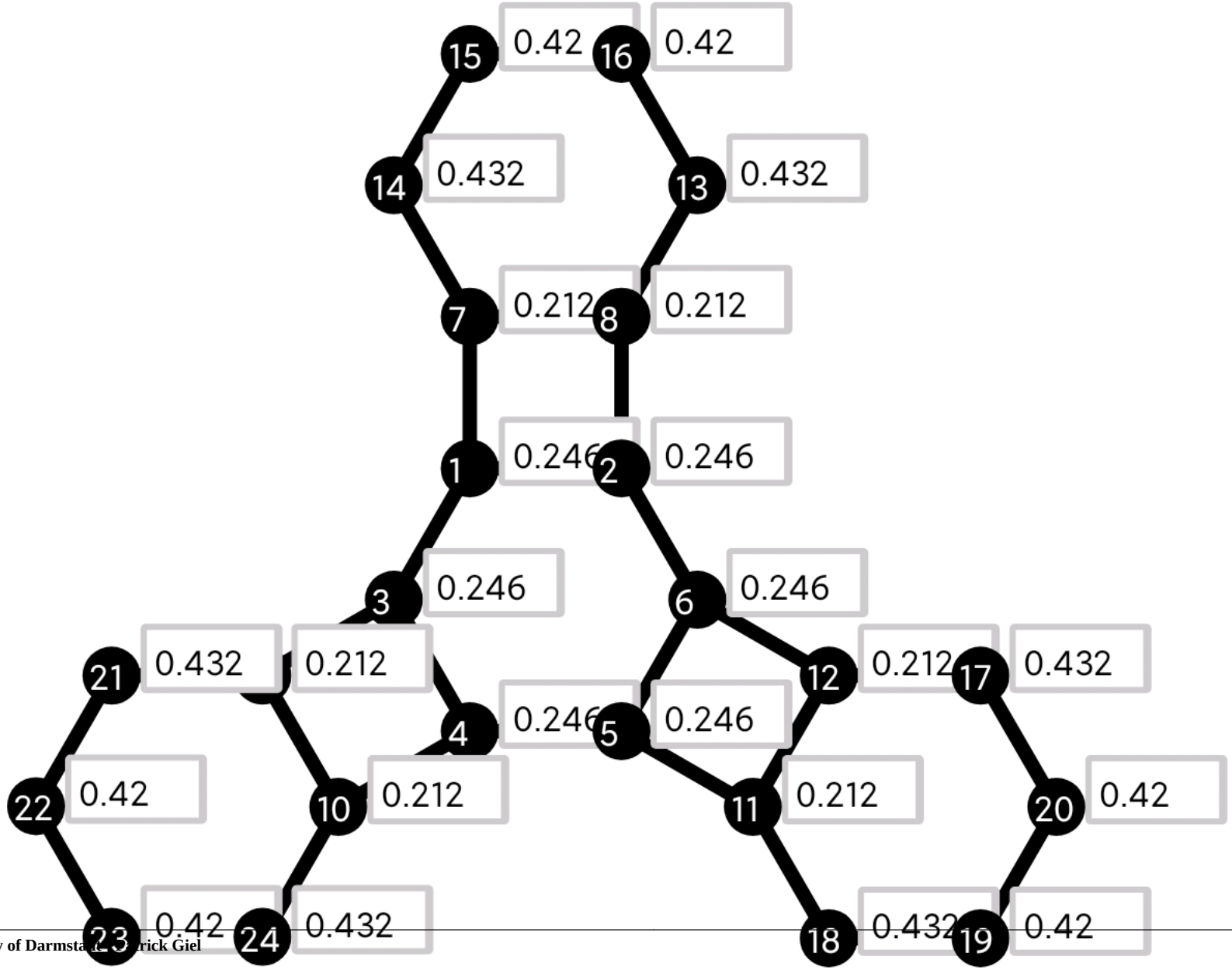


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
0.246	0.246	0.246	0.246	0.246	0.246	0.212	0.212	0.212	0.212	0.212	0.212	0.432	0.432	0.42	0.42	0.432	0.432	0.42	0.42	0.432	0.42	0.42	0.432

5.2. Presentation of molecule:

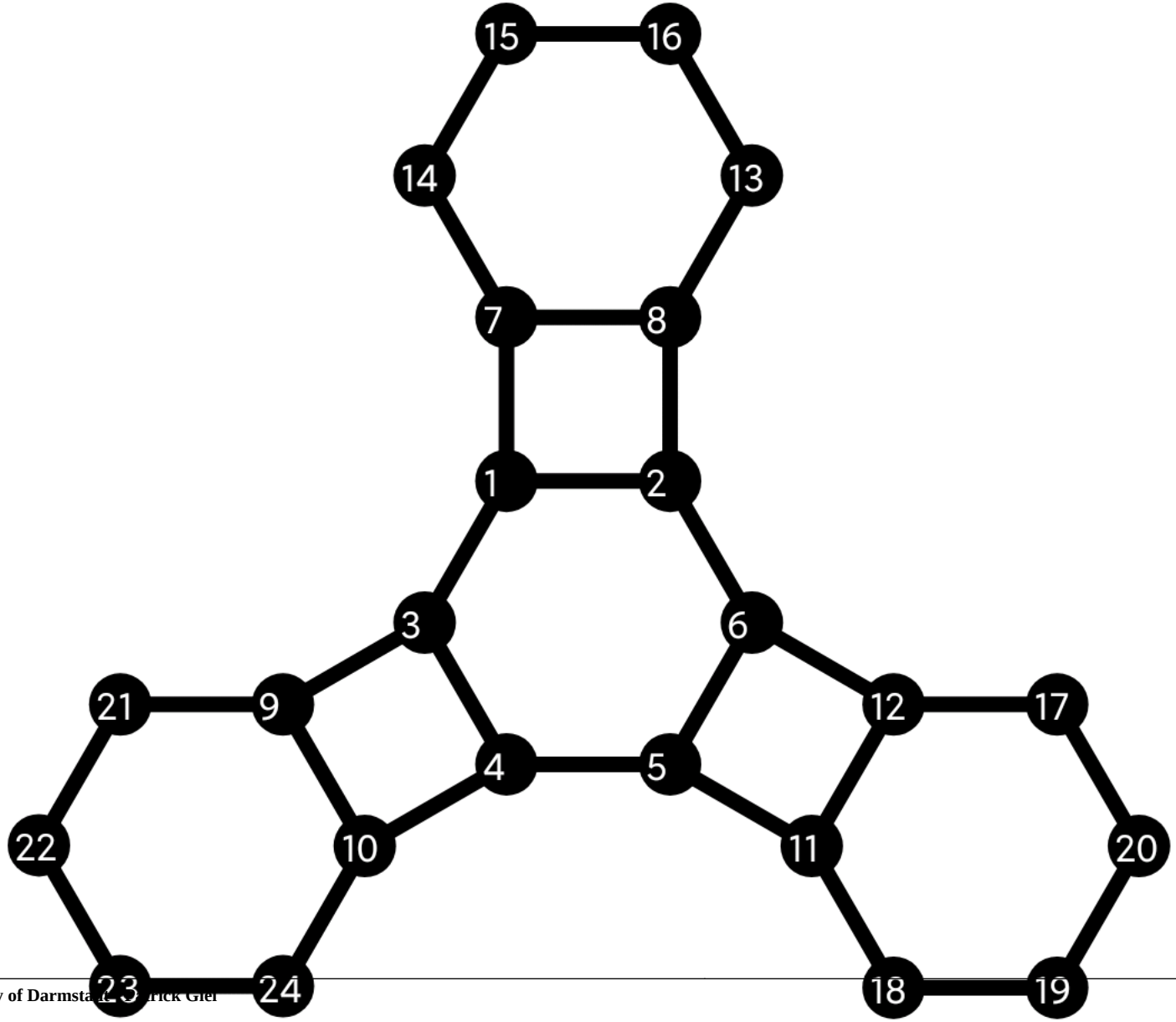

15
0.42
16
0.42
14
0.432
13
0.432
7
0.212
8
0.212
1
0.246
2
0.246
3
0.246
6
0.246
21
0.432
0.212
12
0.212
17
0.432
4
0.246
5
0.246
22
0.42
10
0.212
11
0.212
20
0.42
23
0.42
24
0.432
18
0.432
19
0.42

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	22	23	24
1	0.434																							
2	-0.046	0.434																						
3	-0.25	0.007	0.434																					
4	0.007	-0.047	-0.046	0.434																				
5	-0.047	0.007	0.007	-0.25	0.434																			
6	0.007	-0.25	-0.047	0.007	-0.046	0.434																		
7	-0.022	0.046	0.009	-0.008	0.006	-0.055	0.401																	
8	0.046	-0.022	-0.055	0.006	-0.008	0.009	-0.107	0.401																
9	0.009	-0.008	-0.022	0.046	-0.055	0.006	-0.003	0.001	0.401															
10	-0.055	0.006	0.046	-0.022	0.009	-0.008	0.001	-0.015	-0.107	0.401														
11	0.006	-0.055	-0.008	0.009	-0.022	0.046	-0.015	0.001	0.001	-0.003	0.401													
12	-0.008	0.009	0.006	-0.055	0.046	-0.022	0.001	-0.003	-0.015	0.001	-0.107	0.401												
13	-0.012	0.018	0.004	-0.011	0.0	-0.045	0.002	-0.159	-0.002	0.002	-0.01	0.001	0.424											
14	0.018	-0.012	-0.045	0.0	-0.011	0.004	-0.159	0.002	0.001	-0.01	0.002	-0.002	-0.072	0.424										
15	-0.002	0.018	0.0	-0.009	0.002	-0.044	0.021	-0.093	-0.002	0.0	-0.011	0.001	0.02	-0.139	0.422									
16	0.018	-0.002	-0.044	0.002	-0.009	0.0	-0.093	0.021	0.001	-0.011	0.0	-0.002	-0.139	0.02	-0.161	0.422								
17	0.0	-0.045	-0.011	0.004	-0.012	0.018	-0.01	0.001	0.002	-0.002	0.002	-0.159	-0.01	0.0	-0.009	0.0	0.424							
18	-0.011	0.004	0.0	-0.045	0.018	-0.012	0.002	-0.002	-0.01	0.001	-0.159	0.002	0.0	-0.003	0.001	-0.002	-0.072	0.424						
19	0.002	-0.044	-0.009	0.0	-0.002	0.018	-0.011	0.001	0.0	-0.002	0.021	-0.093	-0.009	0.001	-0.009	0.0	0.02	-0.139	0.422					
20	-0.009	0.0	0.002	-0.044	0.018	-0.002	0.0	-0.002	-0.011	0.001	-0.093	0.021	0.0	-0.002	0.0	-0.002	-0.139	0.02	-0.161	0.422				
21	-0.045	0.0	0.018	-0.012	0.004	-0.011	0.001	-0.01	-0.159	0.002	-0.002	0.002	0.0	-0.01	0.0	-0.009	-0.003	0.0	-0.002	0.001	0.424			
22	0.0	-0.009	-0.002	0.018	-0.044	0.002	-0.002	0.0	0.021	-0.093	0.001	-0.011	-0.002	0.0	-0.002	0.0	0.001	-0.009	0.0	-0.009	-0.139	0.422		
23	-0.044	0.002	0.018	-0.002	0.0	-0.009	0.001	-0.011	-0.093	0.021	-0.002	0.0	0.001	-0.009	0.0	-0.009	-0.002	0.0	-0.002	0.0	0.02	-0.161	0.422	
24	0.004	-0.011	-0.012	0.018	-0.045	0.0	-0.002	0.002	0.002	-0.159	0.001	-0.01	-0.003	0.0	-0.002	0.001	0.0	-0.01	0.0	-0.009	-0.072	0.02	-0.139	0.424

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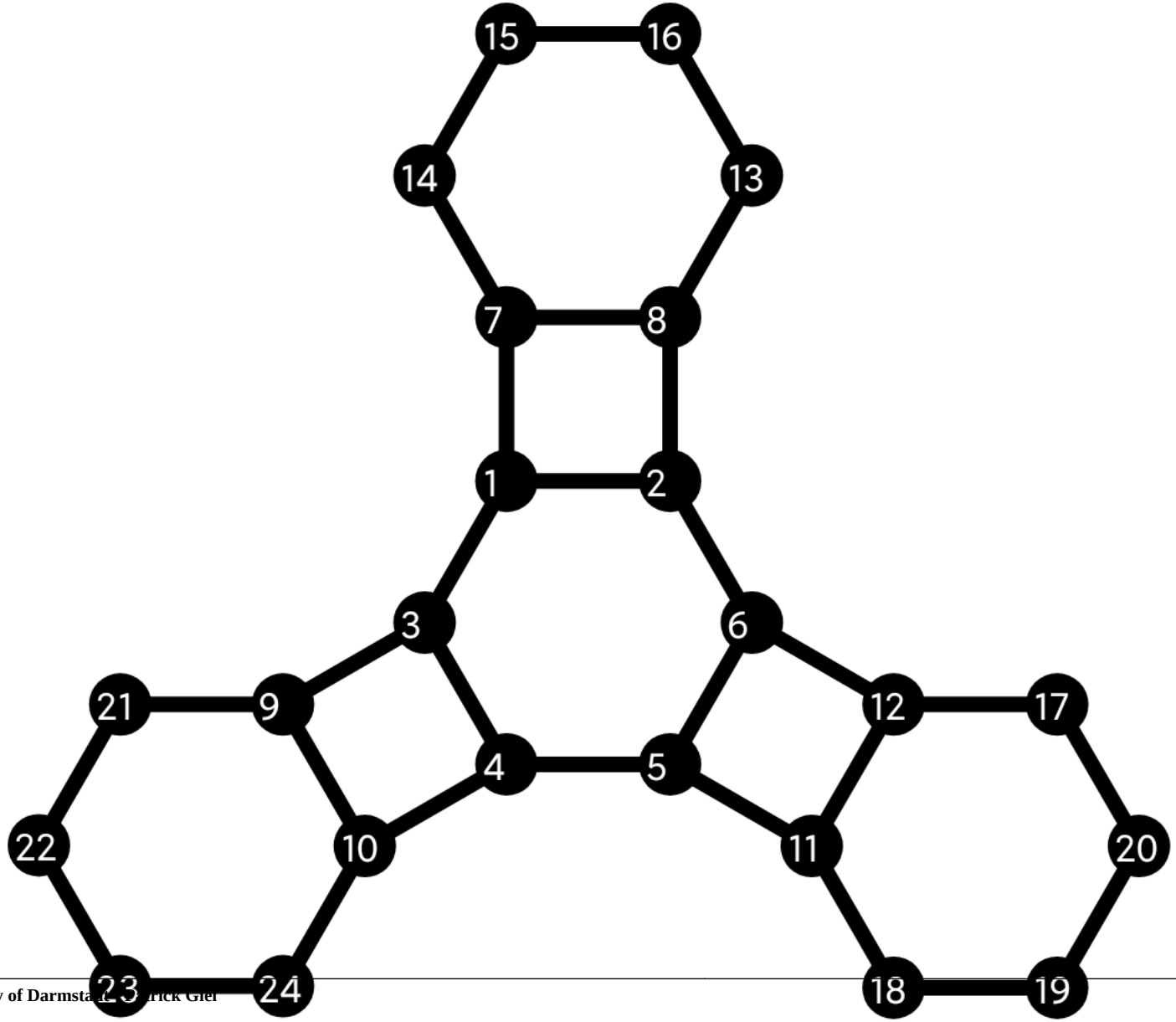
7. Bond-Atom-Polarizability

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	22	23	24
1 2	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	0.0	0.0	0.0	0.0	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	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 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2 6	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	0.0	0.0	0.0	0.0	0.0	0.0
2 8	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	0.0	0.0	0.0	0.0	0.0	0.0
3 4	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	0.0	0.0	0.0	0.0	0.0	0.0
3 9	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	0.0	0.0	0.0	0.0	0.0	0.0
4 5	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	0.0	0.0	0.0	0.0	0.0	0.0
4 10	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	0.0	0.0	0.0	0.0	0.0	0.0
5 6	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	0.0	0.0	0.0	0.0	0.0	0.0
5 11	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	0.0	0.0	0.0	0.0	0.0	0.0
6 12	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	0.0	0.0	0.0	0.0	0.0	0.0
7 8	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	0.0	0.0	0.0	0.0	0.0	0.0
7 14	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	0.0	0.0	0.0	0.0	0.0	0.0
8 13	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	0.0	0.0	0.0	0.0	0.0	0.0
9 10	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	0.0	0.0	0.0	0.0	0.0	0.0
9 21	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	0.0	0.0	0.0	0.0	0.0	0.0
10 24	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	0.0	0.0	0.0	0.0	0.0	0.0
11 12	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	0.0	0.0	0.0	0.0	0.0	0.0
11 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
12 17	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	0.0	0.0	0.0	0.0	0.0	0.0
13 16	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	0.0	0.0	0.0	0.0	0.0	0.0
14 15	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	0.0	0.0	0.0	0.0	0.0	0.0
15 16	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	0.0	0.0	0.0	0.0	0.0	0.0
17 20	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	0.0	0.0	0.0	0.0	0.0	0.0
18 19	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	0.0	0.0	0.0	0.0	0.0	0.0
19 20	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	0.0	0.0	0.0	0.0	0.0	0.0
21 22	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	0.0	0.0	0.0	0.0	0.0	0.0
22 23	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	0.0	0.0	0.0	0.0	0.0	0.0
23 24	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	0.0	0.0	0.0	0.0	0.0	0.0

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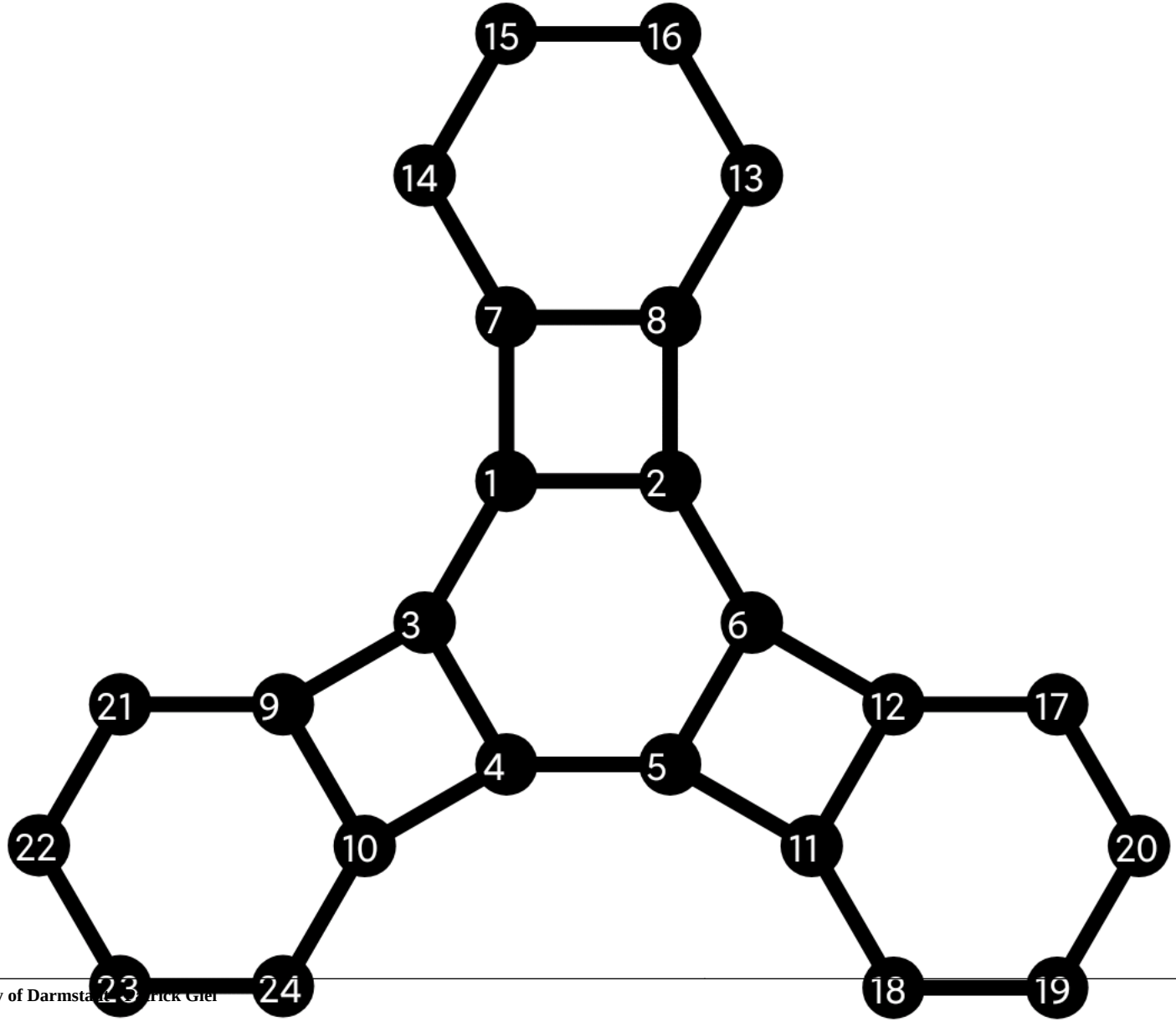
8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3	1 7	2 6	2 8	3 4	3 9	4 5	4 10	5 6	5 11	6 12	7 8	7 14	8 13	9 10	9 21	10 24	11 12	11 18	12 17	13 16	14 15	15 16	17 20	18 19	19 20	21 22	22 23	23 24
1 2	0.387																													
1 3	-0.143	0.183																												
1 7	-0.133	-0.074	0.394																											
2 6	-0.143	0.045	0.06	0.183																										
2 8	-0.133	0.06	-0.021	-0.074	0.394																									
3 4	0.113	-0.143	-0.028	-0.039	-0.057	0.387																								
3 9	-0.028	-0.074	0.038	0.011	0.016	-0.133	0.394																							
4 5	-0.039	0.045	0.011	0.045	0.011	-0.143	0.06	0.183																						
4 10	-0.057	0.06	0.016	0.011	0.032	-0.133	-0.021	-0.074	0.394																					
5 6	0.113	-0.039	-0.057	-0.143	-0.028	0.113	-0.057	-0.143	-0.028	0.387																				
5 11	-0.057	0.011	0.032	0.06	0.016	-0.028	0.016	-0.074	0.038	-0.133	0.394																			
6 12	-0.028	0.011	0.016	-0.074	0.038	-0.057	0.032	0.06	0.016	-0.133	-0.021	0.394																		
7 8	0.023	0.026	-0.121	0.026	-0.121	0.012	-0.016	-0.002	-0.008	0.012	-0.008	-0.016	0.294																	
7 14	0.037	0.015	-0.09	-0.036	0.036	0.016	-0.015	-0.007	-0.008	0.029	-0.016	-0.006	-0.145	0.253																
8 13	0.037	-0.036	0.036	0.015	-0.09	0.029	-0.006	-0.007	-0.016	0.016	-0.008	-0.015	-0.145	0.087	0.253															
9 10	0.012	0.026	-0.016	-0.002	-0.008	0.023	-0.121	0.026	-0.121	0.012	-0.016	-0.008	0.008	0.007	0.003	0.294														
9 21	0.016	0.015	-0.015	-0.007	-0.008	0.037	-0.09	-0.036	0.036	0.029	-0.006	-0.016	0.007	0.007	0.003	-0.145	0.253													
10 24	0.029	-0.036	-0.006	-0.007	-0.016	0.037	0.036	0.015	-0.09	0.016	-0.015	-0.008	0.003	0.003	0.008	-0.145	0.087	0.253												
11 12	0.012	-0.002	-0.008	0.026	-0.016	0.012	-0.008	0.026	-0.016	0.023	-0.121	-0.121	0.008	0.003	0.007	0.008	0.003	0.007	0.294											
11 18	0.029	-0.007	-0.016	-0.036	-0.006	0.016	-0.008	0.015	-0.015	0.037	-0.09	0.036	0.003	0.008	0.003	0.007	0.003	0.007	-0.145	0.253										
12 17	0.016	-0.007	-0.008	0.015	-0.015	0.029	-0.016	-0.036	-0.006	0.037	0.036	-0.09	0.007	0.003	0.007	0.003	0.008	0.003	-0.145	0.087	0.253									
13 16	-0.015	0.027	-0.03	0.008	0.008	-0.024	0.006	0.009	0.013	-0.019	0.01	0.01	0.116	-0.079	-0.213	-0.003	-0.003	-0.007	-0.004	-0.005	-0.005	0.284								

	1 2	**1 3**	**1 7**	**2 6**	**2 8**	**3 4**	**3 9**	**4 5**	**4 10**	**5 6**	**5 11**	**6 12**	**7 8**	**7 14**	**8 13**	**9 10**	**9 21**	**10 24**	**11 12**	**11 18**	**12 17**	**13 16**	**14 15**	**15 16**	**17 20**	**18 19**	**19 20**	**21 22**	**22 23**	**23 24**
14 15	-0.015	0.008	0.008	0.027	-0.03	-0.019	0.01	0.009	0.01	-0.024	0.013	0.006	0.116	-0.213	-0.079	-0.004	-0.005	-0.005	-0.003	-0.007	-0.003	0.123	0.284							
15 16	0.016	-0.008	-0.007	-0.008	-0.007	0.019	-0.009	-0.007	-0.01	0.019	-0.01	-0.009	-0.072	0.123	0.123	0.004	0.004	0.005	0.004	0.005	0.004	-0.216	-0.216	0.261						
17 20	-0.019	0.009	0.01	0.008	0.01	-0.024	0.013	0.027	0.006	-0.015	-0.03	0.008	-0.004	-0.005	-0.005	-0.003	-0.007	-0.003	0.116	-0.079	-0.213	0.004	0.004	-0.004	0.284					
18 19	-0.024	0.009	0.013	0.027	0.006	-0.019	0.01	0.008	0.01	-0.015	0.008	-0.03	-0.003	-0.007	-0.003	-0.004	-0.005	-0.005	0.116	-0.213	-0.079	0.004	0.006	-0.004	0.123	0.284				
19 20	0.019	-0.007	-0.01	-0.008	-0.009	0.019	-0.01	-0.008	-0.009	0.016	-0.007	-0.007	0.004	0.005	0.004	0.004	0.005	0.004	-0.072	0.123	0.123	-0.004	-0.004	0.004	-0.216	-0.216	0.261			
21 22	-0.019	0.008	0.01	0.009	0.01	-0.015	0.008	0.027	-0.03	-0.024	0.006	0.013	-0.004	-0.005	-0.005	0.116	-0.213	-0.079	-0.003	-0.003	-0.007	0.004	0.004	-0.004	0.006	0.004	-0.004	0.284		
22 23	0.019	-0.008	-0.009	-0.007	-0.01	0.016	-0.007	-0.008	-0.007	0.019	-0.009	-0.01	0.004	0.004	0.005	-0.072	0.123	0.123	0.004	0.004	0.005	-0.004	-0.004	0.004	-0.004	-0.004	0.004	-0.216	0.261	
23 24	-0.024	0.027	0.006	0.009	0.013	-0.015	-0.03	0.008	0.008	-0.019	0.01	0.01	-0.003	-0.003	-0.007	0.116	-0.079	-0.213	-0.004	-0.005	-0.005	0.006	0.004	-0.004	0.004	0.004	-0.004	0.123	-0.216	0.284

8.2. Presentation of molecule: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