

Report generated by:root, 20.01.2020 - 17:53:21

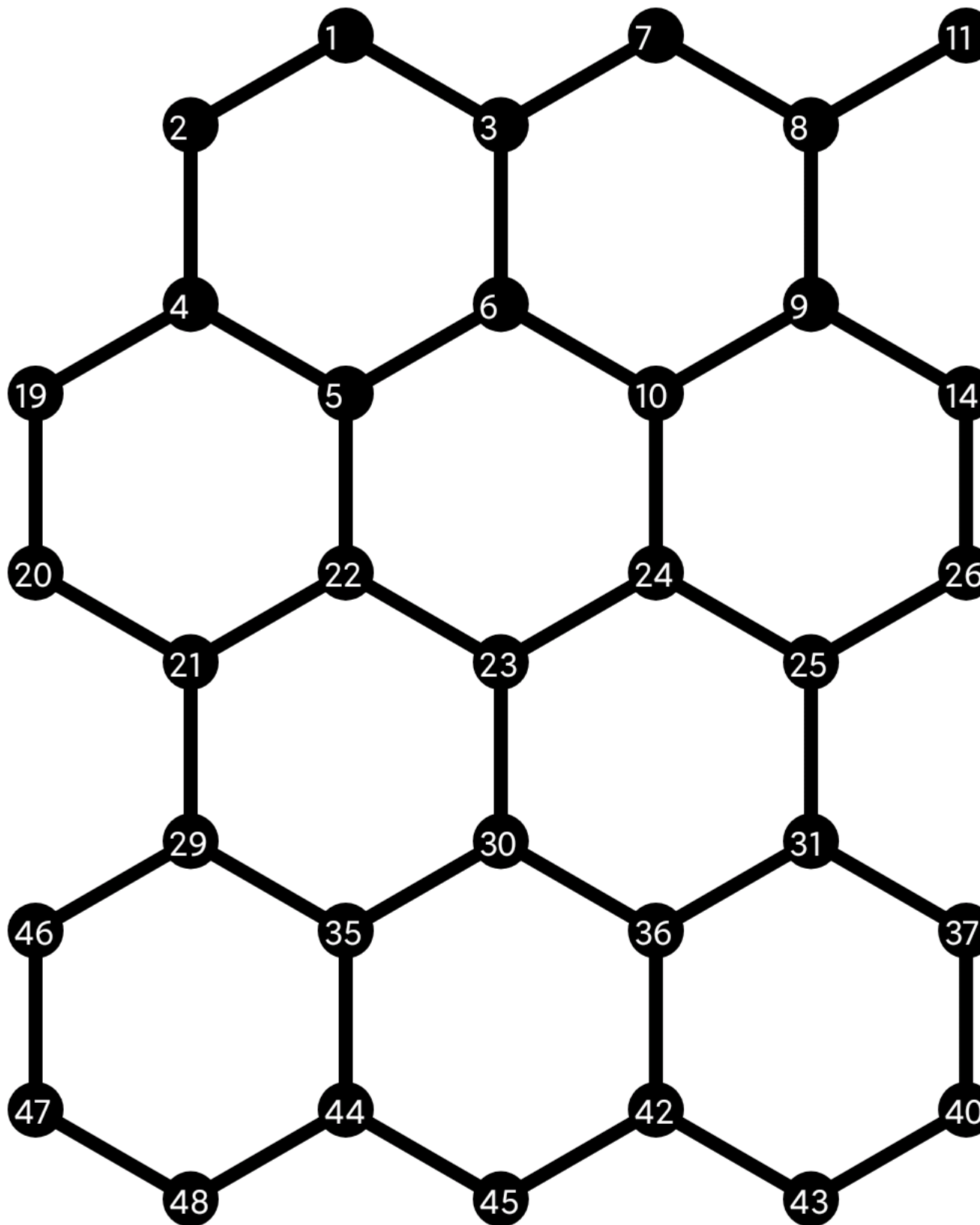
[illegible]

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It is about this molecule:

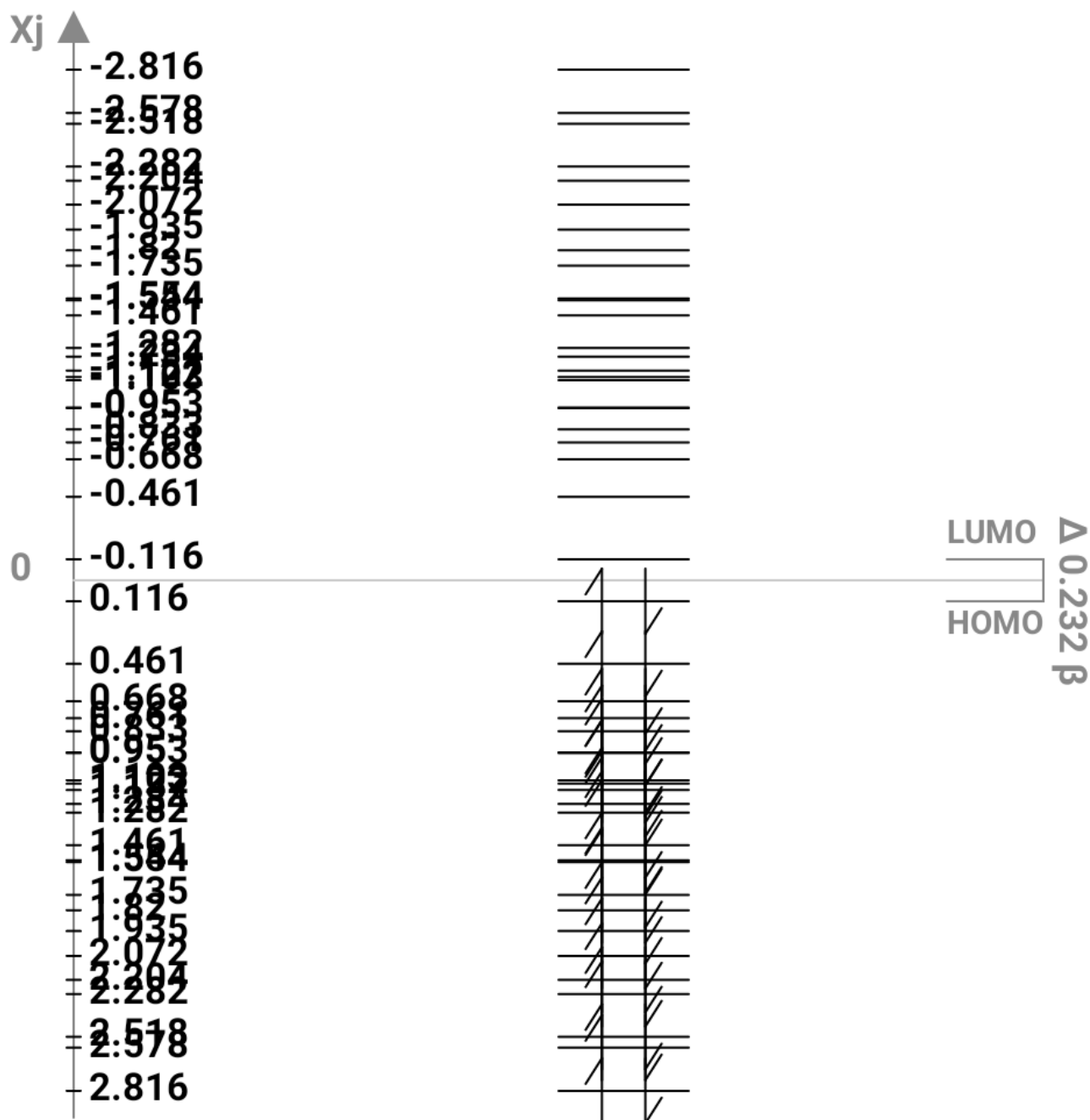
HMO-Energies

x1 = 2.816; x2 = 2.578; x3 = 2.518; x4 = 2.282; x5 = 2.204; x6 = 2.072; x7 = 1.935; x8 = 1.82;
x9 = 1.735; x10 = 1.554; x11 = 1.544; x12 = 1.461; x13 = 1.282; x14 = 1.234; x15 = 1.157; x16 = 1.122;
x17 = 1.103; x18 = 0.953; x19 = 0.95; x20 = 0.833; x21 = 0.761; x22 = 0.668; x23 = 0.461; x24 = 0.116;
x25 = -0.116; x26 = -0.461; x27 = -0.668; x28 = -0.761; x29 = -0.833; x30 = -0.95; x31 = -0.953; x32 = -1.103;
x33 = -1.122; x34 = -1.157; x35 = -1.234; x36 = -1.282; x37 = -1.461; x38 = -1.544; x39 = -1.554; x40 = -1.735;
x41 = -1.82; x42 = -1.935; x43 = -2.072; x44 = -2.204; x45 = -2.282; x46 = -2.518; x47 = -2.578; x48 = -2.816;



1. Energy-eigenvalues

1.1. Calculated values:



total Power $E\pi$: $48\alpha + 70.318\beta$ -

this corresponds to one π electron: 1.465β

2.1. Calculated values:

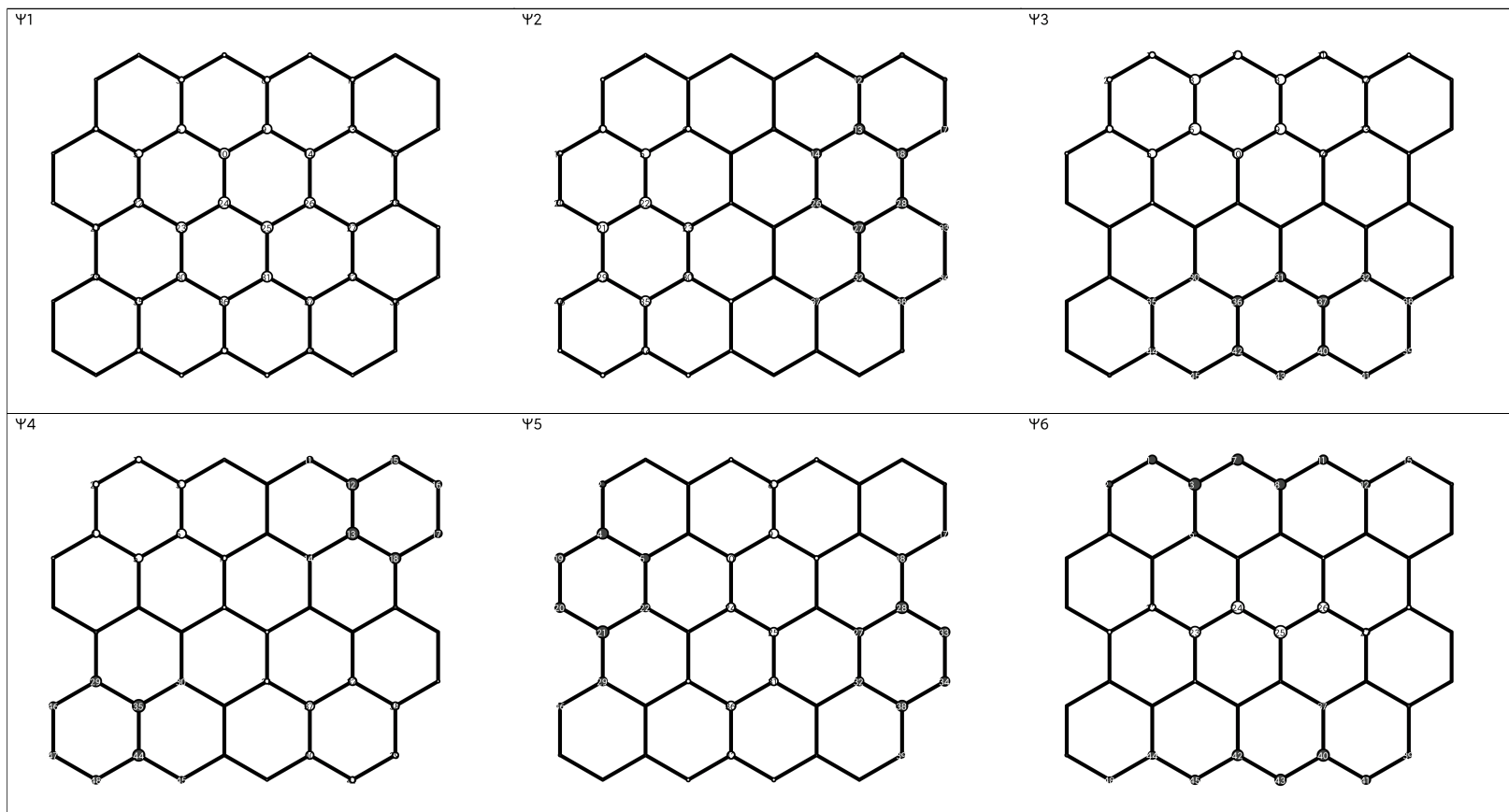
	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11	Psi 12	Psi 13	Psi 14	Psi 15	Psi 16	Psi 17	Psi 18	Psi 19	Psi 20	Psi 21	Psi 22	Psi 23	Psi 24	Psi 25	Psi 26	Psi 27	Psi 28	Psi 29	Psi 30	Psi 31	Psi 32	Psi 33	Psi 34	Psi 35	Psi 36	Psi 37	Psi 38	Psi 39	Psi 40	Psi 41	Psi 42	Psi 43	Psi 44	Psi 45	Psi 46	Psi 47	Psi 48
	x1 = 2.8 16	x2 = 2.5 78	x3 = 2.5 18	x4 = 2.2 82	x5 = 2.2 04	x6 = 2.0 72	x7 = 1.9 35	x8 = 1.8 2	x9 = 1.7 35	x1 0= 1.5 54	x1 1= 1.5 44	x1 2= 1.4 61	x1 3= 1.2 82	x1 4= 1.2 34	x1 5= 1.1 57	x1 6= 1.1 22	x1 7= 1.1 03	x1 8= 0.9 53	x1 9= 0.9 5	x2 0= 0.8 33	x2 1= 0.7 61	x2 2= 0.6 68	x2 3= 0.4 61	x2 4= 0.1 16	x2 5= - 0.1 16	x2 6= - 0.4 61	x2 7= - 0.6 68	x2 8= - 0.7 61	x2 9= - 0.8 33	x3 0= - 0.9 5	x3 1= - 0.9 53	x3 2= - 1.1 03	x3 3= - 1.1 22	x3 4= - 1.1 57	x3 5= - 1.2 34	x3 6= - 1.2 82	x3 7= - 1.4 61	x3 8= - 1.5 44	x3 9= - 1.5 54	x4 0= - 1.7 35	x4 1= - 1.8 2	x4 2= - 1.9 35	x4 3= - 2.0 72	x4 4= - 2.2 04	x4 5= - 2.2 82	x4 6= - 2.5 18	x4 7= - 2.5 78	x4 8= - 2.8 16
1	0.0 63	0.0 58	0.1 32	0.1 3	- 0.0 52	- 0.1 86	- 0.0 09	0.2 22	- 0.0 51	- 0.2 18	- 0.0 99	0.0 2	0.2 75	- 0.0 88	- 0.0 3	0.0 94	0.1 93	0.0 08	- 0.0 48	- 0.2 7	- 0.1 7	- 0.0 06	0.2 44	0.1 32	- 0.1 32	- 0.2 44	- 0.0 06	0.1 7	0.2 7	- 0.0 48	- 0.0 08	0.1 93	- 0.0 94	- 0.0 3	0.0 88	0.2 75	- 0.0 2	- 0.0 99	0.2 18	- 0.0 51	0.2 22	0.0 09	- 0.1 86	- 0.0 52	- 0.1 3	0.1 32	0.0 58	0.0 63
2	0.0 59	0.0 82	0.1 11	0.1 28	- 0.1 29	- 0.1 32	0.0 98	0.1 94	- 0.1 63	- 0.1 2	- 0.0 2	- 0.1 84	0.2 28	- 0.1 46	0.0 9	- 0.0 72	0.0 91	- 0.0 94	- 0.1 85	- 0.1 77	- 0.2 34	0.1 68	0.2 15	0.0 78	0.0 78	0.2 15	- 0.1 68	0.2 34	- 0.1 77	0.1 85	- 0.0 94	- 0.0 91	- 0.0 72	- 0.0 9	- 0.1 46	- 0.2 28	- 0.1 84	0.0 2	- 0.1 2	0.1 63	- 0.1 94	0.0 98	0.1 32	0.1 29	0.1 28	- 0.1 11	- 0.0 82	- 0.0 59
3	0.1 19	0.0 68	0.2 2	0.1 69	0.0 15	- 0.2 54	- 0.1 15	0.2 09	0.0 75	- 0.2 18	- 0.1 33	0.2 13	0.1 25	0.0 37	- 0.1 25	0.1 78	0.1 22	0.1 01	0.1 39	- 0.0 48	0.1 05	- 0.1 72	- 0.1 03	- 0.0 63	- 0.0 63	- 0.1 03	0.1 72	- 0.1 05	- 0.0 48	- 0.1 39	0.1 01	- 0.1 22	0.1 78	0.1 25	0.0 37	- 0.1 25	0.2 13	0.1 33	- 0.2 18	- 0.0 75	- 0.2 09	- 0.1 15	0.2 54	- 0.0 15	0.1 69	- 0.2 2	- 0.0 68	- 0.1 19
4	0.1 03	0.1 53	0.1 49	0.1 62	- 0.2 33	- 0.0 86	0.1 98	0.1 32	- 0.2 32	0.0 31	0.0 69	- 0.2 89	0.0 17	- 0.0 92	0.1 35	- 0.1 75	- 0.0 92	- 0.0 97	- 0.1 28	0.1 23	- 0.0 08	0.1 18	- 0.1 45	- 0.1 23	0.1 45	0.1 18	- 0.0 08	- 0.1 23	- 0.1 28	0.0 97	- 0.0 92	0.1 75	0.1 35	0.0 92	0.0 17	0.2 89	0.0 69	- 0.0 31	- 0.2 32	0.1 32	- 0.1 98	- 0.0 86	- 0.2 33	- 0.1 62	0.1 49	0.1 53	0.1 03	
5	0.1 69	0.2 9	0.1 75	- 0.1 84	- 0.0 21	0.1 38	0.0 61	0.0 12	0.1 54	- 0.0 3	- 0.0 81	- 0.0 97	0.2 76	0.1 32	0.0 84	- 0.1 86	- 0.0 81	0.0 45	0.3 25	- 0.0 62	0.0 85	- 0.0 74	0.0 23	0.0 23	- 0.0 74	- 0.0 85	0.0 62	0.3 25	- 0.0 45	- 0.0 81	0.1 86	0.0 84	- 0.1 32	0.2 76	0.0 97	- 0.0 81	0.0 3	0.1 54	- 0.0 12	- 0.0 61	0.1 38	0.0 21	0.1 84	0.1 75	- 0.1 9	- 0.2 1	- 0.1 69	
6	0.1 83	0.1 18	0.2 48	0.2 01	0.0 05	- 0.1 07	- 0.0 64	0.1 42	0.1 29	0.1 3	- 0.1 79	0.0 97	- 0.0 84	0.1 32	- 0.0 77	0.1 88	- 0.2 3	0.1 71	- 0.0 41	0.1 46	0.2 07	- 0.0 62	- 0.0 16	- 0.1 51	- 0.1 16	- 0.0 62	0.2 07	- 0.1 46	- 0.0 41	- 0.1 71	- 0.2 3	- 0.1 88	- 0.0 77	- 0.1 32	- 0.0 84	- 0.0 97	- 0.1 79	- 0.1 3	0.1 29	0.1 42	0.0 64	- 0.1 07	0.0 05	- 0.2 01	0.2 48	0.1 18	0.1 83	
7	0.0 9	0.0	0.1 75	0.0 54	0.0 81	- 0.2 34	- 0.1 49	0.0 17	0.0 52	- 0.2 51	0.0 73	0.1 94	- 0.0 31	0.0 02	- 0.0 38	- 0.0 84	0.1 71	- 0.0 82	0.2 21	0.0 84	0.0 43	- 0.0 48	- 0.2 76	- 0.2 9	0.2 76	- 0.0 48	0.0 43	- 0.0 84	0.2 21	0.0 82	0.1 71	0.0 84	- 0.0 38	- 0.0 02	- 0.0 31	- 0.1 94	0.0 73	0.2 51	0.0 52	0.0 17	0.1 49	- 0.2 34	0.0 81	- 0.0 54	0.1 75	0.0 9		
8	0.1 33	- 0.0 69	0.2 2	- 0.0 45	0.1 63	- 0.2 3	- 0.1 74	- 0.1 78	0.0 15	- 0.1 73	0.2 45	0.0 7	- 0.1 65	- 0.0 34	0.0 81	- 0.2 71	0.0 67	- 0.1 8	0.0 71	0.1 18	- 0.0 72	0.1 41	- 0.0 25	0.0 29	0.0 29	- 0.0 25	- 0.1 41	0.0 72	0.1 18	- 0.0 71	- 0.1 8	- 0.0 67	- 0.2 71	0.1 81	0.0 34	0.1 65	0.0 7	- 0.2 45	- 0.1 73	- 0.0 15	0.1 78	- 0.1 74	0.2 3	- 0.1 63	- 0.0 45	- 0.2 2	0.0 69	- 0.1 33
9	0.2 02	- 0.0 9	0.2 34	- 0.0 27	0.2	- 0.0 51	- 0.2 03	- 0.1 33	- 0.0 54	0.1 8	0.1 75	0.0 18	- 0.0 18	- 0.1 42	- 0.0 62	- 0.1 57	0.2 31	- 0.1 56	- 0.0 75	0.0 62	- 0.1 79	- 0.0 76	0.2 24	- 0.0 59	- 0.2 24	- 0.0 76	- 0.1 79	0.0 62	- 0.0 75	0.1 56	- 0.2 31	0.1 57	- 0.0 62	- 0.0 42	- 0.0 18	- 0.0 18	0.1 75	- 0.1 8	- 0.0 54	- 0.1 33	0.2 03	- 0.0 51	0.2 27	0.2 34	- 0.0 9	0.2 02		
10	0.2 26	0.0 36	0.2 15	0.1 14	0.1 79	0.0 55	- 0.1 47	- 0.0 13	0.1 36	0.2 66	- 0.1 14	0.0 1	- 0.1 35	- 0.1 51	- 0.0 95	- 0.0 5	- 0.1 89	0.1 42	- 0.2 23	- 0.1 55	0.1 14	0.0 46	0.1 69	0.0 58	0.1 69	- 0.0 46	0.2 18	0.0 81	- 0.0 77	- 0.0 79	0.1 42	0.1 89	- 0.0 5	0.0 95	- 0.1 35	0.1 1	0.2 66	- 0.1 36	0.0 13	- 0.1 47	- 0.0 55	- 0.1 79	0.1 14	- 0.2 15	- 0.0 36	- 0.2 26		
11	0.0 84	- 0.0 88	0.1 46	- 0.1 3	0.0 78	- 0.1 92	0.0 16	- 0.2 08	0.0 28	- 0.1 97	0.1 31	- 0.1 09	- 0.1 62	0.0 98	0.1 94	- 0.0 64	0.1 34	0.0 67	- 0.0 79	0.0 77	0.0 81	0.2 18	0.0 4	0.3 53	- 0.3 53	- 0.0 4	0.2 18	0.0 81	- 0.0 77	- 0.0 79	- 0.0 67	0.1 34	0.0 64	0.1 94	- 0.0 98	- 0.1 62	0.1 09	0.1 31	0.1 97	0.0 28	- 0.2 08	- 0.0 16	- 0.1 92	0.1 78	0.1 3	0.1 46	- 0.0 88	0.0 84
12	0.1 02	- 0.1 58	0.1 48	- 0.2 51	- 0.0 09	- 0.1 67	0.2 04	- 0.2	0.0 34	- 0.1 34	- 0.0 43	- 0.2 3	- 0.0 43	0.1 55	0.1 43	0.1 99	0.0 81	0.2 44	- 0.1 46	- 0.0 54	0.1 34	0.0 05	0.0 43	0.0 12	0.0 12	0.0 43	- 0.0 05	- 0.1 34	- 0.0 54	0.1 46	- 0.0 44	0.1 99	- 0.1 43	0.1 55	0.0 43	- 0.2 3	0.0 43	- 0.1 34	- 0.0 34	0.2 04	0.2 67	- 0.0 09	- 0.2 51	- 0.1 48	0.1 58	- 0.1 02		
13	0.1 54	- 0.2 26	0.1 48	- 0.2 67	- 0.0 34	- 0.0 41	0.1 6	- 0.0 39	- 0.0 65	0.1 07	0.0 18	- 0.0 41	0.2 57	0.0 45	0.1 51	0.1 84	- 0.1 3	0.1 98	0.1 88	- 0.1 85	0.0 34	0.0 2	- 0.1 44	0.1 05	0.1 44	0.0 2	0.0 34	0.0 85	0.1 88	- 0.1 98	- 0.1 3	- 0.1 84	0.1 51	- 0.0 45	0.2 57	0.0 41	0.0 18	- 0.1 07	- 0.0 65	- 0.0 39	- 0.1 6	- 0.0 41	- 0.0 34	0.2 67	0.1 48	- 0.2 26	0.1 54	

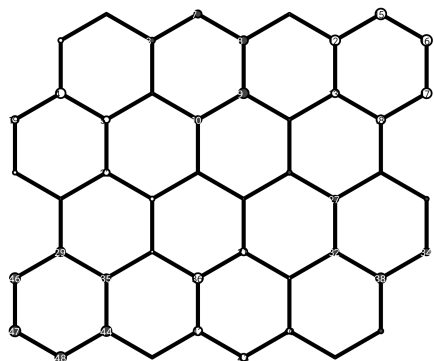
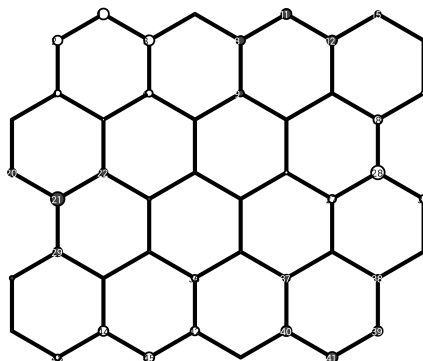
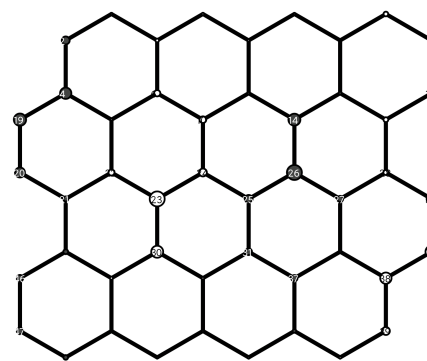
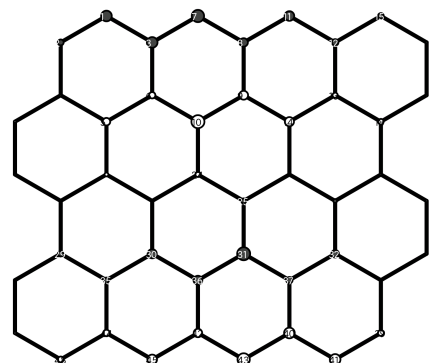
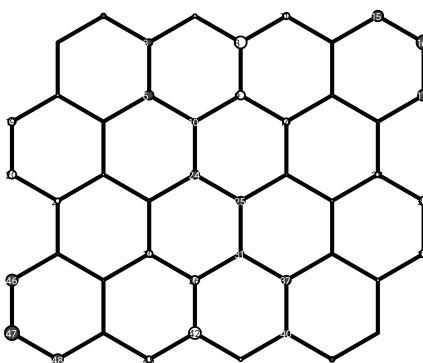
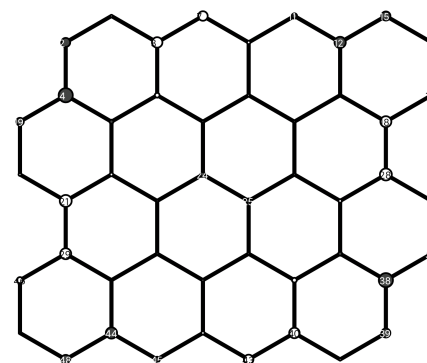
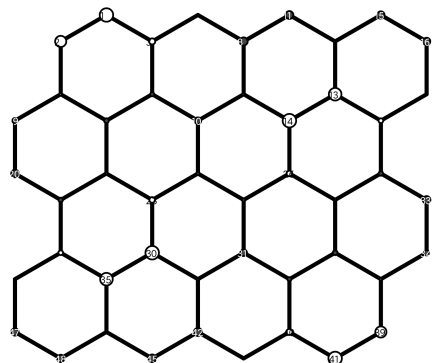
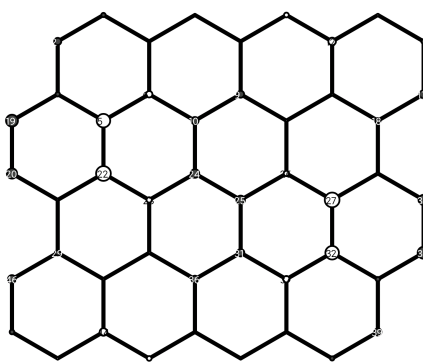
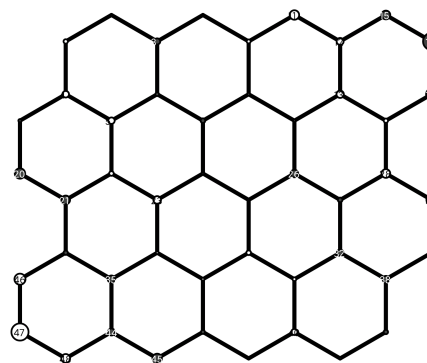
	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11	Psi 12	Psi 13	Psi 14	Psi 15	Psi 16	Psi 17	Psi 18	Psi 19	Psi 20	Psi 21	Psi 22	Psi 23	Psi 24	Psi 25	Psi 26	Psi 27	Psi 28	Psi 29	Psi 30	Psi 31	Psi 32	Psi 33	Psi 34	Psi 35	Psi 36	Psi 37	Psi 38	Psi 39	Psi 40	Psi 41	Psi 42	Psi 43	Psi 44	Psi 45	Psi 46	Psi 47	Psi 48	
14	0.209	-0.2	0.154	-0.131	0.098	0.069	-0.072	-0.051	-0.245	0.187	0.138	-0.055	0.277	0.01	-0.057	0.145	-0.133	-0.112	0.081	-0.015	-0.179	-0.238	0.041	0.093	0.093	-0.041	-0.041	0.238	0.179	-0.015	-0.081	0.112	0.133	0.145	0.057	0.01	-0.277	-0.055	-0.187	0.187	0.245	0.051	-0.072	-0.051	-0.098	-0.131	-0.154	0.209	-0.209
15	0.05	-0.093	0.079	-0.176	0.023	0.113	0.219	-0.118	0.096	0.118	0.215	-0.186	0.151	0.049	-0.18	0.104	0.085	-0.033	-0.0247	0.063	-0.014	-0.235	0.124	0.246	0.246	-0.124	0.235	-0.014	-0.063	0.124	0.14	0.163	0.0	0.33	0.85	-0.104	0.18	0.151	0.096	-0.118	-0.215	-0.113	-0.023	0.176	0.079	-0.05	0.05		
16	0.038	-0.082	0.05	-0.15	0.061	0.067	0.219	-0.015	0.132	-0.049	0.289	-0.041	0.105	-0.095	-0.351	-0.083	0.013	-0.275	0.07	-0.189	-0.144	-0.162	0.14	-0.041	-0.041	0.014	0.162	0.144	0.107	0.089	-0.275	-0.13	-0.083	0.351	-0.095	0.15	-0.041	-0.289	-0.049	-0.132	0.015	0.219	0.067	0.061	-0.05	-0.038			
17	0.058	-0.119	0.048	-0.166	-0.11	-0.027	0.205	0.091	0.133	0.041	-0.231	0.125	-0.042	0.166	-0.226	-0.197	-0.071	-0.229	0.163	0.026	-0.096	0.127	-0.118	0.241	0.118	0.241	-0.118	-0.096	0.127	-0.096	0.026	0.163	0.229	-0.071	0.226	-0.197	-0.225	0.091	0.133	0.041	-0.231	0.125	-0.042	0.166	-0.11	-0.027	0.205		
18	0.124	0.225	0.07	-0.228	0.183	0.12	0.178	0.181	0.099	0.114	-0.068	0.224	0.096	0.11	0.089	-0.138	-0.091	0.056	0.243	-0.085	0.071	0.246	-0.069	0.069	0.069	-0.069	0.246	-0.071	-0.085	0.085	0.043	0.091	-0.138	-0.089	0.11	-0.096	0.224	0.068	0.114	-0.099	0.181	0.12	0.178	0.07	0.225	0.124			
19	0.062	0.111	0.074	0.067	-0.2	0.047	-0.016	-0.251	0.014	0.155	-0.157	-0.109	-0.244	-0.067	-0.08	-0.207	0.082	0.19	-0.046	0.29	0.174	0.208	-0.115	-0.115	-0.208	0.174	-0.209	0.082	0.07	-0.08	0.0	0.07	-0.208	0.067	0.244	0.151	-0.057	-0.155	0.014	0.155	-0.109	-0.251	0.047	-0.016	-0.2	0.062			
20	0.07	0.134	0.037	-0.009	-0.208	0.033	0.087	-0.161	-0.204	-0.009	0.171	0.059	-0.157	0.209	-0.211	-0.059	0.085	0.175	-0.146	0.228	-0.161	0.235	0.049	0.109	-0.109	-0.235	0.049	-0.235	0.109	0.161	0.146	0.085	-0.204	-0.157	0.009	-0.208	0.033	0.087	-0.161	-0.204	-0.009	0.134	0.037	-0.009	0.07				
21	0.137	0.235	0.019	-0.088	-0.258	0.093	0.021	-0.277	-0.103	-0.028	0.09	0.244	-0.092	-0.015	-0.178	0.142	0.1	0.085	0.119	-0.088	-0.116	0.018	0.231	0.128	0.128	0.231	-0.018	-0.088	0.119	-0.16	-0.088	0.142	0.09	0.244	-0.092	-0.103	-0.277	0.093	0.021	-0.258	-0.088	-0.235	0.137	0.235	0.019				
22	0.191	0.246	0.081	0.037	-0.178	0.149	0.132	-0.161	0.124	0.079	0.065	0.073	-0.058	0.301	0.095	0.08	0.117	-0.15	0.211	0.002	-0.246	0.0	0.126	-0.026	0.126	-0.026	0.0	-0.246	0.126	-0.026	0.11	0.17	-0.08	0.095	-0.301	0.037	0.081	0.032	-0.178	0.149	0.132	-0.161	0.246	0.081					
23	0.231	0.198	-0.005	-0.004	0.05	0.236	0.097	-0.078	0.306	-0.003	0.021	-0.056	0.115	0.11	0.156	-0.136	0.215	-0.148	0.36	-0.235	-0.009	0.102	-0.099	0.153	-0.153	0.099	0.102	-0.099	-0.235	-0.009	-0.148	-0.156	0.11	-0.115	-0.003	-0.078	0.306	0.097	-0.078	0.236	0.05	-0.004	-0.005	0.231					
24	0.252	0.066	0.06	0.086	0.191	0.271	-0.017	-0.032	0.162	0.103	-0.171	-0.1	-0.071	-0.176	0.028	-0.087	0.253	0.21	-0.096	0.213	0.06	0.169	-0.131	0.086	0.086	0.131	0.169	-0.086	-0.131	0.06	0.213	0.253	0.086	0.096	0.176	-0.032	0.162	0.103	-0.171	-0.017	0.066	0.252							
25	0.252	-0.066	-0.06	0.086	0.191	0.271	0.017	0.032	-0.162	0.103	-0.171	0.1	-0.071	0.176	-0.028	0.087	0.253	0.21	0.096	0.213	-0.06	0.169	-0.131	0.086	0.086	-0.131	-0.169	0.06	-0.213	-0.096	-0.253	0.086	0.096	-0.176	0.032	-0.162	0.103	-0.171	-0.017	0.066	0.252								
26	0.231	-0.198	-0.005	-0.004	0.05	0.236	-0.097	0.078	-0.306	0.003	0.021	0.056	-0.115	0.11	-0.156	0.136	-0.215	-0.148	0.36	0.235	0.009	-0.102	-0.099	-0.153	-0.153	0.099	-0.102	-0.099	0.235	-0.009	-0.148	-0.156	0.11	-0.115	0.003	0.078	-0.306	0.021	0.056	-0.115	-0.136	-0.215	0.231						
27	0.191	-0.246	-0.081	0.037	-0.178	0.149	-0.132	0.161	-0.124	-0.079	0.065	0.073	-0.058	0.301	-0.095	-0.08	0.117	-0.15	0.211	0.002	0.246	0.0	0.126	0.026	0.126	0.026	0.0	-0.246	0.126	-0.026	0.11	-0.17	-0.08	0.095	-0.301	0.037	0.081	0.032	-0.178	0.149	0.132	-0.161	0.246	0.081					
28	0.137	-0.235	-0.019	-0.088	-0.258	0.093	-0.021	0.277	0.103	0.028	0.09	0.244	-0.092	-0.015	-0.178	-0.142	0.1	0.085	-0.119	0.088	0.116	0.018	0.231	-0.128	0.128	-0.231	-0.018	-0.088	0.119	-0.16	-0.088	0.142	0.09	0.244	-0.092	-0.103	-0.277	0.093	0.021	-0.258	-0.088	-0.235	0.137	0.235	0.019				
29	0.124	0.225	-0.07	-0.228	0.183	0.12	-0.178	-0.181	-0.099	-0.114	-0.068	0.224	0.096	-0.11	-0.089	0.138	-0.091	0.056	-0.243	-0.085	-0.071	0.246	-0.069	-0.069	0.069	0.069	-0.246	-0.071	-0.085	-0.043	-0.056	-0.091	0.138	0.089	-0.224	-0.068	0.114	-0.099	-0.114	-0.068	0.224	0.096	-0.11	-0.089	0.138				
30	0.209	0.2	-0.154	-0.131	0.098	0.069	0.072	0.051	0.245	-0.187	0.138	-0.055	0.277	0.01	0.057	-0.145	-0.133	-0.112	0.081	-0.015	-0.179	-0.238	0.041	0.093	0.093	-0.041	-0.041	0.238	0.179	-0.015	-0.081	0.112	0.133	0.145	0.057	-0.01	0.277	-0.055	-0.187	0.187	0.245	0.051	-0.072	-0.051	-0.098	-0.131	-0.154	0.209	

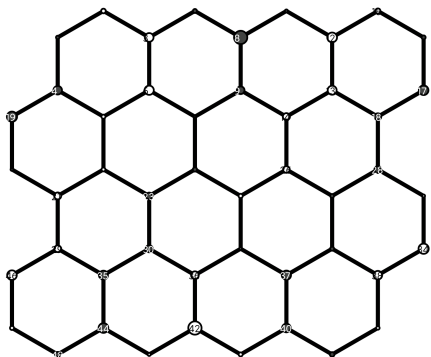
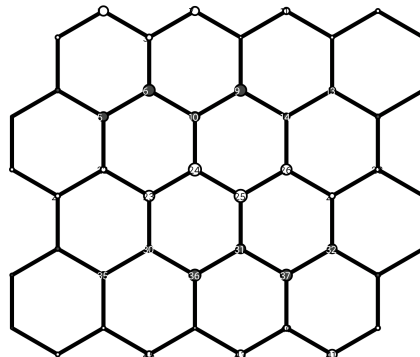
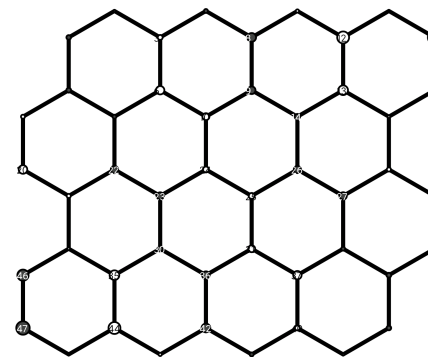
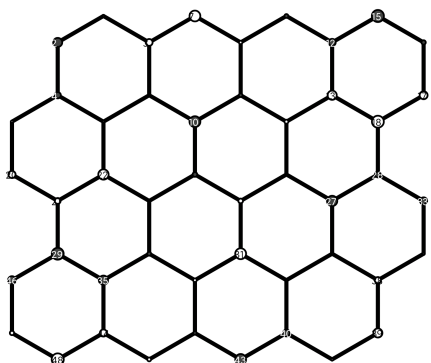
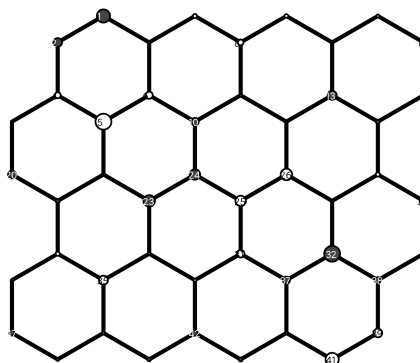
	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11	Psi 12	Psi 13	Psi 14	Psi 15	Psi 16	Psi 17	Psi 18	Psi 19	Psi 20	Psi 21	Psi 22	Psi 23	Psi 24	Psi 25	Psi 26	Psi 27	Psi 28	Psi 29	Psi 30	Psi 31	Psi 32	Psi 33	Psi 34	Psi 35	Psi 36	Psi 37	Psi 38	Psi 39	Psi 40	Psi 41	Psi 42	Psi 43	Psi 44	Psi 45	Psi 46	Psi 47	Psi 48
31	0.226	-0.036	-0.215	0.114	0.179	0.055	0.147	0.013	-0.136	-0.266	-0.114	0.011	-0.135	-0.151	0.095	0.05	-0.189	0.142	0.223	0.155	-0.114	0.046	0.169	-0.058	-0.169	0.046	0.046	-0.114	-0.155	0.223	-0.142	-0.189	-0.05	0.095	0.151	-0.135	-0.011	-0.114	0.266	-0.136	0.013	-0.147	0.055	0.179	-0.114	-0.215	-0.036	0.226
32	0.169	-0.29	-0.119	0.175	-0.184	-0.021	-0.138	0.061	-0.012	-0.154	-0.003	-0.081	-0.097	-0.276	0.132	-0.084	-0.186	-0.081	-0.045	-0.325	0.062	0.085	-0.074	0.085	0.062	0.025	0.045	0.081	-0.186	0.084	-0.132	-0.276	-0.097	0.081	-0.003	0.154	-0.012	0.054	-0.012	0.061	0.138	-0.021	-0.184	-0.119	-0.29	0.169		
33	0.07	-0.134	-0.037	-0.009	0.208	0.033	-0.087	0.161	0.204	0.009	0.171	0.059	-0.157	-0.209	0.211	0.059	0.085	0.175	-0.146	0.161	-0.228	-0.235	0.049	-0.109	0.049	0.235	0.228	0.261	0.146	0.175	0.175	-0.085	0.059	-0.211	-0.209	0.157	0.059	-0.171	0.009	-0.204	-0.161	0.208	-0.087	0.033	0.204	0.009	0.171	-0.07
34	0.062	-0.111	-0.074	0.067	-0.226	-0.047	0.116	0.251	-0.014	0.155	-0.157	-0.109	-0.244	0.067	0.208	-0.007	0.82	-0.082	-0.019	0.046	-0.29	-0.174	-0.208	0.115	-0.115	0.208	-0.174	-0.209	-0.046	-0.019	-0.082	-0.019	0.082	0.198	0.198	-0.207	0.244	-0.109	0.155	0.067	-0.226	-0.047	0.116	-0.251	-0.014	0.155	0.062	
35	0.154	0.226	-0.148	-0.267	-0.034	-0.041	-0.16	0.039	0.065	-0.107	0.18	0.041	-0.257	0.045	-0.151	-0.184	-0.103	0.198	-0.188	0.185	-0.034	0.02	-0.144	0.105	-0.144	-0.042	-0.034	0.085	0.188	0.198	0.13	-0.184	0.151	0.045	-0.257	-0.041	-0.018	-0.065	-0.039	-0.16	0.041	-0.257	-0.041	0.154				
36	0.202	0.09	-0.234	-0.027	0.251	-0.003	0.233	0.154	-0.18	-0.18	0.175	0.18	-0.142	0.062	0.157	-0.231	-0.156	0.075	0.062	0.179	-0.076	0.224	0.059	0.059	0.224	0.076	-0.179	0.062	-0.075	-0.156	0.231	0.157	-0.062	0.18	0.018	0.018	0.018	-0.175	-0.154	0.133	0.203	0.051	-0.234	0.027	0.251	-0.003	0.202	
37	0.183	-0.118	-0.248	0.201	0.005	-0.107	0.064	-0.142	-0.129	-0.103	-0.179	0.097	-0.084	0.132	0.077	-0.188	-0.203	0.171	0.041	-0.146	-0.207	-0.062	-0.016	-0.151	-0.151	-0.016	0.062	0.207	-0.146	-0.041	0.171	0.23	-0.188	-0.077	0.132	0.084	0.097	0.179	-0.103	0.129	0.142	0.064	0.107	-0.107	0.005	0.183		
38	0.103	-0.153	-0.149	0.162	-0.233	-0.086	-0.198	-0.132	0.232	-0.031	0.069	-0.289	-0.092	-0.135	0.175	-0.092	-0.097	-0.028	0.123	0.018	-0.118	0.118	-0.145	0.123	0.123	-0.145	-0.118	-0.023	-0.128	-0.097	0.092	0.175	0.135	-0.092	0.017	-0.289	-0.031	-0.232	0.132	-0.198	0.086	0.233	0.149	0.153	-0.103			
39	0.059	-0.082	-0.111	0.128	-0.129	-0.132	-0.098	-0.194	0.163	0.12	-0.02	-0.184	0.228	-0.146	-0.009	0.072	0.091	-0.085	0.177	0.134	0.268	0.115	0.215	0.268	0.115	0.215	0.268	-0.177	0.185	0.094	0.091	-0.072	-0.009	0.146	0.228	0.184	-0.012	0.163	-0.194	0.098	-0.132	-0.129	-0.132	0.128	0.059			
40	0.119	-0.068	-0.22	0.169	0.015	-0.254	0.115	-0.209	-0.075	0.218	-0.133	0.113	0.037	0.125	0.125	-0.178	0.122	0.101	-0.139	0.048	-0.105	0.172	-0.103	0.063	-0.063	0.103	-0.172	-0.105	-0.048	-0.139	-0.101	0.122	0.178	0.125	-0.037	0.125	-0.209	-0.254	0.115	-0.209	0.169	-0.22	0.119					
41	0.063	-0.058	-0.132	0.13	-0.052	-0.186	0.009	-0.222	0.051	0.218	-0.099	0.02	0.275	-0.088	0.003	-0.094	0.193	0.008	0.048	0.27	0.17	-0.006	0.244	-0.132	0.244	0.006	-0.17	0.27	-0.048	0.008	-0.093	-0.094	-0.003	-0.088	-0.275	0.009	0.099	0.222	0.051	0.218	0.009	0.186	0.052	0.13	0.063			
42	0.133	0.069	-0.22	-0.045	0.163	-0.23	0.174	0.178	-0.015	0.173	0.245	0.007	-0.165	-0.034	-0.081	0.271	0.067	-0.18	-0.071	0.018	0.141	-0.025	-0.029	0.029	0.025	0.141	0.072	0.118	-0.071	0.18	0.067	-0.281	-0.034	-0.165	-0.007	0.273	-0.015	0.173	-0.23	0.174	0.178	-0.015	0.173	0.245	0.007	0.133		
43	0.09	0.075	-0.154	0.081	-0.234	0.149	-0.017	-0.052	0.251	0.073	0.194	-0.031	0.002	0.038	0.084	0.171	-0.082	-0.221	-0.084	-0.043	-0.048	-0.276	-0.29	-0.276	0.048	0.043	-0.084	0.221	-0.082	-0.171	-0.082	-0.171	0.038	0.031	0.194	-0.052	0.251	0.073	0.149	-0.017	0.081	-0.234	0.149	0.09				
44	0.102	0.158	-0.148	-0.251	0.009	-0.167	0.204	0.2	-0.034	0.134	-0.043	0.23	-0.043	0.155	-0.143	-0.199	0.081	0.244	0.146	0.054	-0.134	0.005	0.043	-0.012	0.012	-0.043	0.005	-0.134	-0.054	0.146	-0.244	0.081	0.199	-0.155	-0.043	0.23	-0.043	-0.167	0.204	0.2	-0.034	0.134	-0.043	0.251	0.102			
45	0.084	0.088	-0.146	-0.13	0.078	-0.192	-0.016	0.208	-0.028	0.197	0.131	-0.109	-0.162	0.098	-0.194	0.064	0.134	0.067	0.079	-0.077	-0.081	0.218	0.04	-0.353	0.353	-0.218	0.081	-0.077	-0.079	0.067	-0.134	0.094	0.198	0.162	-0.109	-0.131	0.197	0.028	-0.208	0.192	-0.016	0.078	-0.13	0.146	-0.088	0.084		
46	0.058	0.119	-0.048	-0.166	-0.11	-0.027	0.205	-0.091	-0.133	-0.041	0.231	-0.242	0.166	0.226	0.197	-0.071	-0.229	-0.163	-0.026	0.196	0.127	-0.118	-0.241	-0.241	-0.118	-0.127	-0.096	0.163	-0.229	0.171	0.197	-0.226	-0.166	0.042	0.225	-0.131	-0.041	0.133	-0.242	0.166	0.226	0.197	-0.071	0.231	-0.242	0.119	0.058	
47	0.038	0.082	-0.05	-0.15	-0.061	-0.067	0.219	0.015	-0.132	-0.049	-0.289	-0.041	-0.15	-0.095	0.351	0.083	0.013	-0.275	0.089	-0.107	0.144	-0.162	0.014	0.041	-0.041	-0.014	-0.162	0.144	0.107	0.089	0.275	0.13	-0.083	0.351	0.095	-0.15	0.041	-0.289	-0.061	-0.067	0.219	0.015	-0.132	-0.049	0.038			

	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	Psi 25	Psi 26	Psi 27	Psi 28	Psi 29	Psi 30	Psi 31	Psi 32	Psi 33	Psi 34	Psi 35	Psi 36	Psi 37	Psi 38	Psi 39	Psi 40	Psi 41	Psi 42	Psi 43	Psi 44	Psi 45	Psi 46	Psi 47	Psi 48	
48	0.05	0.093	-0.079	-0.176	-0.023	-0.113	-0.219	0.118	-0.096	0.118	-0.215	-0.186	-0.151	0.049	0.18	-0.014	0.085	-0.033	0.247	-0.063	0.014	-0.235	0.124	0.246	0.246	0.124	0.235	-0.014	-0.063	-0.047	-0.033	-0.085	-0.104	-0.18	0.049	0.151	-0.186	0.215	0.113	0.096	-0.118	-0.219	0.118	0.023	-0.176	0.079	0.0	-0.093	-0.05

2.2. Molecule orbital presentation:



Ψ_7  Ψ_8  Ψ_9  Ψ_{10}  Ψ_{11}  Ψ_{12}  Ψ_{13}  Ψ_{14}  Ψ_{15} 

Ψ_{16}  Ψ_{17}  Ψ_{18}  Ψ_{19}  Ψ_{20} 

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

3. Bond Order

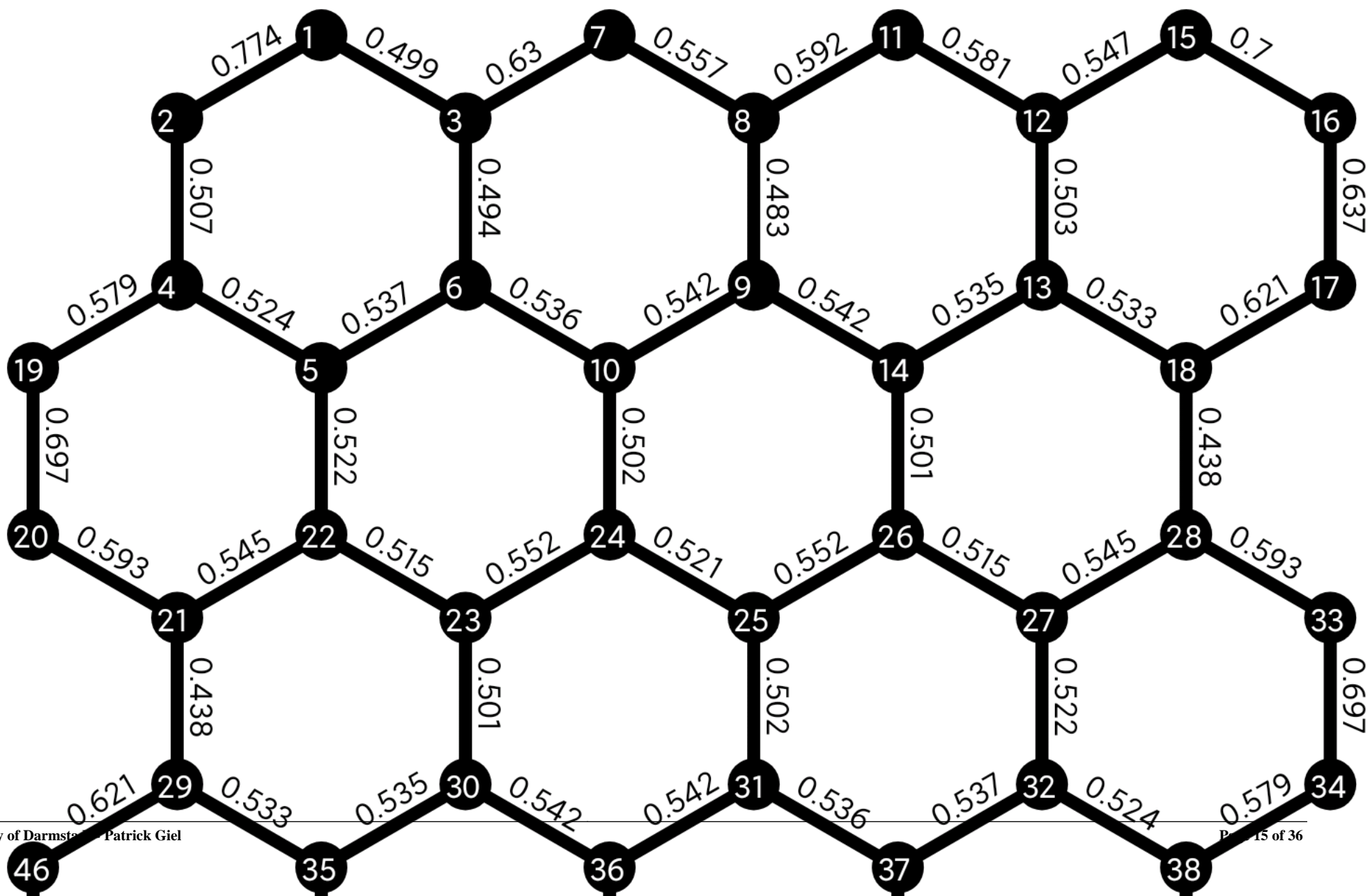
3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48					
1	1.0																																																				
2	0.7 74	1.0																																																			
3	0.4 99	0.0	1.0																																																		
4	0.0	0.5 07	- 0.1 62	1.0																																																	
5	- 0.2 31	0.0	0.0	0.5 24	1.0																																																
6	0.0	- 0.2 13	0.4 94	0.0	0.5 37	1.0																																															
7	0.0	- 0.2 24	0.6 3	0.0	- 0.0 34	0.0	1.0																																														
8	- 0.0 93	0.0	0.0	0.0 66	0.0	- 0.1 66	0.5 57	1.0																																													
9	0.0	0.1 13	- 0.1 81	0.0	- 0.0 71	0.0	0.0	0.4 83	1.0																																												
10	0.0 12	0.0	0.0	- 0.0 77	0.0	0.5 36	- 0.2 68	0.0	0.5 42	1.0																																											
11	0.0	0.0 84	- 0.1 51	0.0	0.0 56	0.0	0.0	0.5 92	0.0	0.0	1.0																																										
12	0.0 26	0.0	0.0	- 0.0 25	0.0	0.0 7	- 0.1 16	0.0	- 0.1 7	0.0	0.5 81	1.0																																									
13	0.0	- 0.0 56	0.0 86	0.0	- 0.0 11	0.0	0.0	- 0.1 75	0.0	- 0.0 75	0.0	0.5 03	1.0																																								
14	0.0 13	0.0	0.0	0.0 06	0.0	- 0.0 8	0.0 13	0.0	0.5 42	0.0	- 0.2 79	0.0	0.5 35	1.0																																							
15	0.0	- 0.0 27	0.0 46	0.0	- 0.0 33	0.0	0.0	- 0.1 22	0.0	0.0 24	0.0	0.5 47	0.0	0.0 22	1.0																																						
16	- 0.0 07	0.0	0.0	0.0 09	0.0	- 0.0 34	0.0 41	0.0	0.0 94	0.0	- 0.1 56	0.0	- 0.2 28	0.0	0.7	1.0																																					

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48								
17	0.0 28	0.0 - 0.0 46		0.0 31	0.0	0.0	0.1 01	0.0 - 0.0 09	0.0	0.0 - 0.2 31	0.0	0.0 - 0.0 85	0.0	0.0 0.6 37	1.0																																									
18	- 0.0 1	0.0	0.0	0.0 06	0.0	0.0 1	0.0 14	0.0 - 0.0 88	0.0	0.0 25	0.0	0.5 33	0.0 - 0.2 95	0.0 0.0 21	1.0																																									
19	- 0.1 98	0.0	0.0	0.5 79	0.0 - 0.0 4	0.1 62	0.0	- 0.0 47	0.0	- 0.0 99	0.0	0.0 54	0.0 0.0 43	0.0 - 0.0 45	0.0	1.0																																								
20	0.0	- 0.1 27	0.0 86	0.0 - 0.2 33	0.0	0.0	- 0.0 49	0.0	0.0 78	0.0	0.0 24	0.0	- 0.0 17	0.0 - 0.0 11	0.0 0.0 01	0.6 97	1.0																																							
21	0.1 58	0.0	0.0	- 0.2 41	0.0 - 0.0 28	- 0.1 25	0.0	0.0 58	0.0	0.0 73	0.0	- 0.0 48	0.0 - 0.0 3	0.0 0.0 34	0.0	0.0 0.5 93	1.0																																							
22	0.0	- 0.0 01	- 0.0 59	0.0	0.5 22	0.0	0.0	0.0 5	- 0.1 71	0.0	- 0.0 33	0.0	0.0 64	0.0	0.0 23	0.0 - 0.0 19	- 0.2 48	0.0	0.5 45	1.0																																				
23	0.0 13	0.0	0.0	- 0.0 1	0.0 - 0.2 18	0.1 5	0.0	- 0.0 45	0.0	- 0.1 12	0.0	0.0 7	0.0	0.0 53	0.0 - 0.0 61	0.0	0.0 - 0.0 63	0.0	0.5 15	1.0																																				
24	0.0	0.0 35	- 0.0 33	0.0 - 0.1 79	0.0	0.0	- 0.0 43	0.0	0.5 02	0.0	0.0 49	0.0	- 0.1 72	0.0 - 0.0 45	0.0	0.0 0.0 64	0.0 0.0 87	0.0	- 0.0 89	0.0	0.5 52	1.0																																		
25	- 0.0 22	0.0	0.0	0.0 31	0.0 - 0.0 28	0.0 42	0.0	- 0.2 1	0.0	0.1 18	0.0	- 0.0 55	0.0	- 0.0 73	0.0	0.0 0.0 89	0.0	- 0.0 18	0.0 - 0.0 59	0.0	0.5 21	1.0																																		
26	0.0	- 0.0 37	0.0 41	0.0 0.0 72	0.0	0.0	- 0.0 31	0.0 - 0.1 77	0.0	- 0.0 55	0.0	0.0 01	0.0	0.0 0.0 71	0.0	- 0.1 52	- 0.0 18	0.0 0.0 07	0.0 - 0.0 85	0.0	0.5 52	1.0																																		
27	0.0 13	0.0	0.0	- 0.0 21	0.0 0.0 44	- 0.0 45	0.0	- 0.0 4	0.0	0.0 75	0.0	- 0.1 87	0.0	0.0 0.0 68	0.0 - 0.0 85	0.0	0.0 0.0 24	0.0 - 0.0 11	0.0 																																					

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48			
34	0.0	-0.018	0.017	0.024	0.0	0.0	-0.011	0.0	-0.055	0.0	0.0	-0.009	0.088	0.039	0.0	-0.097	-0.002	0.0	-0.004	0.0	0.0	-0.018	0.0	0.087	0.0	-0.248	0.0	0.0	0.0	0.0	0.0	0.697	1.0																		
35	-0.041	0.0	0.054	0.0	0.083	-0.032	0.0	-0.039	0.0	0.067	0.0	-0.016	0.0	0.052	0.0	0.056	0.0	0.0	-0.072	0.0	-0.187	0.0	-0.055	0.0	0.07	0.0	-0.048	0.533	0.535	-0.075	-0.011	0.0	0.054	1.0																	
36	0.033	0.0	-0.044	0.0	0.075	-0.095	0.0	0.077	0.0	0.027	0.0	-0.039	0.0	0.008	0.0	-0.001	0.0	0.0	0.066	0.0	-0.004	0.0	-0.21	0.0	-0.045	0.0	0.058	-0.088	0.542	0.542	-0.071	0.0	-0.047	0.0	1.0																
37	-0.016	0.0	0.021	0.0	-0.052	0.061	0.0	0.075	0.0	-0.124	0.0	0.083	0.0	0.051	0.0	-0.056	0.0	0.0	-0.034	0.0	0.044	0.0	-0.028	0.0	-0.218	0.0	-0.028	0.01	-0.008	0.536	0.537	0.0	-0.004	0.0	0.0	1.0															
38	0.005	0.0	-0.006	0.0	0.021	-0.024	0.0	-0.044	0.0	0.063	0.0	0.054	0.0	-0.107	0.0	0.121	0.0	0.0	0.011	0.0	-0.021	0.0	0.031	0.0	-0.001	0.0	-0.241	0.006	0.006	-0.077	0.524	0.0	0.579	0.0	0.0	0.0	1.0														
39	0.0	0.011	-0.012	0.0	0.005	0.0	0.01	0.0	0.011	0.0	0.0	0.0	-0.032	0.0	-0.018	0.0	0.045	-0.018	0.0	0.023	0.0	-0.037	0.0	0.035	0.0	-0.001	0.0	0.0	0.0	0.0	0.0	-0.127	0.0	-0.056	0.113	-0.213	0.507	1.0													
40	0.0	-0.012	0.012	0.0	-0.003	0.0	-0.008	0.0	-0.016	0.0	-0.005	0.0	0.037	0.0	0.012	0.0	-0.022	0.017	0.0	-0.026	0.0	0.041	0.0	-0.033	0.0	-0.059	0.0	0.0	0.0	0.0	0.0	0.086	0.0	0.086	-0.181	0.494	-0.162	0.0	1.0												
41	-0.006	0.0	0.005	0.0	-0.016	0.022	0.0	0.033	0.0	-0.053	0.0	-0.041	0.089	0.0	-0.095	0.0	0.0	-0.006	0.0	0.013	0.0	-0.022	0.0	0.013	0.0	0.158	-0.001	0.013	0.012	-0.231	0.0	-0.198	0.0	0.0	0.0	0.774	0.499	1.0													
42	0.0	0.01	-0.008	0.0	-0.005	0.0	-0.001	0.0	0.024	0.0	0.004	0.0	-0.014	0.0	-0.005	0.0	0.005	-0.011	0.0	0.026	0.0	-0.031	0.0	-0.043	0.0	0.005	0.0	0.0	0.0	0.0	0.0	-0.049	0.0	-0.175	0.483	-0.166	0.066	0.0	0.0	-0.093	1.0										
43	0.022	0.0	-0.024	0.0	0.061	-0.079	0.0	-0.095	0.0	0.164	0.0	-0.032	0.0	-0.133	0.0	0.14	0.0	0.031	0.0	-0.045	0.0	0.042	0.0	0.15	0.0	-0.125	0.014	0.013	-0.268	-0.034	0.0	0.162	0.0	0.0	0.0	-0.224	0.63	0.0	0.557	1.0											
44	0.0	-0.005	0.019	0.0	0.0	0.0	0.004	0.0	-0.004	0.0	-0.001	0.0	-0.004	0.0	-0.001	0.0	0.004	-0.009	0.0	-0.008	0.0	-0.055	0.0	0.049	0.0	-0.033	0.0	0.0	0.0	0.0	0.0	0.024	0.0	0.503	-0.17	0.07	-0.025	0.0	0.0	0.026	0.0	-0.116	1.0								
45	-0.053	0.0	0.063	0.0	-0.124	0.164	0.0	0.027	0.0	-0.188	0.0	0.067	0.024	0.0	-0.13	0.0	0.0	-0.082	0.0	0.075	0.0	0.118	0.0	-0.112	0.0	0.073	0.025	-0.279	0.0	0.056	0.0	-0.099	0.0	0.0	0.0	0.0	0.084	-0.151	0.0	0.592	0.0	0.581	1.0								
46	-0.095	0.0	0.021	0.0	-0.056	0.14	0.0	-0.01	0.0	-0.13	0.0	0.056	0.078	0.0	-0.082	0.0	0.0	-0.18	0.0	-0.085	0.0	0.089	0.0	-0.061	0.0	0.034	0.621	-0.085	-0.009	0.031	0.0	-0.045	0.0	0.0	0.0	0.028	-0.046	0.0	0.101	0.0	-0.231	0.0	1.0								
47	0.0	-0.018	0.012	0.0	-0.007	0.0	-0.005	0.0	-0.001	0.0	-0.001	0.0	0.014	0.0	0.004	0.0	-0.009	0.039	0.0	-0.082	0.0	0.071	0.0	-0.045	0.0	0.023	0.0	0.0	0.0	0.0	0.0	-0.011	0.0	-0.228	0.094	-0.034	0.009	0.0	0.0	-0.007	0.0	0.041	0.0	-0.156	0.637	1.0					
48	0.089	0.0	-0.107	0.0	0.051	-0.133	0.0	0.008	0.0	0.124	0.0	-0.052	0.0	-0.075	0.0	0.078	0.0	0.0	0.137	0.0	0.068	0.0	-0.073	0.0	0.053	0.0	-0.003	-0.295	0.022	0.024	-0.033	0.0	0.043	0.0	0.0	0.0	-0.027	0.046	0.0	-0.122	0.0	0.547	0.0	0.0	0.7	1.0					

3.2. Presentation of bond order:



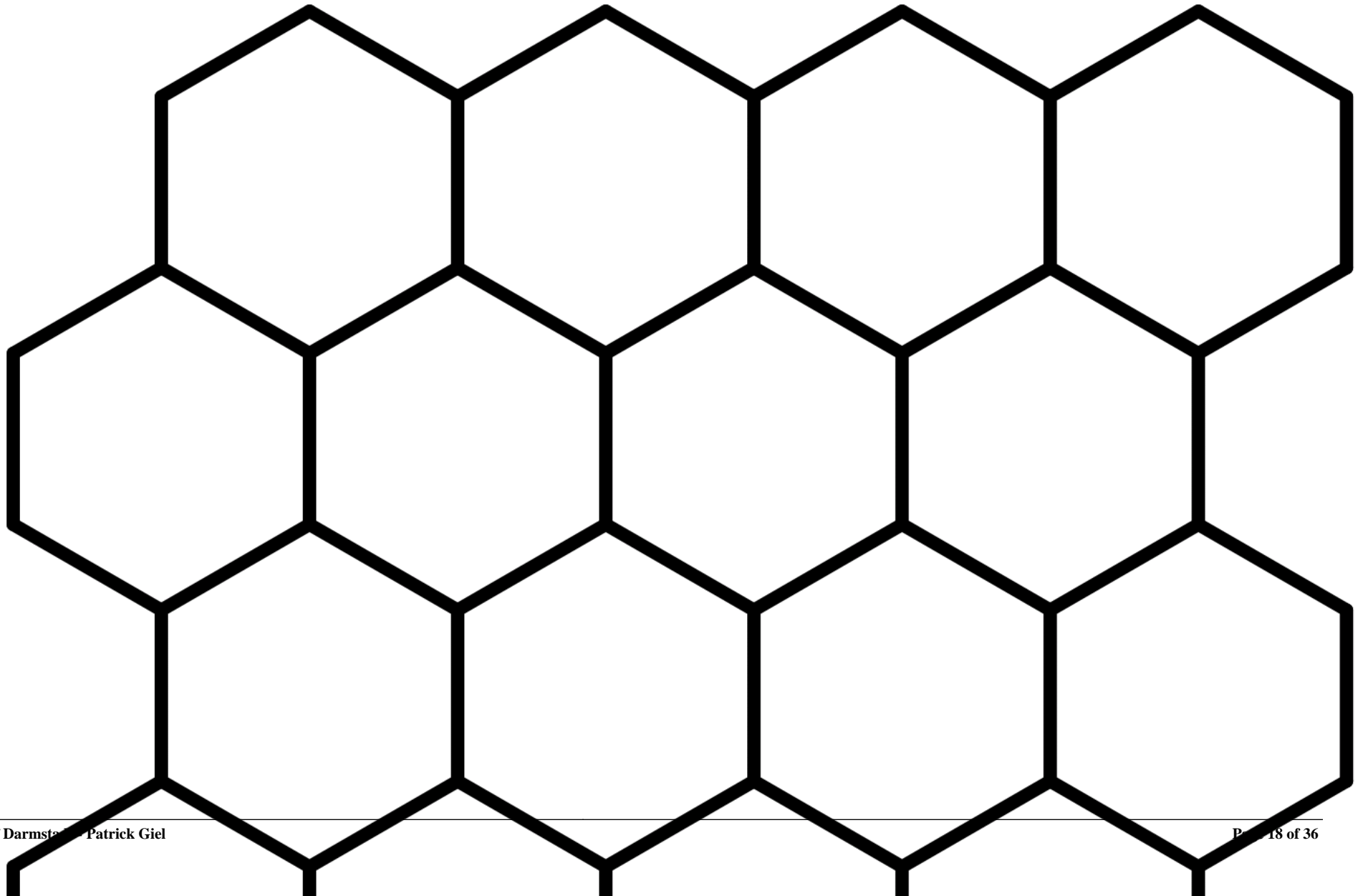
4. Net Charge

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	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48
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																								
25																									0.0																							
26																										0.0																						

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48				
37																																					0.0															
38																																						0.0														
39																																							0.0													
40																																								0.0												
41																																									0.0											
42																																										0.0										
43																																											0.0									
44																																												0.0								
45																																													0.0							
46																																														0.0						
47																																															0.0					
48																																																		0.0		

4.2. Presentation of molecule:

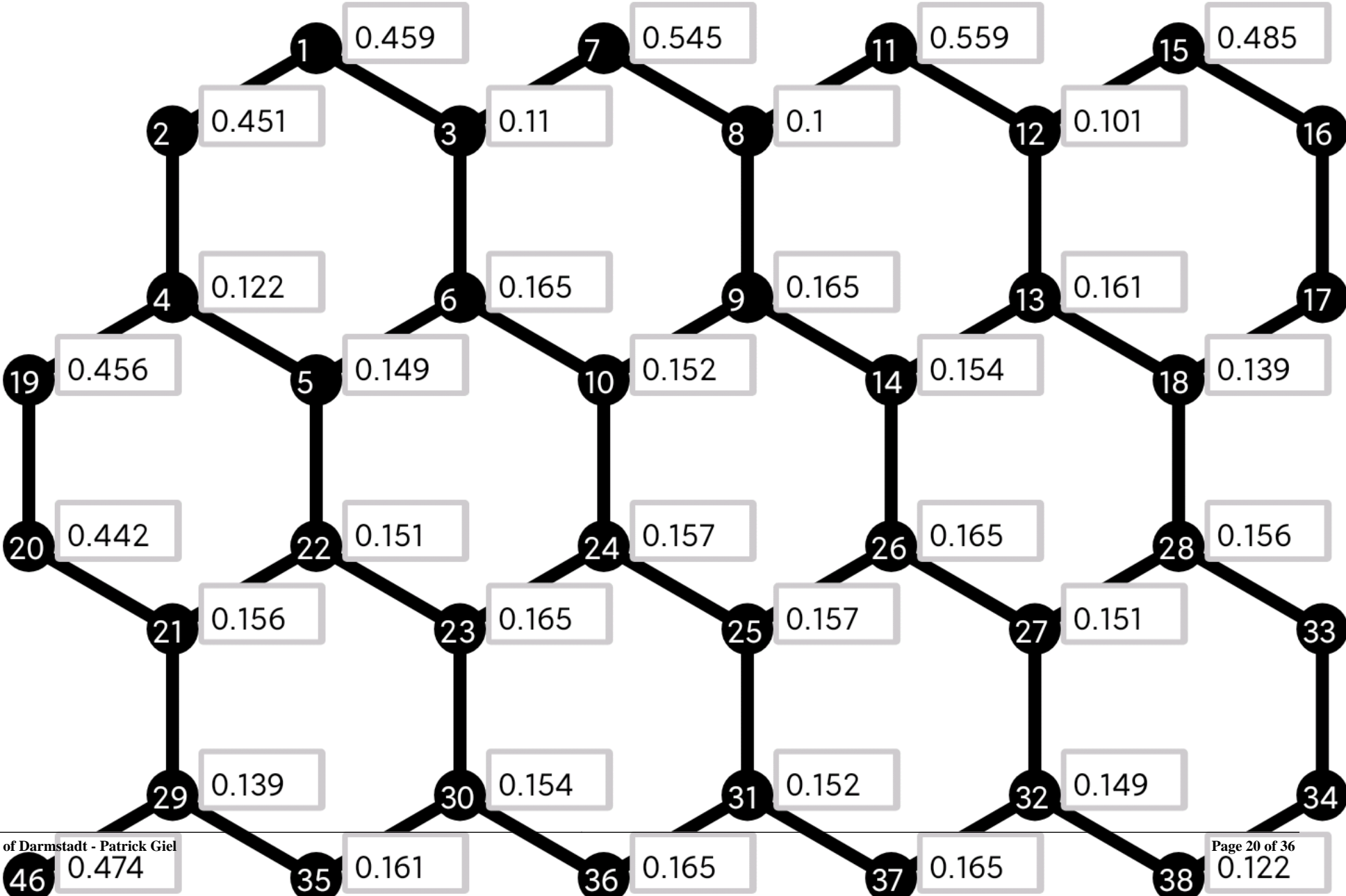


5. Free valences

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	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48
0.459	0.451	0.11	0.122	0.149	0.165	0.545	0.1	0.165	0.152	0.559	0.101	0.161	0.154	0.485	0.396	0.474	0.139	0.456	0.442	0.156	0.151	0.165	0.157	0.165	0.151	0.156	0.139	0.154	0.152	0.149	0.442	0.456	0.161	0.165	0.165	0.122	0.451	0.459	0.1	0.545	0.149	0.165	0.485	0.474	0.396	0.456	

5.2. Presentation of molecule:



6. Atom-Atom-Polarizability

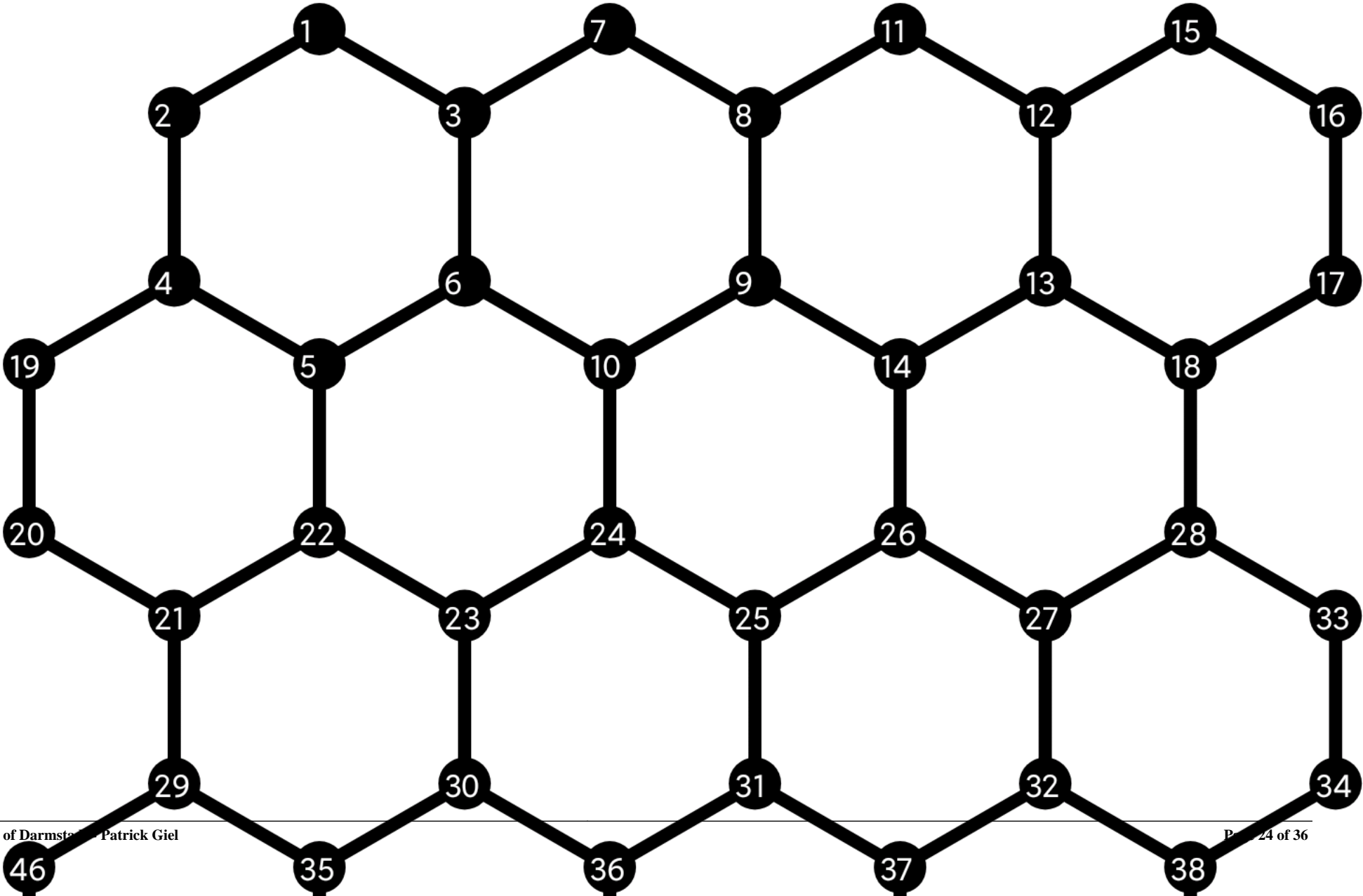
6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48						
1	0.4 59																																																					
2	- 0.2 73	0.4 43																																																				
3	- 0.0 62	0.0 14	0.3 36																																																			
4	0.0 21	- 0.0 65	- 0.0 19	0.3 49																																																		
5	- 0.0 46	0.0 05	0.0 04	- 0.0 79	0.3 52																																																	
6	0.0 06	- 0.0 37	- 0.0 63	0.0 09	- 0.0 85	0.3 73																																																
7	0.0 6	- 0.0 75	- 0.1 51	0.0 26	- 0.0 01	0.0 33	0.6 41																																															
8	- 0.0 07	0.0 01	0.0 06	- 0.0 05	0.0 01	- 0.0 2	- 0.0 9	0.3 29																																														
9	0.0 04	- 0.0 17	- 0.0 26	0.0	- 0.0 05	0.0 08	0.0 07	- 0.0 58	0.3 67																																													
10	- 0.0 05	0.0 04	0.0 05	- 0.0 07	0.0 06	- 0.0 86	- 0.0 81	0.0 04	- 0.0 88	0.3 56																																												
11	0.0 27	- 0.0 22	- 0.0 32	0.0 21	- 0.0 05	0.0 38	0.1 65	- 0.1 16	0.0 14	- 0.0 07	0.7 3																																											
12	- 0.0 01	0.0	0.0	- 0.0 01	0.0	- 0.0 06	- 0.0 13	0.0 06	- 0.0 22	0.0 01	- 0.1 06	0.3 29																																										
13	0.0 05	- 0.0 07	- 0.0 11	0.0 03	0.0	0.0 02	0.0 21	- 0.0 24	0.0 05	- 0.0 06	0.0 29	- 0.0 67	0.3 65																																									
14	- 0.0 02	0.0 01	0.0 02	- 0.0 01	0.0	- 0.0 09	- 0.0 12	0.0 04	- 0.0 89	0.0 07	- 0.0 97	0.0 05	- 0.0 86	0.3 59																																								
15	0.0 08	- 0.0 04	- 0.0 06	0.0 07	- 0.0 03	0.0 15	0.0 51	- 0.0 15	0.0 09	- 0.0 02	0.1 25	- 0.0 85	0.0 07	- 0.0 11	0.5 26																																							
16	0.0	0.0	0.0	0.0	0.0	- 0.0 02	- 0.0 04	0.0	- 0.0 11	0.0	- 0.0 28	0.0 08	- 0.0 43	0.0 03	- 0.1 9	0.3 98																																						

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	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48					
34	0.0 01	- 0.0 01	- 0.0 01	0.0 01	- 0.0 01	0.0 03	0.0 06	0.0	0.0 02	- 0.0 05	0.0 14	0.0	0.0 01	- 0.0 09	0.0 1	- 0.0 02	0.0 13	- 0.0 08	- 0.0 01	0.0 01	- 0.0 01	0.0	- 0.0 03	0.0 01	- 0.0 12	0.0 09	- 0.0 56	0.0 23	0.0 01	0.0 02	0.0 01	0.0 05	- 0.1 8	0.4 52																			
35	- 0.0 03	0.0	0.0	- 0.0 04	0.0 02	- 0.0 13	- 0.0 08	0.0	- 0.0 05	0.0	- 0.0 23	0.0	- 0.0 01	0.0 01	- 0.0 14	0.0	- 0.0 14	0.0 01	0.0 01	- 0.0 04	0.0 04	- 0.0 3	0.0 1	- 0.0 03	0.0 04	- 0.0 11	0.0	- 0.0 08	- 0.0 83	- 0.0 86	- 0.0 06	0.0	0.0 01	- 0.0 09	0.3 65																		
36	- 0.0 05	0.0 01	0.0 01	- 0.0 06	0.0	- 0.0 08	- 0.0 23	0.0	- 0.0 08	0.0 03	- 0.0 06	0.0	- 0.0 05	0.0	- 0.0 01	0.0	- 0.0 01	0.0	0.0 02	- 0.0 07	0.0 05	- 0.0 01	0.0 09	- 0.0 42	0.0 06	- 0.0 01	0.0 03	- 0.0 05	- 0.0 08	- 0.0 89	- 0.0 88	- 0.0 05	0.0	- 0.0 04	0.0 05	0.3 67																	
37	- 0.0 04	0.0 01	0.0 01	- 0.0 04	0.0	- 0.0 12	- 0.0 28	0.0	- 0.0 08	0.0 01	- 0.0 6	0.0	- 0.0 13	0.0 05	- 0.0 2	0.0	- 0.0 2	0.0 01	0.0 03	- 0.0 05	0.0 04	- 0.0 03	0.0 09	- 0.0 02	0.0 09	- 0.0 52	0.0 07	- 0.0 03	- 0.0 01	- 0.0 09	- 0.0 86	- 0.0 85	0.0 07	- 0.0 03	0.0 02	0.0 08	0.3 73																
38	- 0.0 01	0.0	0.0	- 0.0 01	0.0	- 0.0 04	- 0.0 1	0.0	- 0.0 06	0.0	- 0.0 28	0.0	- 0.0 04	0.0 01	- 0.0 34	0.0 01	- 0.0 35	0.0 05	0.0 01	- 0.0 02	0.0 01	- 0.0 01	0.0 03	- 0.0 01	0.0 04	- 0.0 05	0.0 04	- 0.0 61	0.0	- 0.0 01	- 0.0 07	- 0.0 16	- 0.1 1	0.0 03	0.0	0.0	0.0 09	0.3 49															
39	0.0	0.0	0.0	0.0	0.0	0.0 01	0.0 02	0.0	0.0 01	0.0	0.0 06	0.0	0.0	- 0.0 02	0.0 05	0.0 06	- 0.0 02	- 0.0 01	- 0.0 01	0.0 01	- 0.0 01	0.0	- 0.0 02	0.0	- 0.0 02	0.0 02	- 0.0 02	0.0 1	0.0	0.0 01	0.0 04	0.0 05	- 0.0 14	0.0 28	- 0.0 07	- 0.0 17	- 0.0 37	- 0.0 65	0.4 43														
40	0.0	0.0	0.0	0.0	0.0	0.0 01	0.0 02	0.0	0.0 01	- 0.0 01	0.0 04	0.0	0.0	- 0.0 02	0.0 02	0.0 03	- 0.0 01	- 0.0 01	0.0 01	- 0.0 01	0.0 01	- 0.0 01	0.0	- 0.0 02	0.0	- 0.0 01	0.0 04	- 0.0 03	0.0 02	0.0	0.0 02	0.0 05	0.0 04	0.0 09	0.0 06	- 0.0 11	- 0.0 26	- 0.0 63	- 0.0 19	0.0 14	0.3 36												
41	- 0.0 01	0.0	0.0	- 0.0 01	0.0	- 0.0 04	- 0.0 1	0.0	- 0.0 05	0.0	- 0.0 26	0.0	- 0.0 03	0.0 01	- 0.0 3	0.0	- 0.0 31	0.0 02	0.0 01	- 0.0 02	0.0 01	- 0.0 01	0.0 02	- 0.0 01	0.0 02	- 0.0 05	0.0 02	- 0.0 46	0.0 01	- 0.0 02	- 0.0 05	- 0.0 46	0.0 04	- 0.0 53	0.0 05	0.0 04	0.0 06	0.0 21	- 0.2 73	- 0.0 62	0.4 59												
42	0.0	0.0	0.0	0.0	0.0	0.0 01	0.0 01	0.0	0.0	- 0.0 01	0.0 01	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0 01	- 0.0 01	0.0	- 0.0 01	0.0 02	- 0.0 01	0.0	- 0.0 03	0.0 01	0.0 01	0.0 04	0.0 04	0.0 01	- 0.0 04	0.0 01	- 0.0 24	- 0.0 58	- 0.0 2	- 0.0 05	0.0 01	0.0 06	- 0.0 07	0.3 29											
43	- 0.0 1	0.0 02	0.0 02	- 0.0 1	0.0 01	- 0.0 28	- 0.0 68	0.0 01	- 0.0 23	0.0 01	- 0.1 58	0.0	- 0.0 08	0.0 07	- 0.0 95	0.0 01	- 0.0 97	0.0 05	0.0 06	- 0.0 11	0.0 08	- 0.0 06	0.0 16	- 0.0 05	0.0 14	- 0.0 62	0.0	- 0.0 54	- 0.0 03	- 0.0 12	- 0.0 81	- 0.0 01	0.0 13	- 0.0 64	0.0 21	0.0 07	0.0 33	0.0 26	- 0.0 75	- 0.1 51	0.0 6	- 0.0 9	0.6 41										
44	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0 01	- 0.0 02	0.0	- 0.0 02	0.0	- 0.0 02	0.0	0.0 03	0.0 05	0.0 01	- 0.0 01	0.0	- 0.0 67	- 0.0 22	- 0.0 06	- 0.0 01	0.0	0.0	- 0.0 01	0.0 06	- 0.0 13	0.3 29										
45	- 0.0 26	0.0 06	0.0 04	- 0.0 28	0.0 01	- 0.0 6	- 0.1 58	0.0 01	- 0.0 06	0.0 04	- 0.2 25	0.0	- 0.0 23	0.0 1	- 0.1 05	0.0 02	- 0.1 07	0.0 05	0.0 14	- 0.0 32	0.0 19	- 0.0 09	0.0 35	- 0.0 32	0.0 08	- 0.0 58	0.0 01	- 0.0 33	- 0.0 13	- 0.0 97	- 0.0 07	- 0.0 05	0.0 14	- 0.0 38	0.0 29	0.0 14	0.0 38	0.0 21	- 0.0 22	- 0.0 32	0.0 27	- 0.1 16	0.1 65	- 0.1 06	0.7 3								
46	- 0.0 31	0.0 06	0.0 03	- 0.0 35	0.0	- 0.0 2	- 0.0 97	0.0	- 0.0 01	0.0 03	- 0.1 07	0.0	- 0.0 14	0.0 05	- 0.0 44	0.0 01	- 0.0 45	0.0 02	0.0 13	- 0.0 46	0.0 33	- 0.0 06	0.0 21	- 0.0 19	0.0 04	- 0.0 2	0.0 01	- 0.0 1	- 0.1 42	- 0.0 13	- 0.0 01	- 0.0 02	0.0 05	- 0.0 11	0.0 14	0.0 03	0.0 13	0.0 07	- 0.0 04	- 0.0 06	0.0 08	- 0.0 14	0.0 46	- 0.0 45	0.0 92	0.5 1							
47	0.0	0.0	0.0	0.0 01	0.0	0.0 01	0.0 01	0.0	0.0	0.0	0.0 02	0.0	0.0	0.0	0.0 01	0.0	0.0 01	0.0	- 0.0 02	- 0.0 05	0.0	- 0.0 05	0.0 01	- 0.0 03	- 0.0 01	- 0.0 01	0.0 01	- 0.0 1	0.0 03	0.0 01	0.0	0.0	0.0	- 0.0 43	- 0.0 11	- 0.0 02	0.0	0.0	0.0	0.0	0.0	0.0	0.0	- 0.0 04	- 0.0 08	- 0.0 28	- 0.1 32	0.3 98					
48	- 0.0 3	0.0 05	0.0 02	- 0.0 34	0.0	- 0.0 2	- 0.0 95	0.0	- 0.0 01	0.0 03	- 0.1 05	0.0	- 0.0 14	0.0 04	- 0.0 44	0.0 01	- 0.0 44	0.0 02	0.0 1	- 0.0 4	0.0 21	- 0.0 05	0.0 15	- 0.0 18	0.0 03	- 0.0 2	0.0 01	- 0.0 1	- 0.0 93	- 0.0 11	- 0.0 02	- 0.0 03	0.0 06	- 0.0 11	0.0 07	0.0 09	0.0 15	0.0 07	- 0.0 04	- 0.0 06	0.0 08	- 0.0 15	0.0 51	- 0.0 85	0.1 25	0.0 76	- 0.1 9	0.5 26					

6.2. Presentation of molecule:



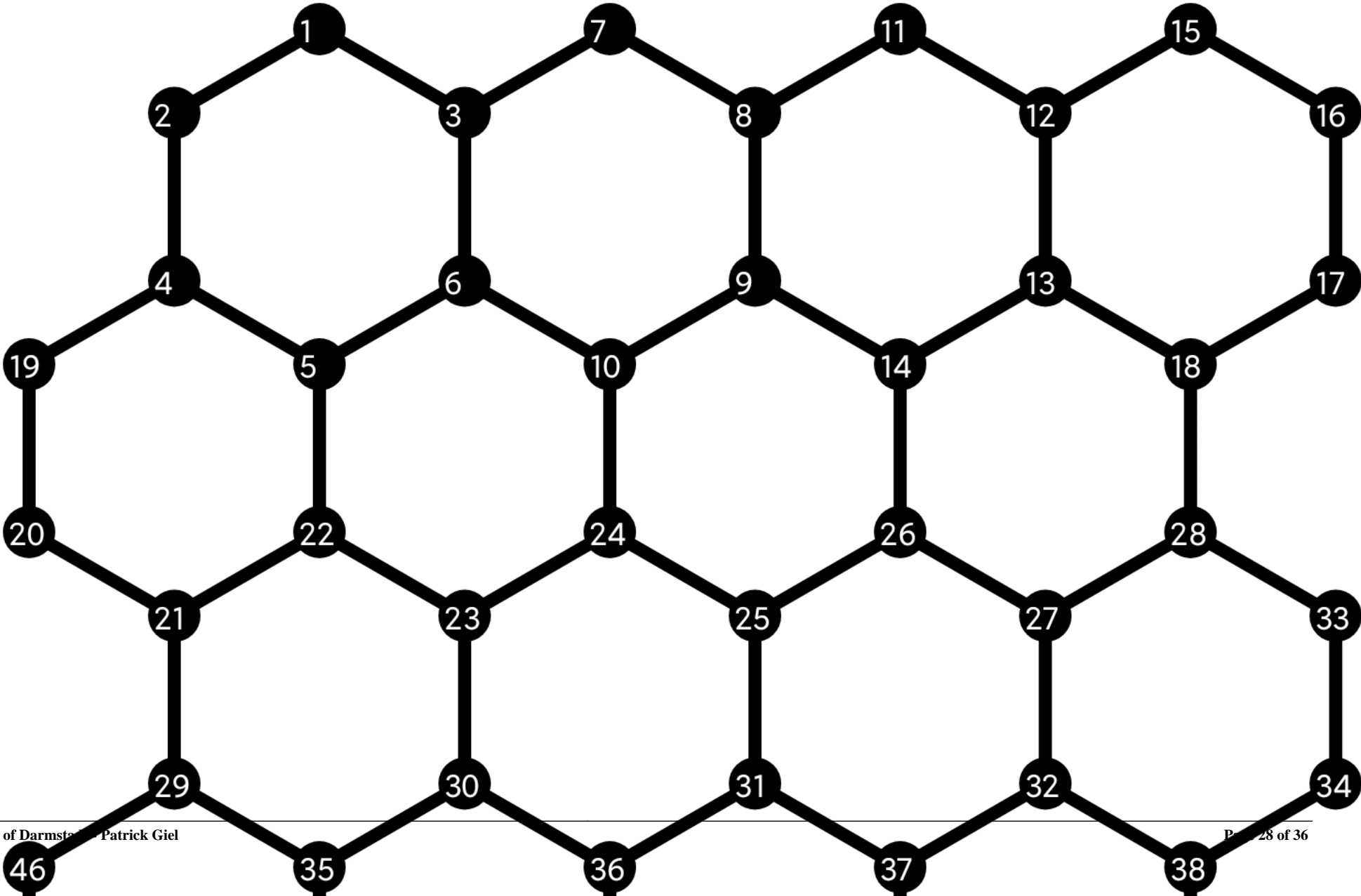
7.1. Calculated values:

[illegible]

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48			
18 28	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
20 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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 29	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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 30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
24 25	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
25 26	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
25 31	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
26 27	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
27 28	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
27 32	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
28 33	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
29 35	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
29 46	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30 35	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30 36	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
31 36	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
31 37	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
32 37	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48					
35 44	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0				
36 42	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0			
37 40	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0		
38 39	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0		
39 41	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
40 41	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
40 43	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
42 43	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
42 45	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
44 45	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
44 48	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
46 47	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
47 48	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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:



8.1. Calculated values:

[illegible]

[illegible]

[illegible]

	1 2	1 3	2 4	3 6	3 7	4 5	4 1 9	5 6	5 2 2	6 1 0	7 8	8 9	8 1 1	9 1 0	9 1 4	1 0 2 4	1 1 1 2	1 2 1 3	1 2 1 5	1 3 1 4	1 3 1 8	1 4 2 6	1 5 1 6	1 6 1 7	1 7 1 8	1 8 2 8	1 9 2 2	2 0 2 1	2 1 2 2	2 1 2 9	2 2 2 3	2 2 2 4	2 3 3 0	2 4 2 5	2 5 2 6	2 5 3 1	2 6 2 7	2 7 2 8	2 7 3 2	2 8 3 3	2 9 3 5	2 9 4 6	3 0 5 5	3 0 6 6	3 1 3 6	3 1 3 7	3 2 3 8	3 2 3 4	3 3 3 8	3 4 3 8	3 5 4 4	3 6 4 2	3 7 4 0	3 8 3 9	3 9 4 1	4 0 4 1	4 0 4 3	4 2 4 3	4 2 4 5	4 4 4 5	4 4 4 8	4 6 4 7	4 7 4 8																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
2 1 2 9	- 0 0 1 2	0 0 0 7	0 0 1 6	0 0 0 1	- 0 0 0 7	- 0 0 0 2	- 0 0 0 9	0 0 4	0 0 0 1	- 0 0 2	0 0 0 2	- 0 0 1	- 0 0 2	- 0 0 2	0 0 0 2	0 0 0 6	- 0 0 0 1	0 0 0 0	- 0 0 3	0 0 0 2	0 0 0 2	- 0 0 1	0 0 0 1	- 0 0 2	0 0 0 0	0 0 4 6	- 0 0 1 6	- 0 0 8	0 0 0 3	- 0 0 2	0 0 1 2	0 0 2 2	0 0 2 5	0 0 2 1	0 0 3 4	0 0 3 7	0 0 4 6	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2 2	0 0 3 3	0 0 4 4	0 0 5 5	0 0 6 6	0 0 7 7	0 0 8 8	0 0 9 9	0 0 0 0	0 0 1 1	0 0 2

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8.2. Presentation of molecule:

