Print calculated values

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

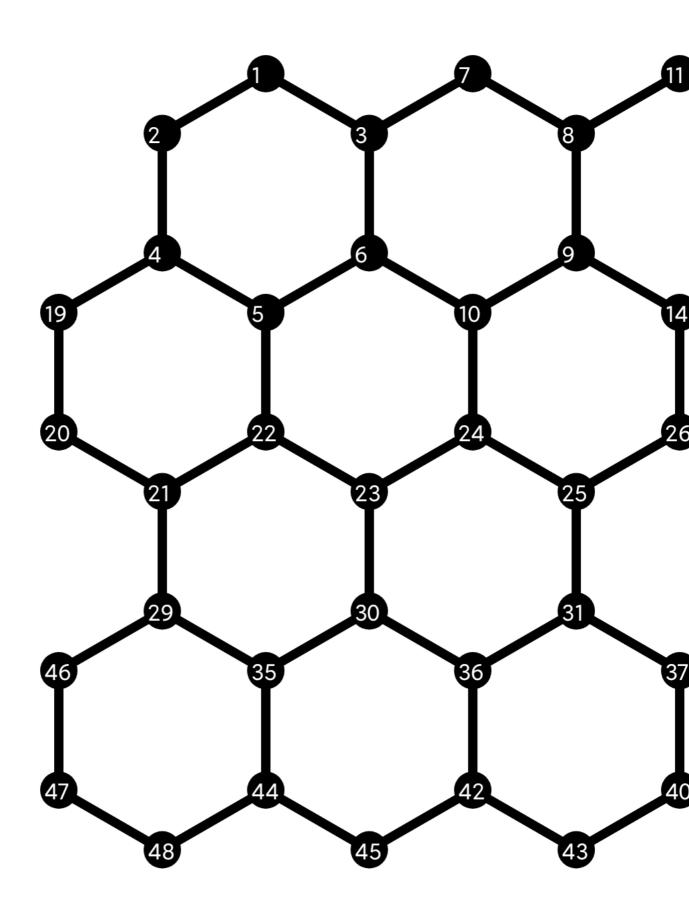
The following determinant is calculated:

 $0\ 0\ 0\ 0\ 0\ 0\ 0\ 1\ 0\ 0\ 0\ 1$

It is about this molecule:

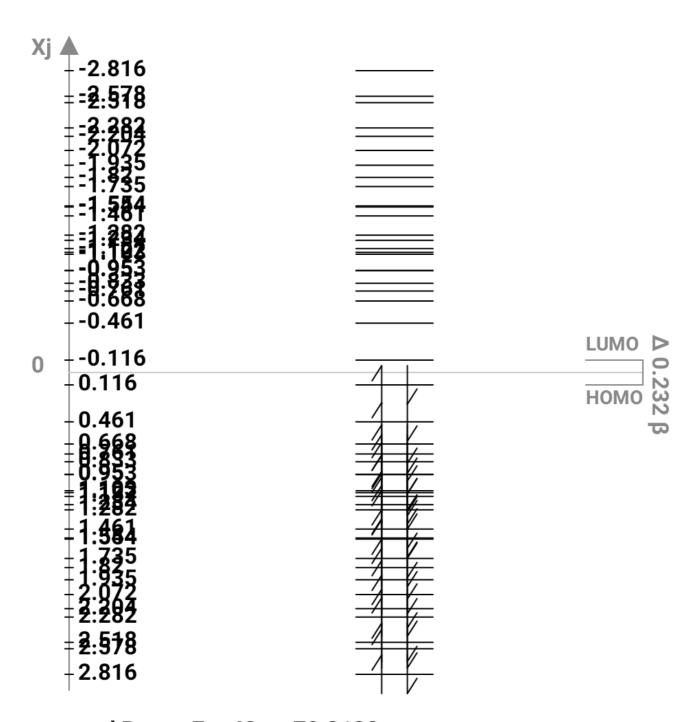
HMO-Energies

```
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 π : 48 α + 70.318 β -

this corresponds to one π electron: 1.465 β

2. Hueckel-coefficient

2.1. Calculated values:

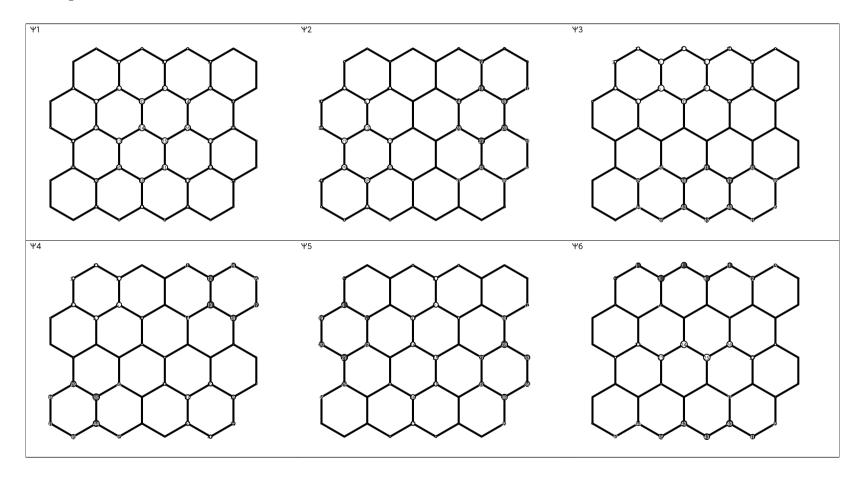
	Psi 1	Psi 2		Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11	Psi 12	Psi 13	Psi 14	Psi 15	Psi 16	Psi 17	Psi 18	Psi 19	Psi 20	Psi 21	Psi 22	Psi 23	Psi 24	Psi 25	Psi 26	Psi 27	Psi 28	Psi 29	Psi 30	Psi 31	Psi 32	Psi 33	Psi 34	Psi 35	Psi 36	Psi 37	Psi 38	Psi 39	Psi 40	Psi 41	Psi 42	Psi 43	Psi 44	Psi 45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

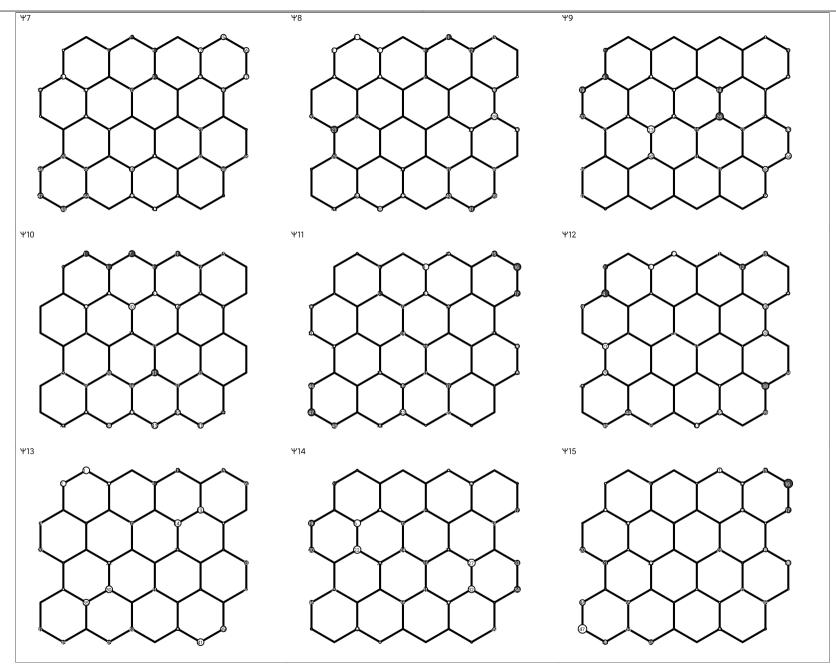
	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7		Psi 9			Psi 12	Psi 13	Psi 14		Psi 16	Psi 17	Psi 18		Psi 20	Psi 21	Psi 22	Psi 23	Psi 24	Psi 25	Psi 26	Psi 27		Psi 29		Psi 31		Psi 33		Psi 35	Psi 36		Psi 38		Psi 40							Psi 47	
14	0.2 09	0.2		- 0.1 31	0.0 98	0.0 69	- 0.0 72	- 0.0 51	0.2 45	0.1 87	0.1 38	- 0.0 55	0.2 77	0.0	- 0.0 57	0.1 45	- 0.1 33	0.1 12	0.0 81	0.0 15	- 0.1 79	- 0.2 38	- 0.0 41	- 0.0 93	- 0.0 93	0.0 41	0.2 38	0.1 79	- 0.0 15	- 0.0 81	0.1 12	0.1 33	0.1 45	0.0 57	0.0	- 0.2 77	0.0 55	0.1	0.1 87	0.2 45	0.0	- 0.0 72	- 0.0 69	- 0.0 98	0.1 31	0.1 54		- 0.2 09
15	0.0 5	- 0.0 93		- 0.1 76	- 0.0 23	- 0.1 13	0.2 19	- 0.1 18	0.0 96	- 0.1 18	- 0.2 15	- 0.1 86	- 0.1 51	0.0 49	- 0.1 8	0.1 04	0.0 85	- 0.0 33	- 0.2 47	0.0 63	- 0.0 14			- 0.2 46	0.2 46	- 0.1 24	- 0.2 35	- 0.0 14	- 0.0 63	- 0.2 47	0.0 33	0.0 85	- 0.1 04			- 0.1 51		- 0.2 15		0.0 96	- 0.1 18	- 0.2 19		- 0.0 23	0.1 76	0.0 79	- 0.0 93	0.0
16	0.0 38	- 0.0 82	0.0 5	- 0.1 5	- 0.0 61	- 0.0 67	0.2 19	- 0.0 15	0.1 32	- 0.0 49	- 0.2 89	- 0.0 41	- 0.1 5	- 0.0 95	- 0.3 51	- 0.0 83	0.0 13	- 0.2 75	- 0.0 89	0.1 07	- 0.1 44	_	0.0 14	- 0.0 41	- 0.0 41	0.0 14	0.1 62	0.1 44	0.1 07	0.0 89	0.2	- 0.0 13	- 0.0 83	0.3 51	- 0.0 95	0.1 5	- 0.0 41	0.2 89	- 0.0 49	- 0.1 32	0.0 15	0.2 19	0.0 67		- 0.1 5	- 0.0 5	0.0 82	- 0.0 38
17	0.0 58	- 0.1 19		- 0.1 66	- 0.1 1			0.0 91		0.0 41	- 0.2 31	0.1 25	- 0.0 42	- 0.1 66	- 0.2 26	- 0.1 97	- 0.0 71	0.2 29	0.1 63	0.0 26	- 0.0 96	0.1 27	- 0.1 18	0.2 41	- 0.2 41	0.1 18	0.1 27	- 0.0 96	- 0.0 26	0.1 63	0.2 29	- 0.0 71	0.1 97	- 0.2 26	0.1 66	- 0.0 42		- 0.2 31	- 0.0 41		0.0 91	- 0.2 05	- 0.0 27	- 0.1 1	0.1 66	0.0 48		0.0 58
18	0.1 24	- 0.2 25	0.0 7	- 0.2 28	- 0.1 83	0.0 12		0.1 81			- 0.0 68	0.2 24		- 0.1 1	0.0 89	- 0.1 38	- 0.0 91		0.2 43	- 0.0 85		0.2 46		0.0 69		0.0	- 0.2 46	- 0.0 71	- 0.0 85	- 0.2 43	0.0 56					- 0.0 96	0.2 24	0.0 68		- 0.0 99	- 0.1 81	0.1 78	- 0.0 12	0.1 83	- 0.2 28	- 0.0 7		- 0.1 24
19	0.0 62	0.1 11	0.0	0.0 67	0.2	- 0.0 26	0.1 47	- 0.0 16	- 0.2 51	0.0 14	0.1 55		- 0.1 09	- 0.2 44	- 0.0 67		- 0.0 07	0.0 82	0.0 19	- 0.0 46	0.2 9	- 0.1 74			- 0.1 15		0.1 74	0.2	- 0.0 46	- 0.0 19	0.0 82	0.0 07			- 0.2 44			- 0.1 55			0.0 16		0.0 26	0.2			- 0.1 11	- 0.0 62
20	0.0 7	0.1 34		- 0.0 09	- 0.2 08		0.0 87			- 0.0 09	0.1 71	0.0 59	- 0.1 57	- 0.2 09	- 0.2 11	- 0.0 59		0.1 75	0.1 46	- 0.1 61	0.2 28	- 0.2 35	0.0 49	0.1 09	- 0.1 09	- 0.0 49	- 0.2 35	0.2 28				0.0 85	0.0 59	- 0.2 11	0.2 09	- 0.1 57	- 0.0 59		0.0 09	- 0.2 04	- 0.1 61	- 0.0 87	0.0 33			0.0 37	0.1 34	0.0
21	0.1 37	0.2 35		- 0.0 88	- 0.2 58	0.0 93	0.0 21	- 0.2 77	- 0.1 03	- 0.0 28	0.1 09	0.2 44	- 0.0 92	- 0.0 15		0.1 42	0.1	0.0 85	0.1 19	- 0.0 88	- 0.1 16			0.1 28			- 0.0 18	0.1 16	- 0.0 88	- 0.1 19	0.0 85	0.1	0.1 42		- 0.0 15				- 0.0 28	0.1 03	0.2 77	0.0 21	- 0.0 93	0.2 58	- 0.0 88	- 0.0 19	- 0.2 35	- 0.1 37
22	0.1 91	0.2 46		0.0 37	- 0.1 78	0.1 49	0.1 32	- 0.1 61			0.0 65		- 0.0 58				0.1 17	- 0.1 5	0.2 11	0.0 02	- 0.2 46	0.0		- 0.0 26	0.0 26		0.0		- 0.0 02	0.2 11	0.1 5	0.1 17	- 0.0 8					0.0 65	- 0.0 79	0.1 24	- 0.1 61	- 0.1 32	0.1 49	- 0.1 78	- 0.0 37		0.2 46	0.1 91
23	0.2 31	0.1 98	- 0.0 05	- 0.0 04	0.0 5			- 0.0 78	0.3 06	- 0.0 03	0.0 21	- 0.0 56		0.1	0.1 56	- 0.1 36	0.2 15	- 0.1 48	0.0 36	- 0.2 35	- 0.0 09					- 0.0 99	0.1 02		- 0.2 35	- 0.0 36	- 0.1 48	- 0.2 15	- 0.1 36	0.1	0.1 1		- 0.0 56					0.0 97	- 0.2 36	- 0.0 5	- 0.0 04	0.0 05	- 0.1 98	0.2 31
24	0.2 52	0.0 66	0.0 6	0.0 86		0.2 71	- 0.0 17	- 0.0 32		0.1 03	- 0.1 71	0.1	- 0.0 71	- 0.1 76	0.0 28	- 0.0 87		0.1 21	- 0.0 96	- 0.2 13	0.0 6		- 0.1 31			0.1 31		0.0 6		- 0.0 96		0.2 53				- 0.0 71			- 0.1 03	0.1 62		0.0 17	0.2 71		1		0.0 66	0.2 52
25	0.2 52	- 0.0 66		0.0 86		0.2 71	0.0 17	0.0	- 0.1 62	- 0.1 03	- 0.1 71	0.1	- 0.0 71	- 0.1 76				0.1 21	0.0 96	0.2 13	- 0.0 6	0.1 69	- 0.1 31	0.0 86		- 0.1 31	- 0.1 69			- 0.0 96	0.1 21	- 0.2 53	0.0 87		- 0.1 76	0.0 71	0.1		- 0.1 03	0.1 62	- 0.0 32	0.0 17	- 0.2 71	- 0.1 91		0.0 6	66	- 0.2 52
26		- 0.1 98	0.0 05	- 0.0 04	0.0 5	0.2 36	- 0.0 97	0.0 78	- 0.3 06	0.0	0.0 21	- 0.0 56	0.1 15	0.1		0.1 36	0.2 15	0.1 48	- 0.0 36	0.2 35	0.0 09	- 0.1 02	- 0.0 99		- 0.1 53		- 0.1 02	0.0 09	- 0.2 35	- 0.0 36	0.1 48	0.2 15	- 0.1 36	- 0.1 56	0.1 1		0.0 56			- 0.3 06	0.0 78		0.2 36			0.0 05	- 0.1 98	0.2 31
27	0.1 91	- 0.2 46	- 0.0 81	0.0 37	- 0.1 78	0.1 49	- 0.1 32	0.1 61	- 0.1 24	- 0.0 79	0.0 65	0.0	- 0.0 58	0.3 01	- 0.0 95	- 0.0 8	0.1 17	0.1 5	- 0.2 11	0.0 02	0.2 46	0.0		0.0 26			0.0	0.2		0.2 11	- 0.1 5	- 0.1 17			0.3 01			- 0.0 65	- 0.0 79	0.1 24	- 0.1 61	- 0.1 32	- 0.1 49	0.1 78	0.0			- 0.1 91
28	0.1 37	- 0.2 35		- 0.0 88	- 0.2 58	0.0 93	- 0.0 21	0.2 77			0.1 09	0.2 44	- 0.0 92	- 0.0 15	0.1 78	- 0.1 42	0.1	0.0 85	- 0.1 19	0.0 88		0.0 18	0.2 31	- 0.1 28	0.1 28	- 0.2 31	0.0 18		- 0.0 88	- 0.1 19	- 0.0 85	0.1	0.1 42		0.0 15		- 0.2 44		- 0.0 28			0.0 21			0.0 88		I I	0.1 37
29		0.2 25		- 0.2 28	- 0.1 83	0.0	- 0.1 78	- 0.1 81	- 0.0 99	- 0.1 14	- 0.0 68	0.2 24	0.0 96	0.1 1	- 0.0 89		- 0.0 91	0.0 56	- 0.2 43	0.0 85	- 0.0 71	0.2 46	- 0.0 69	- 0.0 69	0.0 69	0.0 69	0.2 46	0.0		- 0.2 43			- 0.1 38	- 0.0 89	0.1	0.0 96	- 0.2 24	- 0.0 68	0.1 14	- 0.0 99	- 0.1 81	0.1 78	0.0 12	- 0.1 83	0.2 28	- 0.0 7	0.2 25	0.1 24
30	0.2 09	0.2	0.1 54	- 0.1 31		0.0 69		0.0 51	0.2 45	0.1 87	0.1 38	- 0.0 55	0.2 77	0.0	0.0 57		- 0.1 33	- 0.1 12	- 0.0 81		0.1 79	- 0.2 38	- 0.0 41	0.0 93	- 0.0 93	0.0 41	- 0.2 38	0.1 79	- 0.0 15	- 0.0 81	0.1 12	0.1 33	0.1 45	0.0 57	0.0 1	0.2 77	0.0 55				0.0 51	- 0.0 72		0.0 98	0.1 31	- 0.1 54	0.2	0.2 09

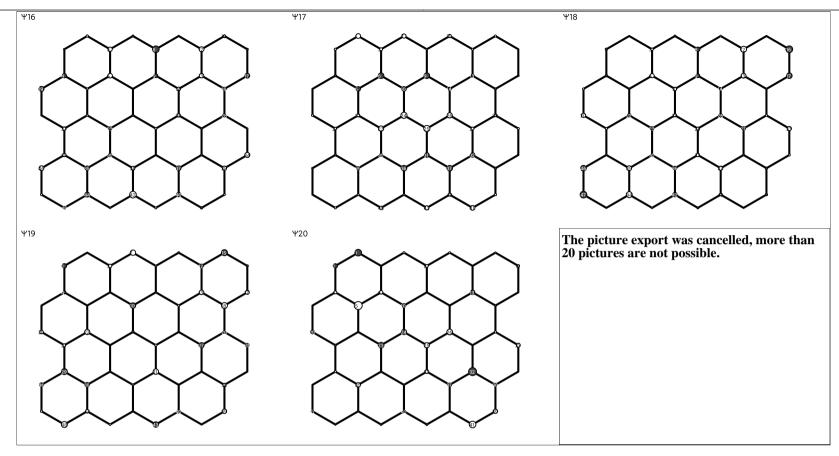
	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11		Psi 13			Psi 16	Psi 17	Psi 18	Psi 19	Psi 20	Psi 21		Psi 23	Psi 24	Psi 25	Psi 26	Psi 27	Psi 28	Psi 29	Psi 30	Psi 31	Psi 32	Psi 33	Psi 1	Psi P	si P	si Ps 7 38	i P	si Ps 9 40	i Ps	Psi 42	Psi 43		Psi 45			Psi 48
31	0.2 26	- 0.0 36		0.1 14			0.1 47	0.0	- 0.1 36	- 0.2 66	- 0.1 14	0.0	0.1 35	- 0.1 51		0.0	- 0.1 89	0.1 42	0.2 23	0.1 55	- 0.1 14	0.0 46	0.1 69	- 0.0 58	0.0 58	- 0.1 69	0.0 46	- 0.1 14	- 0.1 55	0.2 23	- 0.1 42	- 0.1 89			1 0 3		0 - 0 0.1 14				- 0.1 47	0.0 55			- 0.2 15	0.0	0.2 26
32	0.1 69	0.2	-	0.1 75			- 0.1 38	- 0.0 61	0.0	-	-	- 0.0 81	-	0.2	- 0.1 32	- 0.0	- 0.1	- 0.0 81	- 0.0 45	- 0.3 25	0.0	0.0 85	0.0	-	0.0 23	0.0	0.0 85	0.0	0.3 25	_	0.0 81	-	0.0 84	0.1 0	-	0.	+	0.	1 - 4 0.0	1-	0.1	0.0	- 0.1 84	- 0.1	-		0.1 69
33	0.0		- 0.0 37	- 0.0 09	-	0.0 33	-	0.1	0.2	0.0	0.1	0.0	-	- 0.2 09		0.0	0.0	0.1	0.1	0.1	- 0.2 28	- 0.2 35	0.0	0.1	- 0.1 09	0.0 49	0.2	0.2 28	0.1	0.1	0.1 75	_	0.0 59	0.2	0	1 0	0 -		0 -	2 0.1	- 0.0 87	0.0	0.2	- 0.0 09	0.0	0.1	0.0
34	0.0	_	- 0.0 74	0.0	- 0.2	- 0.0	-	0.0	0.2 51	- 0.0 14	0.1 55	- 0.1 57	-	-	0.0 67	08	- 0.0 07	0.0 82	- 0.0 19	0.0 46	_	- 0.1	- 0.2 08	09 0.1 15	-	0.2	- 0.1 74	- 0.2 9	- 0.0 46	- 0.0 19	- 0.0	-0.0	_	0.0	.2 -	1 5	1 0.1 7 55	0.		2 0.0	0.1	-	-0.2	- 0.0			0.0 62
35	0.1 54		- 0.1	- 0.2 67	0.0	-0.0	-		0.0 65	-	0.0 18	-	0.2	0.0	- 0.1 51	-	-	0.1 98	0.1	0.1	-	0.0	- 0.1	0.1 05	0.1	-	-	0.0	0.1	0.1	0.1	0.1	0.1		.0 -	2 0.	- 0 0.0	0.00	1 0.0	- 0.0 39	- 0.1 6	0.0	0.0	+	0.1	0.2	
36	0.2	0.0	+	- 0.0 27	0.2		0.2	0.1	0.0 54	-	0.1 75	0.0	- 0.0 18	- 0.1 42	-	0.1	-	- 0.1 56	0.0 75	0.0 62	0.1	- 0.0 76	0.2 24	0.0 59	0.0 59	0.2		- 0.1 79	0.0 62		- 0.1 56			- 0.0 62	0	0 0. 3 18	0 -	- 0.	-	0.1	0.2	0.0		-	0.2		- 0.2 02
37	0.1	- 0.1 18	-	0.2	0.0 05	-	0.0 64	- 0.1 42	- 0.1 29	- 0.1 3	- 0.1 79	0.0 97	-	0.1	0.0 77	- 0.1 88	-	0.1	0.0 41	- 0.1 46	- 0.2 07	-			- 0.1 51	- 0.0 16	0.0 62	0.2	- 0.1 46	-0.0	0.1		0.1	- (.1 0		_	1 -	0.1	0.1	0.0 64		- 0.0 05	+=	0.2 48	0.1 18	- 0.1 83
38	0.1	- 0.1 53	-	0.1 62	0.2	- 0.0	- 0.1 98	- 0.1 32	0.2	-	0.0	- 0.2 89	0.0	- 0.0 92	- 0.1 35	0.1	-	- 0.0 97	0.1 28	- 0.1 23	0.0	0.1	-	+	0.1	-	- 0.1 18	-0.0	- 0.1	- 0.1	- 0.0 97	0.0 92	0.1	0.1 -	.0 0 2 1	0 0. 7 89			0 0.2 1 32	0.1		0.0 86	0.2		0.1 49	0.1 53	- 0.1 03
39	0.0 59	- 0.0 82	-	0.1 28	0.1	- 0.1	- 0.0 98	- 0.1 94	0.1 63	0.1	- 0.0 2	- 0.1 84	0.2 28	-	0.0		0.0	-	0.1 85	0.1	0.2 34	0.1 68	0.2		0.0 78	-	0.1	0.2	-	0.1	0.0	0.0 91	- 0.0 72		.1 0	2 0.	1 - 0.0	1-	0.1	. -	0.0	- 0.1 32	- 0.1 29			-	0.0 59
40	0.1 19	-	0.2	0.1 69	0.0	- 0.2 54	0.1	-	- 0.0 75	0.2 18	-	0.2	0.1 25	0.0	0.1 25	- 0.1 78	0.1 22	0.1	- 0.1 39	0.0 48	- 0.1 05	- 0.1 72	- 0.1 03	0.0	- 0.0 63	0.1		- 0.1 05	-		- 0.1 01	0.1	0.1	0.1 -	0 2		2 0.1		2 0.0	0.2	- 0.1 15	-	0.0	-	0.2	-	0.1 19
41	0.0 63	-	0.1	0.1	- 0.0 52		0.0 09	- 0.2 22	+	0.2 18		0.0	0.2 75	- 0.0 88	0.0	- 0.0 94	0.1 93		0.0 48	0.2 7	0.1	- 0.0 06	0.2	- 0.1 32	-	0.2 44	0.0	-	0.2	-	0.0 08			- 0.0 3	.0 0	2 0.	0.0	0.		0.2	0.0	+	0.0 52	0.1	0.1	0.0 58	- 0.0 63
42	0.1	0.0 69	0.2	- 0.0 45	0.1 63		0.1 74	0.1 78	- 0.0 15		0.2 45		- 0.1 65	- 0.0 34	- 0.0 81	0.2 71		- 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 72		- 0.0 71		0.0 67		- 0.0 81	.0 - 4 0 6		0.2		- 1 0.0 3 15			0.2		0.0 45	0.2	0.0 69	0.1
43	0.0	0.0	- 0.1 75	0.0 54	0.0 81	- 0.2 34	0.1 49	- 0.0 17	- 0.0 52		0.0 73		- 0.0 31	0.0 02	0.0 38		0.1 71		- 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 0 3	0 1 94	1 - 1 0.0 73) 5	2 0.0			0.2 34	- 0.0 81		0.1 75		- 0.0 9
44	0.1	0.1 58		- 0.2 51		- 0.1 67	- 0.2 04	0.2	- 0.0 34	0.1 34	- 0.0 43	0.2	0.0 43	0.1 55		- 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		- 0.2 44	0.0 81		- 0.1 43	.1 0 5 4		2 - 0.0 43		1 0.0 4 34)	0.2	- 0.1 67		51	- 0.1 48		0.1 02
45	0.0 84	0.0 88	- 0.1 46	- 0.1 3		- 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		0.1 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	- 0.2 18	0.0 81	- 0.0 77		0.0 67	- 0.1 34		0.1 94	.0 0 8 6		- 1 0.1 9 31			0.2	- 0.0 16		- 0.0 78	- 0.1 3		- 0.0 88	
46	0.0 58	0.1 19	- 0.0 48	- 0.1 66		- 0.0 27	- 0.2 05	- 0.0 91		- 0.0 41	0.2 31	0.1 25	- 0.0 42	- 0.1 66		0.1 97	- 0.0 71		- 0.1 63	- 0.0 26	0.0 96		- 0.1 18	- 0.2 41	- 0.2 41	- 0.1 18	- 0.1 27	- 0.0 96	- 0.0 26	0.1 63	- 0.2 29	0.0 71	97	- 0.2 26	.1 0 6 4	0 0.	1 0.2			0.0		0.0 27	0.1 1	- 0.1 66	0.0 48	- 0.1 19	- 0.0 58
47	0.0	0.0 82	0.0 5	0.1 5	- 0.0 61	- 0.0 67	- 0.2 19	0.0 15	- 0.1 32	0.0 49	- 0.2 89	- 0.0 41	0.1 5	- 0.0 95	0.3 51		0.0 13	- 0.2 75	0.0 89	- 0.1 07	0.1 44	- 0.1 62	0.0 14	0.0 41	- 0.0 41	- 0.0 14	- 0.1 62	0.1 44				0.0 13	0.0 83	0.3	5 0 5	1 0.	0 - 0.2 89				0.2 19	- 0.0 67	- 0.0 61	0.1 5	0.0 5		0.0 38

	Psi					Psi																																										
	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
48	0.0	0.0	-	-	-	-	-	0.1	-	0.1	-	-	-	0.0	0.1		0.0	-	0.2	-	0.0	-	0.1	0.2	0.2	0.1	0.2	-	-	-	-	-	-	_	0.0	0.1	-	0.2	0.1	0.0	_	-	0.1	0.0	-	0.0	-	-
	5	93	0.0	0.1	0.0	0.1	0.2	18	0.0	18	0.2	0.1	0.1	49	8	0.1	85	0.0	47	0.0	14	0.2	24	46	46	24	35	0.0	0.0	0.2	0.0	0.0	0.1	0.1	49	51	0.1	15	18	96	0.1	0.2	13	23	0.1	79	0.0	0.0
			79	76	23	13	19		96		15	86	51			04		33		63		35						14	63	47	33	85	04	8			86				18	19			76		93	5

2.2. Molecule orbital presentation:







3. Bond Order

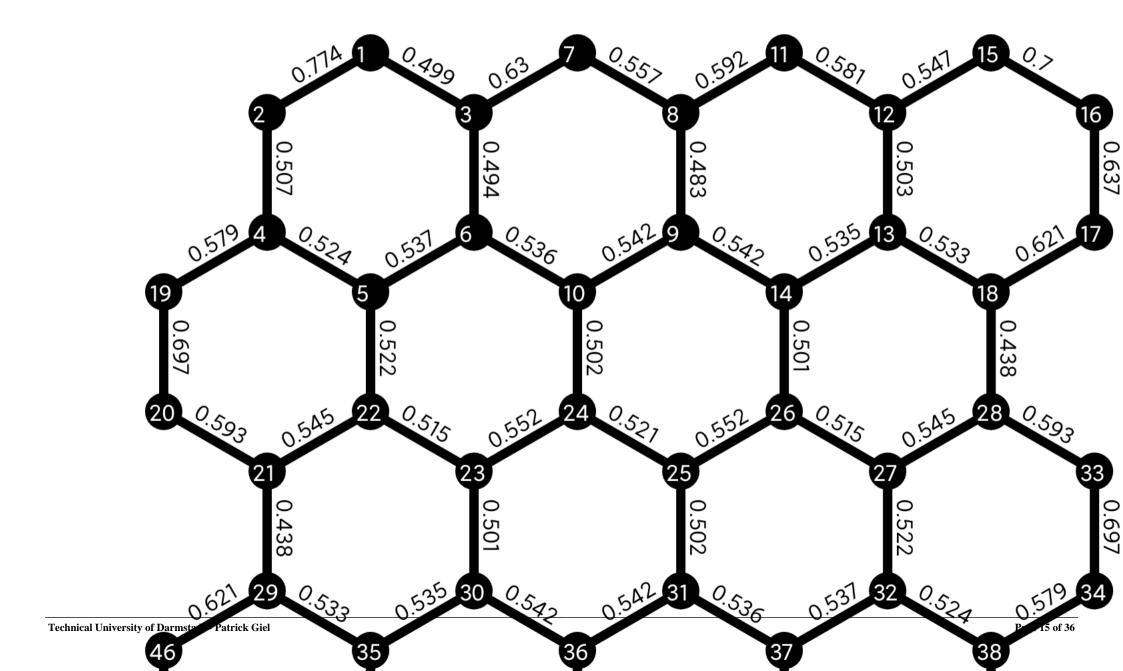
3.1. Calculated values:

	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	5 26	27	7 28	29	30	3	1 32	33	3	4 35	5 3	6 3	7 38	3 3	9 4	10 4	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	1.0																																													
5	0.2 31	0.0	0.0	0.5 24	1.0																																												
6	0.0	- 0.2 13	0.4	0.0	0.5 37	1.0																																											
7	0.0	- 0.2 24	0.6	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	0.1	0.0	0.0	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	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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.5 42	0.0	0.2	0.0	0.5 35	1.0																																			
15	0.0	- 0.0 27	0.0	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	1.0																																		
16	- 0.0 07	0.0	0.0 46	0.0	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
		28	- 0.0 46	0.0	0.0 31	0.0	0.0	0.1 01	0.0	- 0.0 09	0.0	- 0.2 31	0.0	- 0.0 85	0.0	0.6 37	1.0																															
	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	0.6 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																												
20	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	5	0.0	- 0.1 71	0.0	0.0	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	0.0	0.2	0.1 5	0.0	0.0	0.0	0.1	0.0	0.0 7	0.0	0.0 53	0.0	0.0	0.0	0.0	0.0	0.0	0.5 15	1.0																									
25	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 64	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 89	0.0	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	0.5 01	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																						
26 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 68	0.0	- 0.0 85	0.0	0.0	0.0 24	0.0	- 0.0 11	0.0	- 0.0 59	0.0	0.5 15	1.0																					
28	0.0	0.0	- 0.0 26	0.0	- 0.0 24	0.0	0.0	0.0 26	0.0	0.0 7	0.0	- 0.0 08	0.0	- 0.1 57	0.0	- 0.0 82	0.0	0.4 38	- 0.0 04	0.0	0.0	0.0	0.0 07	0.0	- 0.0 89	0.0	0.5 45	1.0																				
29	0.0	0.0 45	- 0.0 22	0.0	- 0.0 13	0.0	0.0	0.0 05	0.0	0.0 34	0.0	0.0 04	0.0	- 0.0 29	0.0	- 0.0 09	0.0	0.0 16	- 0.0 97	0.0	0.4 38	0.0	- 0.1 52	0.0	0.0 64	0.0	- 0.0 19	0.0	1.0																			
30	0.0	- 0.0 32	0.0 37	0.0	- 0.0 57	0.0	0.0	- 0.0 14	0.0	- 0.0 41	0.0	- 0.0 04	0.0	0.0 48	0.0	0.0 14	0.0	- 0.0 29	0.0 88	0.0	- 0.1 57	0.0	0.5 01	0.0	- 0.1 72	0.0	0.0 64	0.0	0.0	1.0																		
31	0.0	11	0.0 16	0.0	52	0.0	0.0	24	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	34	0.0 55	0.0	7	0.0	0.1 77	0.0	0.3	0.0	0.1 71	0.0	0.0	0.0	1.0																	
32	0.0	0.0 05	0.0 03	0.0	0.0 36	0.0	0.0	- 0.0 05	0.0	0.0 52	0.0	0.0 19	0.0	- 0.0 57	0.0	- 0.0 07	0.0	- 0.0 13	0.0 24	0.0	- 0.0 24	0.0	0.0 72	0.0	- 0.1 79	0.0	0.5 22	0.0	0.0	0.0	0.0	1.0																
	- 0.0 06	0.0	0.0	0.0	0.0	0.0 34	0.0 31	0.0	0.0 66	0.0	- 0.0 82	0.0	- 0.0 72	0.0	0.1 37	0.0	0.1 8	0.0	0.0	- 0.0 17	0.0	0.0	0.0	- 0.0 18	0.0	- 0.0 63	0.0	0.5 93	- 0.0 01	- 0.0 17	0.0 78	- 0.2 33	1.0															

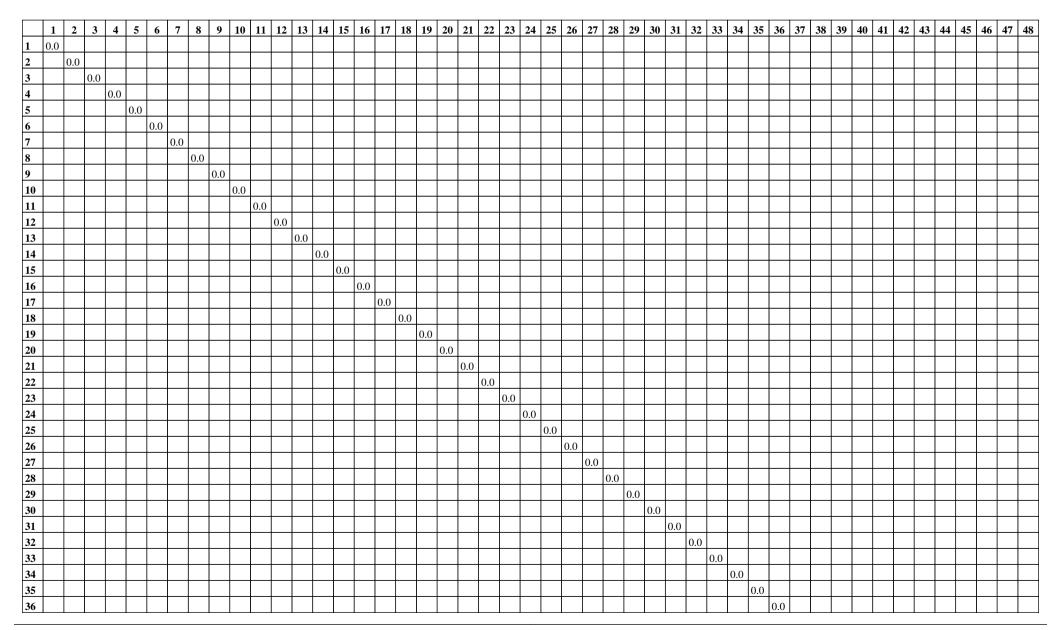
	1	2	3	4	5	6	7	8							15 1						22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48
34		0.0 18	17		24			0.0 11		0.0 55		0.0 09		88	0.0 0.39	9	0.0 97	0.0 02		0.0 04	0.0	- 0.0 18	0.0		0.0		0.0	0.0	0.0	0.0	0.0	0.6 97	1.0														
35	- 0.0 41		0.0	0.0 54	0.0	83	-	0.0	-	0.0	0.0 67	0.0	- 0.0 16	0.0	0.0	مامر	مما	0.0	0.0 72	0.0	_	0.0	0.0 55	0.0	0.0 7	0.0	0.0 48	0.5 33	0.5 35	0.0 75	- 0.0 11	0.0	0.0 54	1.0													
	33			0.0 44		75	0.0 95		77		27		0.0 39		0.0	0.0)		66		0.0 4		0.2	0.0	0.0 45	0.0	58	- 0.0 88	0.5 42	0.5 42	- 0.0 71	0.0	- 0.0 47	0.0	1.0												
37	- 0.0 16			21		0.0 52	61		75		0.1 24		83).0 51	0.0 56			0.0 34		44		0.0 28		0.2 18	:	0.0		0.0	0.5 36	37		0.0	0.0													
	05			0.0 06		21	0.0 24		0.0 44		63		54		0.1 0.7	21			11		0.0 21		31		1	4	41			- 0.0 77					0.0	0.0	1.0										
39	0.0	11	0.0 12		05			1		11				0.0 32	0.0 0. 13	0	45	0.0 18		23		0.0 37		35		0.0 01				0.0		0.1 27		0.0 56		0.2 13		1.0									
40			12		- 0.0 03			- 0.0 08		- 0.0 16		0.0 05		37	0.0 0.	2	0.0 22	17		0.0 26		41		- 0.0 33		- 0.0 59	0.0	0.0	0.0	0.0	0.0	0.0 86	0.0	86	- 0.1 81	0.4 94	- 0.1 62	0.0	1.0								
	0.0 06			05		0.0 16	22		33		0.0 53		0.0 41		0.0	0.0 95)		0.0 06		13		0.0 22	0.0	0.0 13	0.0	0.1 58	- 0.0 1	0.0 13	12	- 0.2 31		- 0.1 98	0.0	0.0	0.0	0.0	0.7 74		1.0							
42			- 0.0 08	0.0	- 0.0 05	0.0	0.0	- 0.0 01		0.0 24	0.0	0.0 04	0.0	0.0 14	0.0	0.0	0.0	- 0.0 11	0.0	0.0 26	0.0	0.0 31	0.0	0.0 43	0.0	0.0	0.0	0.0	0.0	0.0		- 0.0 49	0.0	0.1 75	0.4 83	0.1 66	66	0.0		- 0.0 93	1.0				į		
	22			0.0 24		61	0.0 79		0.0 95		64		0.0 32		0.1	4			31		0.0 45		42		5		0.1 25	14	13	0.2 68	0.0 34		62					0.2 24	3		57						
			0.0 05		19			04		0.0 04					0.0	0	04			- 0.0 08		- 0.0 55		0.0 49		- 0.0 33		0.0	0.0	0.0		0.0 24	0.0	03	- 0.1 7	7	- 0.0 25		0.0	0.0 26		- 0.1 16	1.0				
45	0.0 53			63		0.1 24	64		27		0.1 88		67		0.1 0.24	0.1			0.0 82	0.0	0.0 75	0.0	0.1 18	0.0	0.1 12	ľ	73	25	0.2 79		56		0.0 99					84	0.1 51		92		81				
46	0.0 95			21		0.0 56	4		0.0 1		0.1 3		56		0.0 78	0.0 82			0.1 8		0.0 85				0.0 61	- 1	34	21	0.0 85	0.0 09	31		0.0 45		0.0	0.0	0.0	0.0 28	- 0.0 46	0.0	0.1 01		- 0.2 31	0.0	1.0		
		0.0 18	12		0.0 07			0.0 05		0.0		0.0 01		14	0.0	4	0.0 09	39		0.0 82		71	0.0	- 0.0 45	0.0	0.0	0.0	0.0	0.0	0.0	0.0	- 0.0 11	0.0	0.2	0.0 94	0.0 34	0.0 09	0.0		0.0 07		41		0.1 56			
48	0.0 89	0.0	0.0	- 0.1 07	0.0	51	- 0.1 33	0.0	0.0 08	0.0	0.1 24	0.0	- 0.0 52	0.0	0.0 75	0.078	0.0	0.0	0.1 37	0.0	0.0 68	0.0	- 0.0 73	0.0	0.0 53	0.0	0.0	- 0.2 95	0.0 22	0.0 24	- 0.0 33	0.0	0.0 43	0.0	0.0	0.0		- 0.0 27	0.0 46	0.0	- 0.1 22	0.0	0.5 47	0.0	0.0	0.7	1.0

3.2. Presentation of bond order:



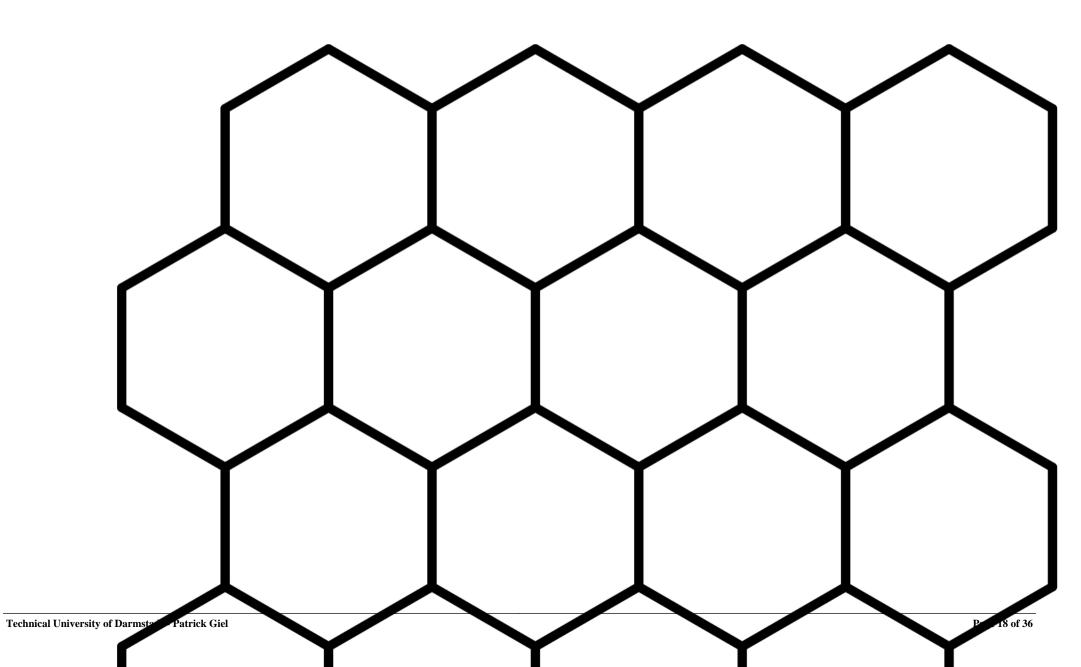
4. Net Charge

4.1. Calculated values:



	1	2	2 3	. 4	4	5	6	7	8	9	10	11	1 1	2 1	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:

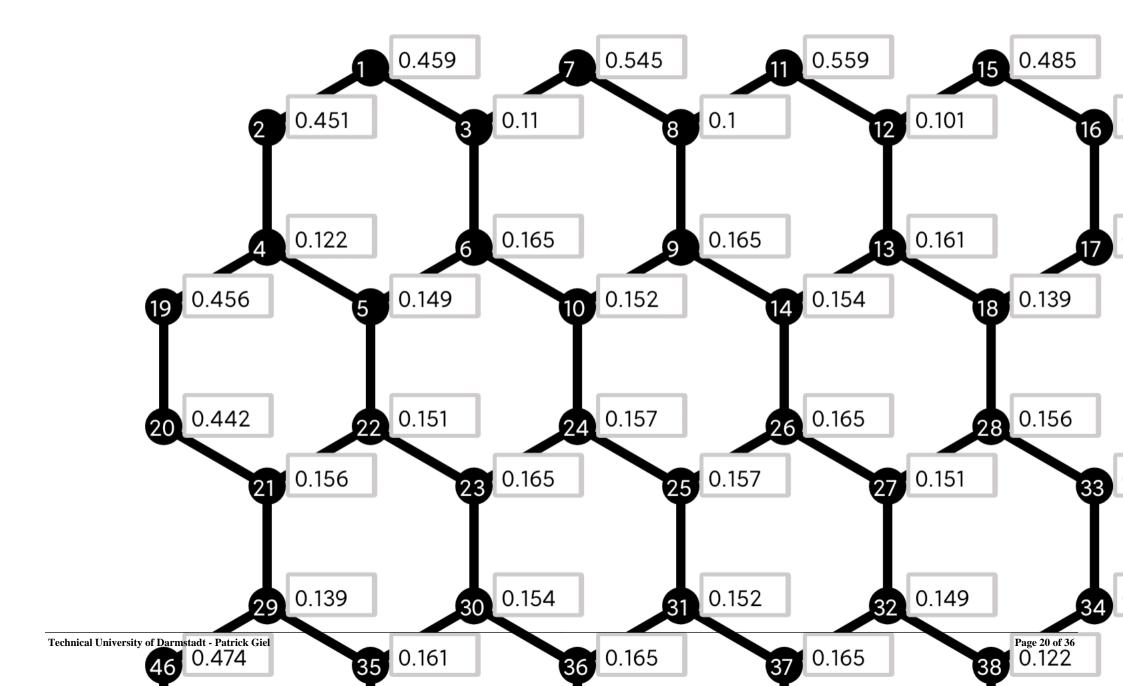


5. Free valences

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
0.4 59 5	0.4	0.1 1	0.1 22	0.1 49	0.1 65	0.5 45	0.1	0.1 65	0.1 52	0.5 59	0.1 01	0.1 61	0.1 54	0.4 85	0.3 96	0.4 74	V	0.4 56	v	0.1 0	.1 1	0.1	0.1 57	0.1 57	0.1 65	0.1 51	0.1 56	0.1 39	0.1 54	0.1 52	0.1 49	0.4 42	0.4 56	0.1 61	0.1 65	· · ·	0.1 22	0.4 51	0.1 1	0.4 59	0.1	0.5 45	0.1 01	0.5 59	0.4 74	0.3 96	0.4 85

5.2. Presentation of molecule:



6. Atom-Atom-Polarizability

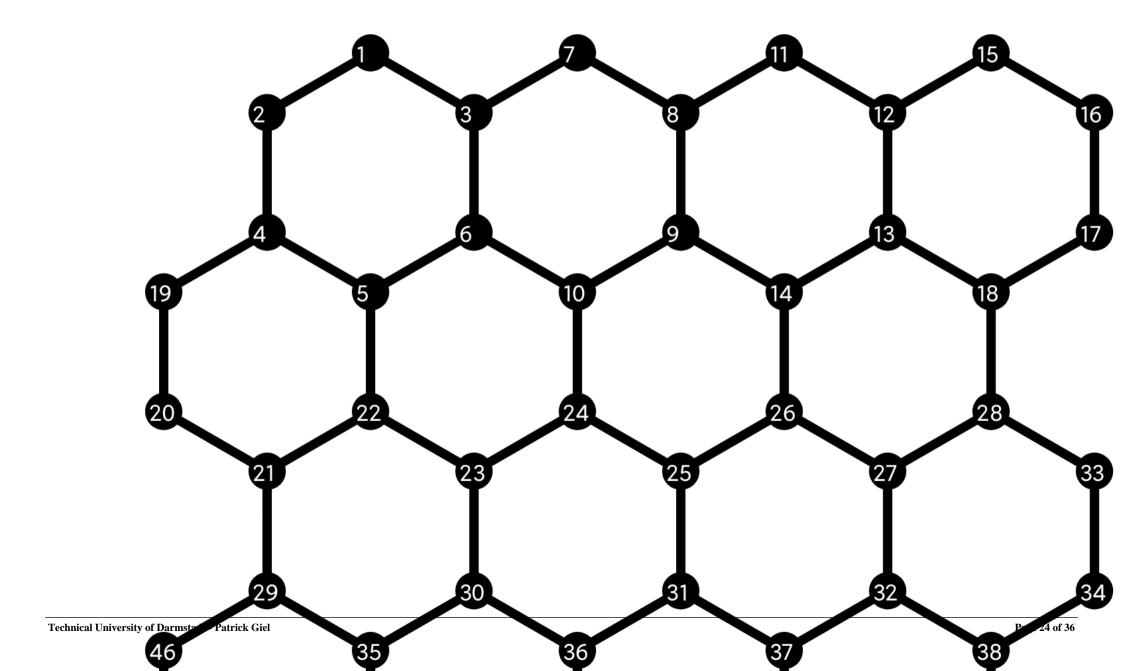
6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13	3 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		0.4 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																																				
13	0.0 05	- 0.0 07	- 0.0 11	0.0	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	3																																		
14	-0.0 -0.0	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	0.0 86	0.3	3																																	
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	0.0 11	0.5																																	
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	$\begin{vmatrix} 0.0\\08 \end{vmatrix}$	0.0 43	0.0	0.1	0.3 98																																

	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
		04	06		02			14		01		45		- 0.0 13		32																																
18	- 0.0 01	0.0	0.0	0.0	0.0	- 0.0 01	- 0.0 03	0.0 01	- 0.0 08	0.0	- 0.0 13	0.0	- 0.0 83	0.0 08	- 0.0 93	0.0	- 0.1 42	0.3 51																														
19	- 0.0 53	0.0 28	0.0 06	- 0.1 1	0.0 05	0.0 03	- 0.0 64	0.0 01	- 0.0 04	0.0 01	- 0.0 38	0.0	- 0.0 09	0.0	- 0.0 11	0.0	- 0.0 11	0.0 01	0.4 52																													
20	0.0 04	- 0.0 14	- 0.0 09	0.0 16	- 0.0 47	0.0 07	0.0 13	- 0.0 04	0.0	- 0.0 09	0.0 14	- 0.0 01	0.0 01	- 0.0 01	0.0 06	0.0	0.0 05	0.0	- 0.1 8	0.4 35																												
21	0.0	0.0	0.0 02	- 0.0	0.0 04	- 0.0 03	- 0.0 54	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.3 72																											
22	0.0 02	- 0.0 02	0.0 03	0.0 04	- 0.0 76	0.0 07	0.0	- 0.0 03	0.0 03	- 0.0 22	0.0 01	- 0.0 02	0.0	0.0 05 0.0	0.0 01	- 0.0 01	0.0 01	- 0.0 01	- 0.0 56	0.0 06	- 0.0 92	0.3 54																										
	0.0	02	04	0.0	06	52	62		0.0	108	58		0.0	05	0.0	01	0.0	01	09	0.0	14	72	/5																									
24	0.0 02	- 0.0 02	- 0.0 01	0.0 04	- 0.0 25	0.0 09	0.0 14	- 0.0 01	0.0 06	- 0.0 66	0.0 08	- 0.0 02	0.0 04	- 0.0 23	0.0	- 0.0 03	0.0 04	- 0.0 05	- 0.0 12	0.0 01	- 0.0 11	0.0 05	- 0.0 99	0.3 61																								
25	- 0.0 01	0.0	0.0	- 0.0 01	0.0 02	0.0 02	- 0.0 05	0.0	- 0.0 42	0.0	- 0.0 32	0.0	- 0.0 03	0.0	- 0.0 18	0.0 01	- 0.0 19	0.0	0.0 01	- 0.0 01	0.0 01	0.0 03	0.0 08	- 0.0 76	0.3 61																							
26	0.0 02	- 0.0 02	- 0.0 02	0.0 03	- 0.0 07	0.0 09	0.0 16	- 0.0 01	0.0 09	- 0.0 25	0.0 35	- 0.0 02	0.0	- 0.0 66	0.0 15	- 0.0 05	0.0 21	- 0.0 17	- 0.0 03	0.0 03	- 0.0 03	0.0	- 0.0 13	0.0 08	- 0.0 99	0.3 75																						
27	- 0.0 01	0.0	0.0	- 0.0 01	0.0	- 0.0 03	- 0.0 06	0.0	- 0.0 01	0.0	- 0.0 09	0.0	- 0.0 3	0.0 06	- 0.0 05	0.0	- 0.0 06	0.0 04	0.0	- 0.0 01	0.0 01	0.0	0.0	- 0.0 03	0.0 05	- 0.0 72	0.3 54																					
	01	0.0	0.0	01	0.0	04	08	0.0	05	0.0	19		04	0.0	21	0.0	33	0.0	0.0	01	0.0	01	0.0	01	0.0	14	- 0.0 92	0.3 72																				
29	0.0 02	- 0.0 02	0.0 01	0.0 05	0.0	0.0 01	0.0 05	0.0	0.0	- 0.0 01	0.0 05	0.0	0.0 01	- 0.0 01	0.0 02	0.0	0.0 02	0.0	- 0.0 08	0.0 15	- 0.0 42	0.0 04	- 0.0 17	0.0 03	- 0.0 05	0.0 01	- 0.0 01	0.0	0.3 51	0.3																		
30	0.0 01	- 0.0 02	0.0 02	0.0 01	- 0.0 02	0.0 05	0.0 07	0.0	0.0	- 0.0 01	0.0	0.0	0.0 01	- 0.0 03	0.0 04	0.0	0.0 05	- 0.0 01	- 0.0 09	0.0 06	- 0.0 18	0.0 06	- 0.0 66	0.0 07	- 0.0 23	0.0 05	- 0.0 05	0.0 02	0.0 08	0.3 59																		
31	0.0	0.0	- 0.0 01	0.0	- 0.0 03	0.0 01	0.0 01	- 0.0 01	0.0	- 0.0 01	0.0 04	0.0	0.0	- 0.0 01	0.0	0.0	0.0	- 0.0 01	- 0.0 05	0.0 01	- 0.0 06	0.0	- 0.0 25	0.0 05	- 0.0 66	0.0 08	- 0.0 22	0.0 04	0.0	0.0 07	0.3 56																	
32	0.0	0.0	0.0	0.0	- 0.0 02	0.0	0.0 01	0.0	0.0	- 0.0 03	0.0 01	0.0	0.0 02	- 0.0 02	0.0	0.0	0.0	0.0	- 0.0 01	0.0	- 0.0 01	0.0	- 0.0 07	0.0 02	- 0.0 25	0.0 06	- 0.0 76	0.0 04	0.0	0.0	0.0 06	0.3																
33	- 0.0 02	0.0 01	0.0 01	- 0.0 02	0.0	0.0 05	- 0.0 11	0.0	- 0.0 07	0.0	- 0.0 32	0.0	- 0.0 04	0.0 06	- 0.0 4	0.0	- 0.0 46	0.0 15	0.0 01	- 0.0 02	0.0 01	- 0.0 01	0.0 03	0.0 01	0.0 01	- 0.0 06	0.0 06	- 0.1 18	0.0	- 0.0 01	- 0.0 09	- 0.0 47	0.4 35															

	1	2	3	4	5	6	7	8	9	10	11	12		_	15	16	17 1	8 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 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	- 0.0 02	3 0 0	.0 8 01	0.0	0.0 01	0.0	- 0.0 03	0.0 01	- 0.0 12		- 0.0 56	0.0 23	0.0 01	0.0	0.0 01	05	0.1 8	0.4 52														
35	0.0 03	0.0		- 0.0 04			- 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	0.0	0.0 04	04	0.0	0.0	0.0 03		- 0.0 11	0.0	0.0	0.0 83	- 0.0 86	0.0	0.0	01		0.3 65													
36	- 0.0 05		0.0 01		0.0	- 0.0 08	0.0	0.0		0.0	- 0.0 06	0.0	- 0.0 05		- 0.0 01		0.0	0.0	0.0	05	0.0	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	0.0	- 0.0 04	0.0 05	0.3 67												
37	- 0.0 04	0.0 01	0.0 01		0.0	0.0	- 0.0 28	0.0	- 0.0 08	0.0 01	- 0.0 6	0.0	- 0.0 13	0.0 05	0.0	0.0	0.0	0.0	0.0 0.0 0.5	04	0.0	0.0 09	- 0.0 02	0.0 09	- 0.0 52	0.0 07	- 0.0	0.0	_	- 0.0	- 0.0	0.0 07	- 0.0 03	0.0	0.0	0.3 73											
38	- 0.0 01	0.0		- 0.0 01		- 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 03	0.0 0	0.0	0.0	0.0	0.0	0.0 03	- 0.0 01		- 0.0 05		- 0.0 61	0.0	- 0.0 01	- 0.0 07	- 0.0 79	0.0 16	- 0.1 1	0.0		0.0 09											
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	05	0.0	6 0	.0 0.0 2 01	0 0 1	0.0 01	0.0	- 0.0 02	0.0	- 0.0 02	0.0 02	- 0.0 02	1	0.0	0.0 01	0.0 04	05	- 0.0 14	0.0 28	0.0 07	0.0 17	- 0.0 37	0.0	0.4 43									
40	0.0	0.0	0.0	0.0		0.0 01		0.0		- 0.0 01	0.0 04	0.0		- 0.0 02	02	0.0	3 0	.0 0.0 1 01	0 01	0.0 01)	- 0.0 02		- 0.0 01	04	0.0 03	02	0.0	0.0 02	0.0 05	04	- 0.0 09		0.0 11			0.0	0.0	0.3 36								
41	- 0.0 01		0.0	- 0.0 01		- 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 0	0.0	0.0	0.0	0.0 01	0.0	- 0.0 01	0.0 02	- 0.0 05	0.0 02	0.0	- 0.0 01	- 0.0 02	- 0.0 05	0.0	0.0	_	0.0	0.0	0.0	0.0	- 0.2 73	- 0.0 62	0.4 59							
42	0.0	0.0	0.0	0.0	0.0	0.0	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 02	- 0.0 01	0.0	0.0 03	0.0	0.0 01	0.0 04	0.0 04	01	- 0.0 04		0.0			- 0.0 05	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	- 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	0.0 0	0.0	0.0	0.0	0.0 06	0.0 16	- 0.0 05	0.0 14	- 0.0 62	0.0	0.0	- 0.0 03	- 0.0 12	- 0.0 81	0.0	0.0	0.0	0.0	07 :	33	26	- 0.0 75	0.1		- 0.0 9	0.6 41					
44																0.0					01	0.0	0.0	0.0	0.0	0.0		03	0.0 05	01		0.0	0.0	0.0			0.0	0.0		0.0		0.0					
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	- 0.2 25	0.0	- 0.0 23	0.0	0.1 05	0.0 -	0.1 0	.0 5 0.0 14	0.0	0.0	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	- 0.0 38	0.0	0.0	0.0 38	0.0	0.0 22	0.0 32	0.0 27	- 0.1 16	0.1 65	- 0.1 06	0.7			
46	0.0 31	06	0.0 03	0.0 35		0.0	0.0 97		0.0 01		0.1 07	0.0	- 0.0 14	0.0 05	- 0.0 44	0.0 01 4	0 0 0 0 5	0.0	0.0 46	0.0	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	- 0.0 11	0.0 14	0.0	0.0	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		
47	0.0	0.0	0.0	0.0	0.0	0.0	01			0.0	0.0 02	0.0	0.0	0.0	0.0 01	0.0	1	0.0	02	0.0 0.5)	- 0.0 05	0.0 01	- 0.0 03		0.0 01		1	03			0.0		0.0 43	o o To	0.0		0.0	0.0	0.0				0.0 28		0.3 98	
48	0.0	0.0 05		0.0 34	0.0		- 0.0 95	0.0	- 0.0 01	0.0	0.1 05	0.0	- 0.0 14	0.0 04	- 0.0 44	0.0 01 04	0.0 0	0.0	0.0	0.0	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	0.0 02	0.0 03	0.0	- 0.0 11	0.0 07	0.0	0.0 15	07	0.0	- 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. Bond-Atom-Polarizability

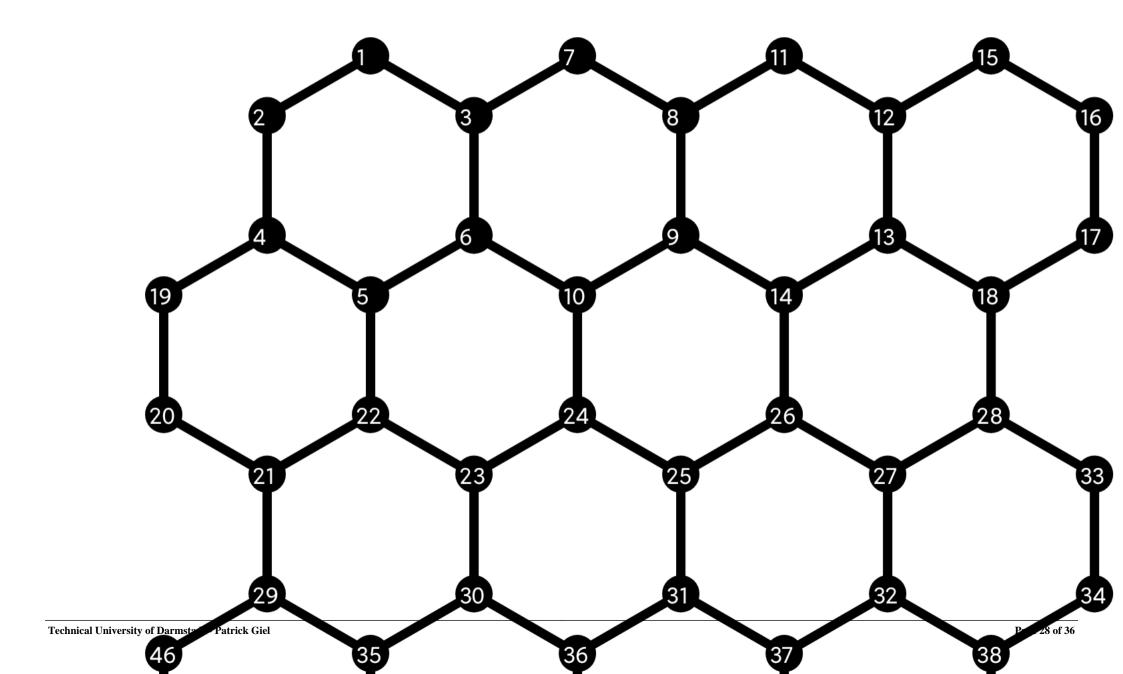
7.1. Calculated values:

	1	2	2 3	3	4	5	6	7	8	9	10	11	12	2 1	3 14	1 1:	5 1	6 1	18	19	20) 2	1 2	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 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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	0.0	0.0	0 0.	.0 0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.	0.0	0.0	0.	0.0	0.0	0.0	0.0	0.	0 0	.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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	0.0	0.0	0 0.	.0 0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.	0.0	0.0	0.	0.0	0.0	0.0	0.0	0.	0 0	.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
56	0.0	0.0	0 0.	.0 0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.	0.0	0.0	0.	0.0	0.0	0.0	0.0	0.	0 0	.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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 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
6 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
78	0.0	0.0	0 0.	.0 0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.	0.0	0.0	0.	0.0	0.0	0.0	0.0	0.	0 0	.0 (0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
89	0.0	0.0	0 0.	.0 0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.	0.0	0.0	0.	0.0	0.0	0.0	0.0	0.	0 0	.0 (0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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 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
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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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
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
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
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
21 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
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
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
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
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
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
25 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
26 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
31 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
27																																																10.0
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
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
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
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
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
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
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
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
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
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
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
38	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
34	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	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											1																					1									<u> </u>	<u>Щ</u>	<u>Щ</u>	<u>Щ</u>	<u>Щ</u>	丄	<u></u>	

	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
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
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
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
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
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
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
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
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
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
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
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
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

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3	2 4	3 6	3 7	4 5	4 1 9	5 6	5 2 2	6 2	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 0	2 0 2 1	2 1 2 2	2 1 2 9	2 2 2 3	2 3 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 3 5	3 0 3 6	3 1 3 6	3 1 3 7	3 2 2 3 7 3	3 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	3 3 4	3 3 4 5 3 4 8 4	3 3 5 6 4 4 1 2	3 3 7 4 4 6 6	3 3 7 8 4 3 9	3 3 3 4 9 1	3 4 9 (0 4 4 1 1	1 4 0 0 1 4 1 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
1 2	0. 1 7 7																																																													
1	-	0. 3 2 5																																																												
2 4	0. 1 8 4	0. 0 8 4	0. 3 2 6																																																											
3 6	0. 0 4 5	- 0. 0 8 7	0. 0 1 5	0. 2 8 9																																																										
3 7	6	0. 1 5 6	0	0. 1 4	0. 2 7 1																																																									
4 5	0. 0 5 5	0. 0 2	0. 1 0 2	3	0. 0 0 0 9	0. 2 7 1																																																								
4 1 9		0. 0 3 7	0. 1 4 1	0. 0 1 1	0. 0 3 5	0. 1 2 5	0. 2 8 4																																																							
5 6		0. 0 5 1	0. 0 5	- 0. 1	0. 0 1	- 0. 1 1 7	0. 0 1 5	0. 2 7 5																																																						
5 2 2	0. 0 0 2	0. 0 1 4	0. 0 0 1	0. 0 1 9	0. 0 0 0	0. 1 0 6	0. 0 6 6	- (0) 1 (1) 1 (2)). 2 7 7																																																					

	1 2	1 1	1 2 4	3 6	3 7	4 5	4 1 9	5 6	5 2 2	6 7 8	7 8	8 8	3 9 1 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 0	2 0 2 1	2 1 2 2	2 1 2 9	2 2 2 2 3 4	2 2 3 3 2 3 4 (2 2 3 4 3 2 5 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 3 9 0 4 3 6 5	3 0 3 6	3 1 3 6	3 1 3 7	3 2 3 7	3 2 3 8	3 3 3 4 3 4	3 3 4 5 3 4 3 4	3 6 4 2	3 7 4 0	3 8 3 9	3 9 4 1	4 0 4 1	4 4 0 2 4 4 3 3	4 2 4 5	4 4 4 5	4 4 4 8	4 6 4 7	4 7 4 8
1	0. 0 0 0 6	 0 0 0 2	0. 0. 0. 0. 0. 2	0. 1 0 7	0. 0 6 7	0. 0 2 7	0. 0 0 1	- (0. (1. 2. 2. 1.	0. 0 0 2 4 7 3 7).																																																
8	0. 0. 0. 2. 5	. 0047	0. 0 2 1	0. 0 6 4	5		0. 0 1 8	- (0 0. (0 0 (0 0 1 8) 0 0 0 0 1 3	0 3 2 2).																																															
9	0. 0 1 1	 0 0 1 7	- 0. 0. 0 0 0	0. 0 1 6	0. 0 5 1		\vdash	2). 0 0 0 4 5 6) 0 0 1 0 5 0 5	8																																															
1	. 0		0. 0. 0 1	0. 0 3 1	0. 0 6 2	0. 0 0 0 8	0. 0 1 2	0. 0 1 4 4). 0 0 0 0 0 1 2). 0 0 1 8 2	0. 0 1 1 8 8	0. 3 0 3	-																																													
1	0. 0. 0. 0. 0. 4	0	0. 0 1 1	0. 0 5 1	0. 0 3 8	0. 0 0 0 5	0. 0 0 0 5	0. 0 2 5). 0) 1 1 2 3 3	0 0 5 9	0 1	. 0. 0 0 4	. 0. 2 7 3																																													
9 1 4	0. 0. 0. 0. 0.	. 0 0 0 3	0 0. 0. 0 0 0 2	0. 0 1 7			_	6	0. 0 0 0 2 2 5 9	0.000		0. 0 6 4	 0. 1 2 6	0. 2 7 4																																												
1 (2 4	0. 0. 0. 0. 0. 2.	1	0. 0 0 0 5	0. 0 1 2	- 0. 0 0 9	0. 0 1 6	0. 0 0 7	0. 0 5 1). 0) 1 1 1 3 1	. 3	0 0 1 4	0.0000000000000000000000000000000000000	 0. 1 0 9	0. 0 4 9	0. 2 9 3																																											
1 1 1 2	0. 0. 0. 0. 4	0 6	0. 0 0 0 4	0. 0 1 4	0. 0 2 2	lo.	0. 0 0 0 5	- 10	0. 0 0 0 0 0 3 2). 0 0 0 5 5	0 0 5 6	 0. 1 6 3		0 3 5	3	0. 3 1 1																																										
1 2 1 3	0.0000000000000000000000000000000000000	 0 0 0 4	0. 0. 0 0 0 0 2	0. 0 0 0 8	0. 0 1 2	0. 0 0 0	0. 0 0 3	0. 0 0 2). 0 0 0 5) 0 0 0 0 2 4	0. 0 0 0 1 1 7	0. 0 5 8	3	0. 0 4 6	0. 0 0 6	- 0. 1 2 8	0. 2 7 7																																									
1 2 1 5	0.0000000000000000000000000000000000000	000000000000000000000000000000000000000	0. 0. 0 0 0 1	0. 0 0 0 5	0. 0 0 8	0. 0 0 0 2	0. 0 0 2	0. 0 0 0 5). - 0. 0 0 0 0 0 2 4	0. 0 0 0 0 2 1 1	0 0 0 2 3	0. 0 5 4	. 0. 0 0 6	0. 0 0 3	0.	- 0. 1 7	0. 0 9 8	0. 3 0 6																																								

	1 2	1 3	2 4	3 6	3 7	4 4 1 9	1 5 1 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 0	2 0 2 1	2 1 2 2	2 1 2 9	2 2 2 3	2 3 2 4	2 3 3 0	2 4 2 5	2 2 5 2 6 3	2 2 5 6 3 2 1 7	2 2	2 2 7 2 3 8 3 3 3 3 3 3 3 3	2 2 7 8 3 3 2 3	2 2 9 3 5 5	2 9 4 6	3 0 3 5	3 0 3 6	3 1 3 6	3 1 3 7	3 3 2 2 3 3 7 8	3 3 3 3 4	3 3 3 4 3 3 4 8	3 3 1 5 3 4 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 2 4 4 2 5 5	1 4 1 4 1 4 5 8	4 6 4 7	4 7 4 8
1 3 1 4	0. 0 0 1	0. 0 0 0 2	0. 0	0 0 (0 7 (- (C) (C) (C) (C) (C)	0. 0	 0. 0 0	0. 0 0 1	- 0. 0 0 5	0. 0 0 1	0. 0 4 9	- 0. 0 3 6	0. 0 2 6	-	_	0.	-	_	0. 2 7 6																																								
1 3 1 8	0. 0 0 1	0. 0 0 2	0. 0 0 1	0. 0 0 0 0 1	- (C) (C) (C) (C) (C) (C) (C)) 0 0 0 0 1		_	0. 0 0 1	0	0. 0 1 6	0. 0 0 4	0. 0 0 8	0. 0 3	0. 0 0 6	_		0. 0 6 9		0. 2 7 5																																							
1 4 2 6	0.	0.	0. 0 0 2	0. - 0 0 7 0). (C)). 0 0 0 0 0 1	. 0. 0 0 7	0. 0 0 0 6	0. 0 1 8	0. 0 0 2	0. 0 1 1	0. 0 1	0. 0 5 2	0. 1 1 3	0	0. 0 2	0. 0 1 9	0. 0 0 6	0. 1 1	0. 0 4 4	0.																																						
1 5 1 6	0.	0. 0 0 1	0. 0	0 0 (0 3 (3	- (CO) (CO) (CO) (CO) (CO) (CO) (CO) (CO)) 0 0 0 0 0 1	. 0. 0. 0 0 2	0. 0 0 2	0. 0 0 2	0. 0 0 8	0. 0 1 4	0. 0 2 2	0. 0 0 0 3	0. 0 0 0 3	0.	0. 0 6 2	0. 0 6	0. 1 7 7	0. 0 1 1	0. 0 5 7	0. 0 0 8	0. 2 4 8																																					
1 6 1 7	0.	0. 0 0 1	0.	- (0 0 (0 0 (3 3	O O.	0 0 0 0 1	. 0.00000000000000000000000000000000000	0. 0 0 1	0. 0 0 2	0. 0 0 7			0. 0 0 1			0. 0 4 8	0.035	0. 1 0 8	0. 0 2 4	0. 0 8 5	0. 0 1 3	0. 2 3 8	0. 3 0 2																																				
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4 7 4 8	0. 0 0 4	0	0. 0 0 0 4	0. 0	0 0 0. 0 0 4 0 2	0. 0 0 8	0	0. (0 0 (0 1		. 0		0.		0. 0 0 2		0. 0). 0 0 0 2	0.	0. 0 0 2		- (0 0. (0 0 (0 0 2) 0 0 0 0 2 0 1	. 0. 0 1 1	0. 0 1 5	0. 0 0 5	0. 0 0 0 2 0 9 5			0.	0. 0. 0 0 5	0. 0 0 0 3		0 0 0 0 0 2 0 1	- 0. 0 5 7	0. 1 1 8	0 0 0 1 0 1 0 3	0. 0 0 0 3	0	- 0 0. 0 0 0 0 1 2	. 0. 0 0 1	- 0. 0 0 1	0. 0 0 0 6 1 4		0. 0	0. 0	0 0 (0 0 (1 1 (3	0 (0. 0 2 2	0. 0 6 2	0. 0. 1 2 7 3 7 8	0. 2 4 8

8.2. Presentation of molecule:

