Tables of the Topological Characteristics of Polyhexes (Condensed Aromatic Hydrocarbons)

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Characterization of the honeycomb or polyhex networks is of particular interest, not only from the view points of graph and combinatorial theories,[1,2] but also from those of chemistry and physics.[3,4] That is to say, the carbon atom skeleton of a cata-condensed aromatic hydrocarbon molecule is nothing else but a polyhex and the stability of this class of molecules is sensitively dependent on the topology of the polyhex network through the wavemechanics of the π-electron, or free electron, delocalizing over the molecular skeleton.[5]

A number of trials have been made to characterize the topology of the molecule and to clarify the relation between the structure and stability.[5-11] In this paper effort was made to list up as many parameters or indices as possible for characterizing the topology of the polyhex.

Polyhexes are classified into catafusene and perifusene according to the structure of the " ring-incidence graph ", which is derived from the original graph by connecting the centers of the hexagons; the ring-incidence graphs of catafusene and perifusene are respectively tree and non-tree.[4]

Explanation of the Tables

No. To each polyhex is given a set of numbers $n_1 A n_2 n_3$. Integer n_1 (≤ 6) is the number of hexagons, A is C (catafusene) or P (perifusene), and n_2 (one figure) represents the number of the points at which three hexagons meet. Note that the parity of n_2 is that of the graph with respect to the number of points. All the polyhexes are classified with a set of numbers $n_1 A n_2$, which is arranged alpha-numerically. The entries within the same group are numbered (n_3) according to the magnitudes of the parameters k, $\#K$, and $\tilde{Z}$ with this order of priority.

Balaban. For catafusenes a shorthand notation by Balaban is given.[11]

k, the number of kinks. Although a " kink " is originally defined for catafusenes as a corner of the ring-incidence graph,[12] in this paper

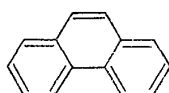k is defined as the number of biphenyl structures.[13]
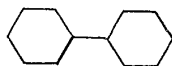
Thus, as shown in Fig. 1, the values of k for 3C0002 (phenanthrene), 4P2001 (pyrene), and 5P2001 (perylene) are respectively 1, 1, and 2.

Fig. 1.

$\#K$, the number of Kekulé structures. For a graph of even parity one can choose $\#K$ different sets of m lines so as to span all the points in the graph as in

which is called as a Kekulé structure by chemists. In what follows m is defined as $[N/2]$, N being the number of points, irrespective of the parity of the graph. In the graph theory $\#K$ is the number of maximum matching. For a graph of odd parity one point is left out in the maximum matching, whose number is given in parentheses.

$\#D$, *the number of Dewar structures.* A Dewar structure is exemplified as in
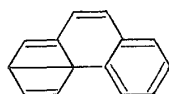
where $m-1$ lines span all the points in the graph except for a pair of non-neighbor points (designated by a long line). A bipartite graph,

or an alternant hydrocarbon, is a graph without an odd-membered ring. It is shown that $\#D$ is expressed as

$$\#D = p(G, \, m-1) - m \cdot p(G, \, m) \tag{1}$$

where $p(G, \, k)$ is the non-adjacent number, which will be explained later.[14]

B, *total benzene character*.[15,16] Let $G \ominus A$ is the subgraph of graph G obtained by deleting subgraph A and all the lines incident to A. The benzene number of a hexagon A is defined as the number of Kekulé structures for $G \ominus A$. The benzene number of ring A in 3C0002 is 2 as shown below.

The sum of the benzene numbers of all the hexagons is defined as B. For the above example $B = 2+1+2 = 5$.

Z, *topological index and $p(G, \, k)$, non-adjacent number*.[9] For graph G a non-adjacent number $p(G, \, k)$ is defined as the number of ways in which such k disconnected lines can be chosen from G. The sum of $p(G, \, k)$ for G is defined as the topological index Z.

$$Z = \sum_{k=0}^{m} p(G, \, k) \, . \tag{2}$$

$\tilde{Z}$, *stability index*.[10] The characteristic polynomial $P(X)$ of a graph is defined as

$$P(X) = (-1)^N \det |A - XE| \, , \tag{3}$$

$$= \sum_{k=0}^{m} a_k X^{N-k} \, , \tag{4}$$

where A is the adjacency matrix and E is the unit matrix of the same order as A. The sum of the absolute values of the coefficients a_{2k} appearing alternately in $P(X)$ is defined as $\tilde{Z}$,

$$\tilde{Z} = \sum_{k=0}^{m} |a_{2k}| \, . \tag{5}$$

E_{π}, *total π-electron energy*. If the roots $\{X_k\}$ of $P(X)$ are numbered according to the decreasing order,

$$X_1 > X_2 > X_3 \cdots > X_N \, ,$$

the double of the half sum of $\{X_k\}$ is defined as E_{π}

$$E_{\pi} = 2 \sum_{k=1}^{m} X_k \tag{6}$$

which gives the relative stability of the π-electron network of a conjugated hydrocarbon molecule.

$\varepsilon_{\text{HOMO}}$. For a bipartite graph the roots $\{X_k\}$ appear as pairs,[17]

$$X_k = - X_{N-k+1} .\qquad(7)$$

The smallest positive root of $P(X)$ is called as the energy of the highest occupied molecular orbital and abbreviated as $\varepsilon_{\text{HOMO}}$. In case $\varepsilon_{\text{HOMO}}$ is equal to zero, the second smallest positive root or the second highest occupied molecular orbital energy $\varepsilon_{\text{SOMO}}$ is given in parentheses.

In Table I all the above quantities except for a_{2k} and $p(G, k)$ are given, which are given in Tables II and III respectively. Analysis of these quantities will be reported elsewhere.

References

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Table I-1.

No.	Balaban	k	#K	#D	B	Z	$\tilde{Z}$	E_π	ε_{HOMO}
1C0001	--	0	2	3	1	18	20	8.0000	1.0000
2C0001	.	0	3	16	2	148	170	13.6832	0.6180
3C0001	0	0	4	48	3	1208	1440	19.3137	0.4142
3C0002	1	1	5	47	5	1233	1489	19.4483	0.6052
3P1001	--	0	(20)	--	-	754	896	17.8272	(1.0000)
4C0001	00	0	5	110	4	9854	12218	24.9308	0.2950
4C0002	01	1	7	112	8	10074	12638	25.1012	0.4523
4C0003	11	2	8	116	10	10244	12960	25.1875	0.5676
4C0004	12	2	8	117	10	10269	13009	25.1922	0.5201
4C0005	1(.)	3	9	117	13	10373	13357	25.2745	0.6840
4P1001	--	1	(36)	--	-	6258	7820	23.5818	(0.7182)
4P2001	--	1	6	87	6	3888	4810	22.5055	0.4450

1C0001

2C0001

3C0001

2

3P1001

4C0001

2

3

4

4P1001

4P2001

5
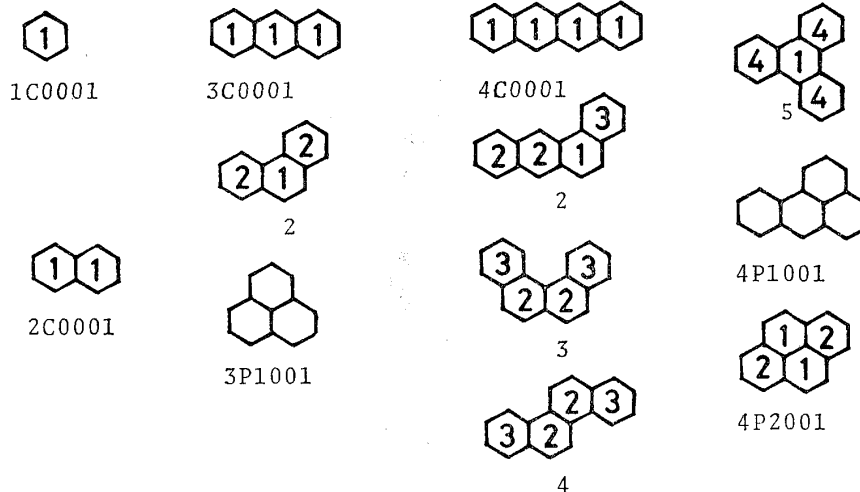
Table I-2.

No.	Balaban	k	#K	#D	B	Z	$\tilde{Z}$	E_π	ε_{HOMO}
5C0001	000	0	6	215	5	80378	103700	30.5401	0.2197
5C0002	001	1	9	231	11	82183	107221	30.7256	0.3271
5C0003	010	1	10	227	13	82314	107300	30.7627	0.4372
5C0004	011	2	11	243	15	83679	109981	30.8338	0.4186
5C0005	012	2	11	245	15	83899	110401	30.8390	0.4048
5C0006	101	2	12	247	18	83988	110840	30.8795	0.4918
5C0007	102	2	12	248	18	84013	110889	30.8805	0.4735
5C0008	111	3	13	257	20	85169	113005	30.9362	0.5355
5C0009	112	3	13	257	20	85314	113278	30.9386	0.5498
5C0010	01(.)	3	13	250	21	84815	113513	30.9418	0.4991
5C0011	121	3	13	259	20	85534	113698	30.9432	0.5019
5C0012	11(.)	4	14	266	23	86180	116040	30.9990	0.5319
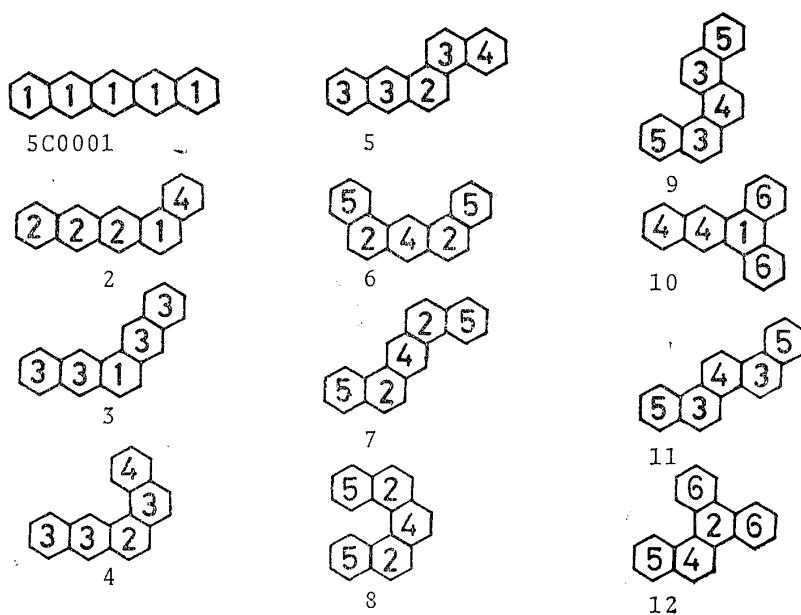
Table I-3.

No.	k	#K	#D	B	Z	$\tilde{Z}$	E_π	ε_{HOMO}
5P1001	1	(55)	--	-	51114	66424	29.2485	(0.5123)
5P1002	2	(60)	--	-	51792	67792	29.3027	(0.5576)
5P1003	2	(62)	--	-	51964	68062	29.3247	(0.6209)
5P1004	2	(64)	--	-	51982	68296	29.3368	(0.6548)
5P1005	2	(64)	--	-	51922	68310	29.3406	(0.7251)
5P1006	2	(65)	--	-	52204	68510	29.3478	(0.6894)
5P2001	2	9	199	12	32246	41904	28.2220	0.3711
5P2002	2	9	194	12	32604	42704	28.2453	0.3473
5P2003	3	11	198	16	32748	43072	28.3361	0.4970
5P3001	2	(52)	--	-	19822	25440	26.6964	(0.6622)

5P1001

2

3

4

5

6

5P2001

2

3

5P3001
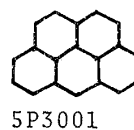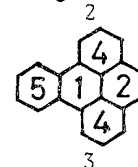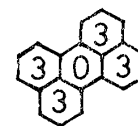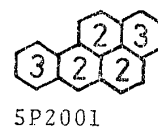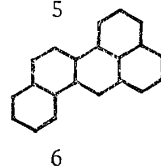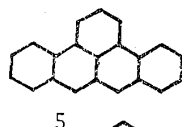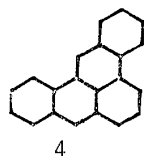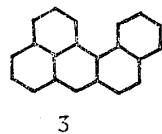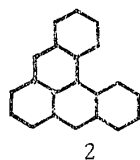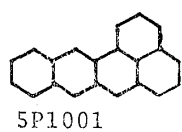
Table I-4.

No.	Balaban	k	#K	#D	B	Z	$\tilde{Z}$	E_π	ε_{HOMO}
6C0001	0000	0	7	378	6	655632	880178	36.1560	0.1694
6C0002	0001	1	11	428	14	670362	909998	36.3413	0.2436
6C0003	0010	1	13	422	18	671516	910358	36.3905	0.3358
6C0004	0011	2	14	459	20	682636	933136	36.4562	0.3071
6C0005	0012	2	14	462	20	684441	936657	36.4613	0.3033
6C0006	0110	2	15	458	22	683528	933338	36.4783	0.3602
6C0007	0120	2	15	462	22	685464	936938	36.4839	0.3482
6C0008	1001	2	16	476	26	685392	940896	36.5169	0.3607
6C0009	1002	2	16	477	26	685417	940945	36.5172	0.3584
6C0010	0101	2	17	472	28	686246	941018	36.5378	0.4484
6C0011	0102	2	17	474	28	686466	941438	36.5390	0.4287
6C0012	0111	3	18	495	30	695748	959056	36.5854	0.4200
6C0013	0112	3	18	494	30	696893	961317	36.5874	0.4322
6C0014	0122	3	18	495	30	697024	961396	36.5879	0.4194
6C0015	0121	3	18	498	30	698829	964917	36.5924	0.4129
6C0016	1011	3	19	508	33	697691	964727	36.6152	0.4505
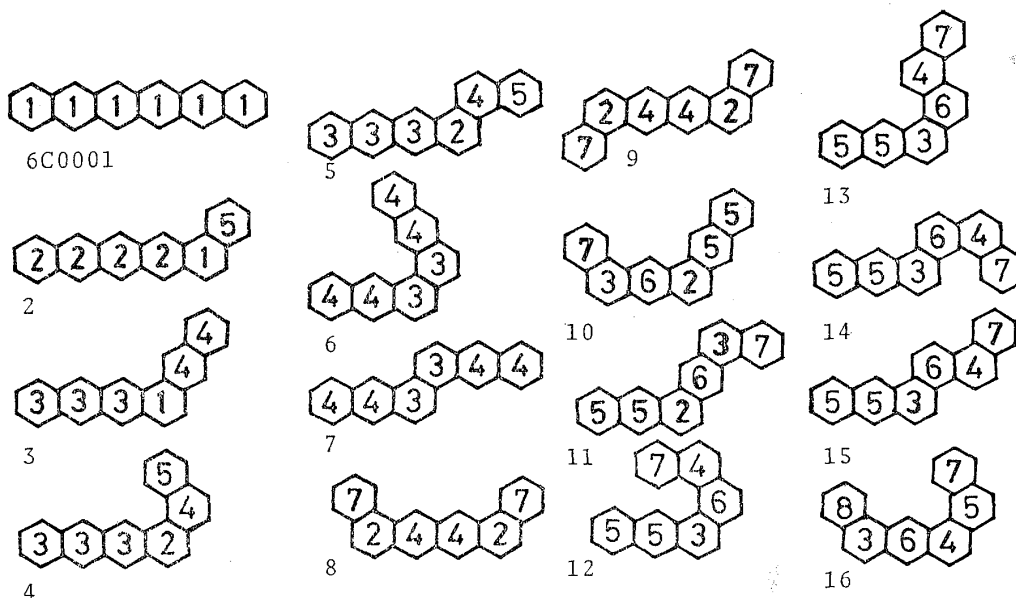
Table I-5.

No.	Balaban	k	#K	#D	B	Z	$\tilde{Z}$	E_π	ε_{HOMO}
6C0017	1022	3	19	508	33	697836	965000	36.6156	0.4507
6C0018	1012	3	19	510	33	699471	968297	36.6198	0.4378
6C0019	1021	3	19	512	33	699691	968717	36.6209	0.4286
6C0020	1111	4	21	532	38	707968	984872	36.6814	0.5463
6C0021	1122	4	21	532	38	708809	986393	36.6828	0.5393
6C0022	1112	4	21	534	38	709313	987623	36.6848	0.5022
6C0023	1121	4	21	534	38	710589	989963	36.6871	0.5066
6C0024	1221	4	21	534	38	710508	990080	36.6874	0.4985
6C0025	1212	4	21	538	38	712444	993680	36.6920	0.4714
6C0026	001(.)	3	17	484	29	691957	962933	36.5705	0.3557
6C0027	01(.)0	3	19	483	34	693532	964882	36.6142	0.5058
6C0028	011(.)	4	19	520	33	703969	984593	36.6406	0.3955
6C0029	01(.)2	4	20	520	36	704652	986064	36.6624	0.4451
6C0030	01(.)1	4	20	520	36	704517	986085	36.6624	0.4466
6C0031	101(.)	4	22	534	43	707147	995427	36.7149	0.5224
6C0032	12(.)1	5	22	554	41	716022	1008324	36.7280	0.5465
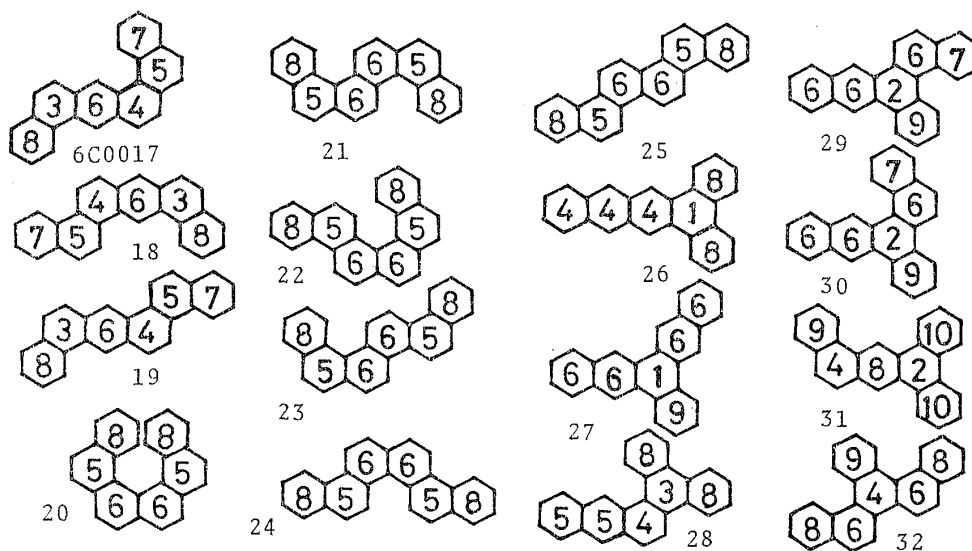
Table I-6.

No.	Balaban	k	#K	#D	B	Z	$\tilde{Z}$	E_π	ε_{HOMO}
6C0033	11(.)2	5	22	556	41	715962	1008492	36.7285	0.5041
6C0034	11(.)1	5	22	561	41	716477	1009885	36.7311	0.4706
6C0035	111(.)	5	23	555	45	716429	1012033	36.7525	0.5451
6C0036	1(.)12	5	23	556	45	717794	1014560	36.7551	0.5364
6C0037	1(.)1(.)	6	24	580	48	723432	1033792	36.7953	0.5115
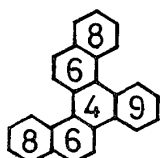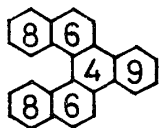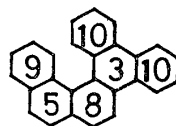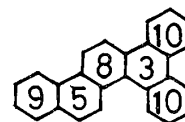
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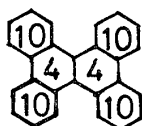
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Table I-7.

No.	k	#K	#D	B	Z	$\tilde{Z}$	E_π	ε_{HOMO}
6P1001	1	(77)	--	-	416974	563644	34.8868	(0.3769)
6P1002	2	(88)	--	-	422934	575676	34.9575	(0.4284)
6P1003	2	(91)	--	-	424454	577684	34.9789	(0.4567)
6P1004	2	(96)	--	-	424606	579996	34.9981	(0.4825)
6P1005	2	(97)	--	-	424604	580184	35.0044	(0.5041)
6P1006	2	(97)	--	-	424076	580304	35.0089	(0.5171)
6P1007	2	(97)	--	-	426566	581524	35.0063	(0.4873)
6P1008	2	(97)	--	-	426104	582460	35.0216	(0.5228)
6P1009	2	(100)	--	-	426344	582908	35.0292	(0.5509)
6P1010	3	(104)	--	-	430364	591104	35.0570	(0.5597)
6P1011	3	(104)	--	-	432734	594862	35.0746	(0.5523)
6P1012	3	(106)	--	-	430066	592676	35.0639	(0.5528)
6P1013	3	(107)	--	-	432124	593672	35.0783	(0.6394)
6P1014	3	(107)	--	-	433516	596168	35.0869	(0.6008)
6P1015	3	(108)	--	-	432034	594156	35.0739	(0.5798)
6P1016	3	(108)	--	-	431656	594416	35.0793	(0.6153)
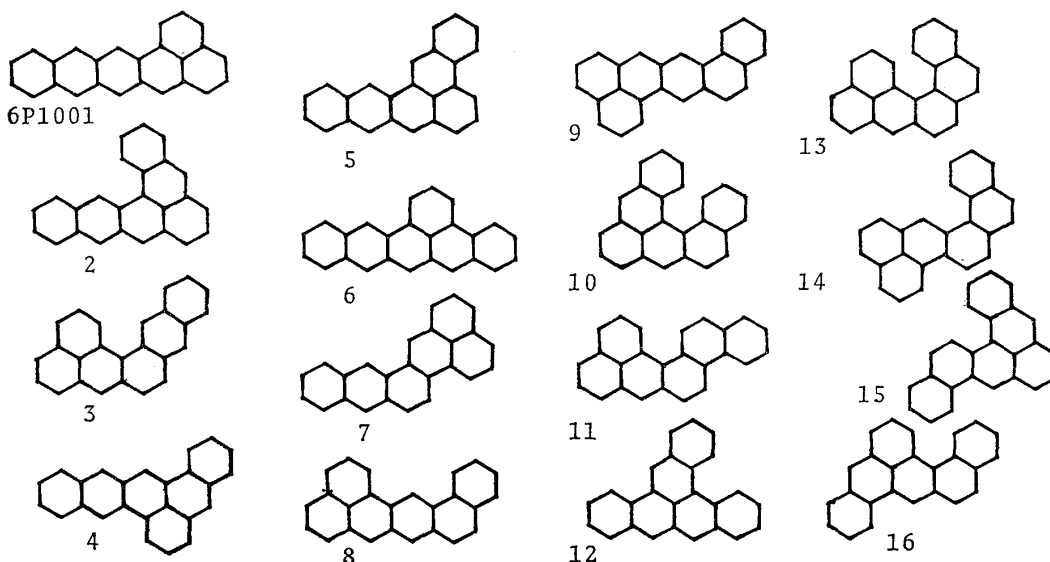
Table I-8.

No.	k	#K	#D	B	Z	$\tilde{Z}$	E_π	ε_{HOMO}
6P1017	3	(110)	--	-	431559	594387	35.0798	(0.6010)
6P1018	3	(110)	--	-	431151	594479	35.0823	(0.6127)
6P1019	3	(110)	--	-	434846	598702	35.0975	(0.5891)
6P1020	3	(112)	--	-	433516	597972	35.0967	(0.5981)
6P1021	3	(114)	--	-	432141	597037	35.0961	(0.6741)
6P1022	3	(115)	--	-	433629	598321	35.1033	(0.6732)
6P1023	3	(115)	--	-	433161	598427	35.1057	(0.6653)
6P1024	4	(117)	--	-	437810	610822	35.1522	(0.6893)
6P2001	2	0	390	0	263296	357192	33.4555	(0.7991)
6P2002	2	9	378	12	265600	361288	33.7981	0.1987
6P2003	2	12	386	16	263364	355890	33.8634	0.3026
6P2004	3	12	404	17	269664	369768	33.9165	0.2648
6P2005	3	13	418	18	267426	365026	33.9278	0.3027
6P2006	3	14	413	21	267476	365320	33.9541	0.3420
6P2007	3	15	410	23	267834	364920	33.9778	0.3965

6P1017   21   6P2001   5

18   22   2   6

19   23   3   7

20   24   4
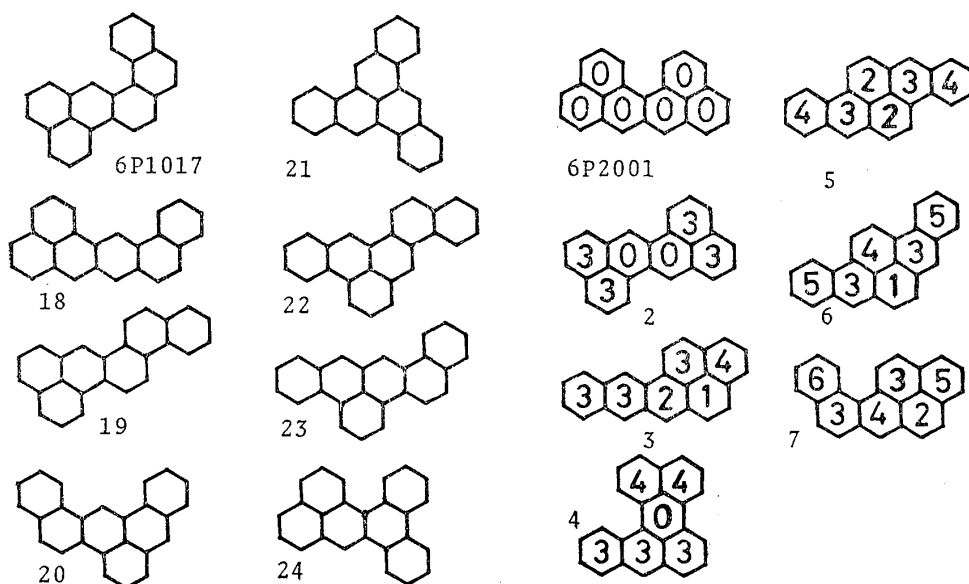
Table I-9.

No.	k	#K	#D	B	Z	$\tilde{Z}$	E_π	ε_{HOMO}
6P2008	3	15	420	23	268964	367090	33.9873	0.3698
6P2009	3	15	403	25	270814	373184	34.0070	0.3514
6P2010	3	16	388	26	267790	365994	34.0059	0.5053
6P2011	4	16	424	26	270928	373032	34.0307	0.3983
6P2012	4	17	415	28	272030	374282	34.0593	0.4400
6P2013	4	17	425	30	271798	375608	34.0646	0.4216
6P2014	5	20	436	38	275782	385866	34.1644	0.5550
6P3001	3	(87)	--	-	164344	221788	32.4373	(0.5618)
6P3002	3	(93)	--	-	164679	222285	32.4517	(0.6092)
6P3003	3	(102)	--	-	167692	228140	32.5095	(0.6180)
6P3004	4	(96)	--	-	166838	227456	32.5062	(0.6580)
6P4001	3	0	306	0	99964	132848	30.8098	(0.8632)
6P4002	3	10	304	12	101217	134885	31.2529	0.2910
6P4003	4	14	336	21	103774	139828	31.4251	0.4392

6P2008

12

9

13

10

11

14

6P3001

2

3

4

6P4001

2

3
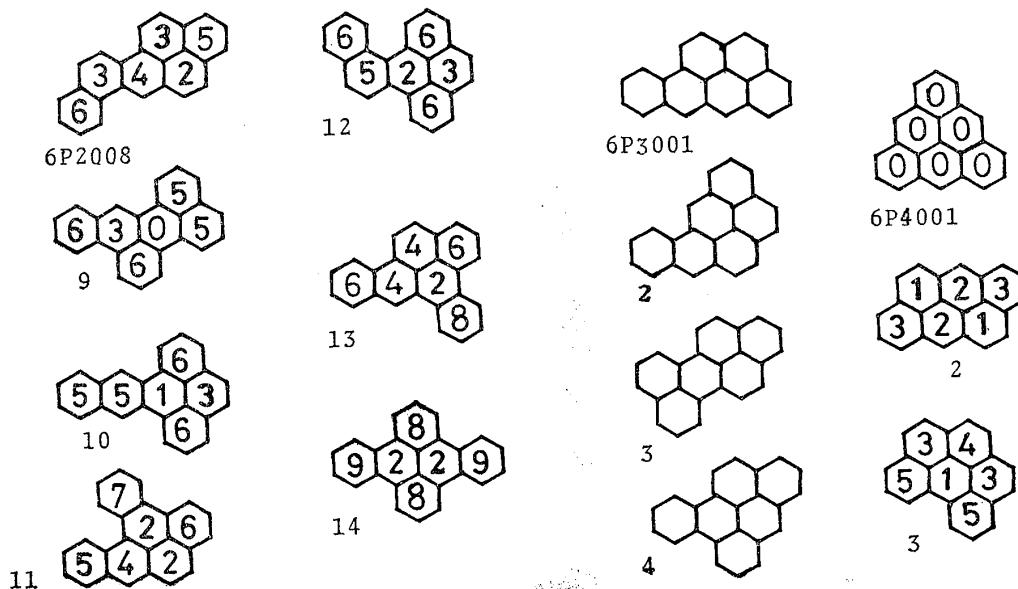
Table II-1.[a]

No.	6	4	2	0
1C0001	1	6	9	4

No.	10	8	6	4	2	0
2C0001	1	11	41	65	43	9

No.	14	12	10	8	6	4	2	0
3C0001	1	16	98	296	473	392	148	16
3C0002	1	16	98	297	479	407	166	25

No.	13	11	9	7	5	3	1
3P1001	1	15	84	226	309	207	54

[a] For 1C0001 one gets $P(X) = X^6 - 6X^4 + 9X^2 - 4$.

Table II-2.

No.	18	16	14	12	10	8	6	4	2	0
4C0001	1	21	180	822	2192	3510	3321	1731	415	25
4C0002	1	21	180	823	2203	3558	3430	1868	505	49
4C0003	1	21	180	824	2213	3599	3518	1972	568	64
4C0004	1	21	180	824	2214	3605	3533	1990	577	64
4C0005	1	21	180	825	2223	3645	3627	2106	648	81

No.	17	15	13	11	9	7	5	3	1
4P1001	1	20	161	681	1655	2367	1947	842	146

No.	16	14	12	10	8	6	4	2	0
4P2001	1	19	143	555	1208	1498	1017	333	36

Table II-3, 4.

No.	22	20	18	16	14	12	10	8	6	4	2	0
5C0001	1	26	287	1768	6725	16498	26429	27292	17399	6230	1009	36
5C0002	1	26	287	1769	6741	16603	26804	28094	18448	7037	1330	81
5C0003	1	26	287	1769	6741	16604	26809	28101	18451	7050	1361	100
5C0004	1	26	287	1770	6756	16697	27125	28746	19254	7630	1568	121
5C0005	1	26	287	1770	6757	16708	27173	28855	19391	7720	1592	121
5C0006	1	26	287	1770	6757	16708	27179	28898	19509	7874	1687	144
5C0007	1	26	287	1770	6757	16708	27180	28904	19524	7892	1696	144
5C0008	1	26	287	1771	6771	16791	27450	29427	20138	8318	1856	169
5C0009	1	26	287	1771	6772	16801	27490	29509	20227	8363	1862	169
5C0010	1	26	287	1771	6771	16796	27492	29556	20321	8438	1885	169
5C0011	1	26	287	1771	6773	16812	27538	29618	20364	8453	1886	169
5C0012	1	26	287	1772	6786	16889	27804	30177	21068	8960	2074	196

No.	21	19	17	15	13	11	9	7	5	3	1
5P1001	1	25	263	1530	5441	12334	17999	16617	9203	2706	305
5P1002	1	25	263	1531	5454	12408	18225	17013	9601	2919	352
5P1003	1	25	263	1531	5455	12414	18245	17064	9687	2997	380
5P1004	1	25	263	1531	5455	12418	18270	17126	9765	3048	394
5P1005	1	25	263	1531	5455	12417	18266	17122	9770	3060	400
5P1006	1	25	263	1531	5456	12425	18294	17178	9834	3096	407

No.	20	18	16	14	12	10	8	6	4	2	0
5P2001	1	24	240	1313	4337	8998	11802	9564	4491	1053	81
5P2002	1	24	240	1314	4350	9066	11985	9834	4695	1114	81
5P2003	1	24	240	1314	4350	9070	12009	9902	4815	1226	121

No.	19	17	15	13	11	9	7	5	3	1
5P3001	1	23	218	1116	3395	6355	7306	4962	1800	264

Table II-5, 6.

No.	26	24	22	20	18	16	14	12	10	8	6	4	2	0
6C0001	1	31	419	3259	16222	54366	125605	201175	221065	161875	74572	19334	2205	49
6C0002	1	31	419	3260	16243	54553	126541	204105	227063	169968	81585	22961	3147	121
6C0003	1	31	419	3260	16243	54554	126551	204140	227110	169976	81584	23049	3271	169
6C0004	1	31	419	3261	16263	54724	127366	206590	231931	176218	86741	25548	3847	196
6C0005	1	31	419	3261	16264	54740	127471	206965	232733	177267	87548	25869	3892	196
6C0006	1	31	419	3261	16263	54725	127375	206619	231966	176216	86724	25592	3921	225
6C0007	1	31	419	3261	16264	54741	127481	206999	232775	177268	87544	25944	3985	225
6C0008	1	31	419	3261	16264	54740	127478	207046	233115	178215	88874	26900	4296	256
6C0009	1	31	419	3261	16264	54740	127478	207046	233116	178221	88889	26918	4305	256
6C0010	1	31	419	3261	16264	54741	127487	207072	233130	178165	88815	26950	4393	289
6C0011	1	31	419	3261	16264	54741	127488	207083	233178	178274	88952	27040	4417	289
6C0012	1	31	419	3262	16283	54896	128204	209153	237073	183066	92709	28796	4839	324
6C0013	1	31	419	3262	16284	54911	128296	209458	237670	183760	93152	28913	4836	324
6C0014	1	31	419	3262	16284	54911	128297	209463	237677	183763	93165	28944	4855	324
6C0015	1	31	419	3262	16285	54927	128402	209838	238479	184812	93972	29265	4900	324
6C0016	1	31	419	3262	16284	54911	128303	209533	238004	184553	94221	29713	5131	361
6C0017	1	31	419	3262	16284	54911	128304	209543	238044	184635	94310	29758	5137	361
6C0018	1	31	419	3262	16285	54927	128408	209908	238807	185608	95043	30052	5185	361
6C0019	1	31	419	3262	16285	54927	128409	209919	238855	185717	95180	30142	5209	361

No.	26	24	22	20	18	16	14	12	10	8	6	4	2	0
6C0020	1	31	419	3263	16303	55067	129033	211687	242180	189918	98706	32030	5793	441
6C0021	1	31	419	3263	16304	55081	129114	211937	242622	190362	98939	32082	5797	441
6C0022	1	31	419	3263	16304	55082	129126	212002	242821	190720	99305	32273	5835	441
6C0023	1	31	419	3263	16305	55097	129219	212312	243425	191417	99761	32421	5851	441
6C0024	1	31	419	3263	16305	55097	129218	212308	243427	191447	99811	32453	5859	441
6C0025	1	31	419	3263	16306	55113	129324	212688	244236	192499	100631	32805	5923	441
6C0026	1	31	419	3262	16283	54900	128262	209473	237962	184404	93754	29108	4785	289
6C0027	1	31	419	3262	16283	54902	128280	209544	238133	184719	94233	29622	5092	361
6C0028	1	31	419	3263	16303	55071	129082	211908	242630	190242	98446	31421	5415	361
6C0029	1	31	419	3263	16303	55072	129091	211950	242762	190527	98854	31789	5602	400
6C0030	1	31	419	3263	16303	55072	129090	211945	242755	190531	98872	31801	5602	400
6C0031	1	31	419	3263	16304	55087	129200	212428	244094	192898	101491	33523	6204	484
6C0032	1	31	419	3264	16323	55242	129903	214368	247452	196508	103772	34265	6292	484
6C0033	1	31	419	3264	16323	55242	129902	214364	247453	196539	103838	34322	6310	484
6C0034	1	31	419	3264	16323	55243	129914	214429	247654	196915	104258	34577	6373	484
6C0035	1	31	419	3264	16323	55242	129912	214458	247829	197368	104914	35125	6618	529
6C0036	1	31	419	3264	16324	55257	130005	214770	248450	198115	105436	35314	6645	529
6C0037	1	31	419	3265	16342	55402	130690	216842	252557	203407	109731	37373	7156	576

Table II-7, 8.

No.	25	23	21	19	17	15	13	11	9	7	5	3	1
6P1001	1	30	390	2899	13696	43231	93234	137904	138032	90268	35920	7490	549
6P1002	1	30	390	2900	13714	43373	93867	139635	141028	93559	38148	8341	690
6P1003	1	30	390	2900	13715	43384	93920	139798	141390	94114	38677	8616	749
6P1004	1	30	390	2900	13715	43388	93965	140001	141877	94798	39248	8881	802
6P1005	1	30	390	2900	13715	43388	93965	140001	141881	94826	39315	8947	825
6P1006	1	30	390	2900	13715	43387	93956	139974	141856	94854	39393	9007	841
6P1007	1	30	390	2900	13716	43400	94027	140188	142237	95238	39570	9006	821
6P1008	1	30	390	2900	13716	43399	94021	140189	142322	95494	39907	9218	873
6P1009	1	30	390	2900	13716	43399	94022	140200	142371	95608	40054	9317	900
6P1010	1	30	390	2901	13733	43526	94557	141573	144570	97792	41347	9730	954
6P1011	1	30	390	2901	13735	43551	94693	142003	145434	98893	42180	10053	998
6P1012	1	30	390	2901	13733	43529	94590	141724	144936	98290	41718	9864	970
6P1013	1	30	390	2901	13734	43537	94614	141768	145036	98523	42036	10077	1025
6P1014	1	30	390	2901	13735	43552	94708	142087	145671	99272	42536	10242	1043
6P1015	1	30	390	2901	13734	43541	94652	141904	145264	98687	42035	10015	1002
6P1016	1	30	390	2901	13734	43540	94644	141884	145261	98754	42154	10099	1024
6P1017	1	30	390	2901	13734	43540	94643	141877	145242	98735	42157	10111	1026
6P1018	1	30	390	2901	13734	43539	94635	141855	145225	98762	42218	10153	1036
6P1019	1	30	390	2901	13736	43567	94800	142393	146281	100017	43073	10443	1070

No.	25	23	21	19	17	15	13	11	9	7	5	3	1
6P1020	1	30	390	2901	13735	43556	94749	142260	146068	99813	42971	10426	1072
6P1021	1	30	390	2901	13734	43545	94696	142113	145812	99535	42807	10395	1078
6P1022	1	30	390	2901	13735	43556	94750	142267	146095	99885	43088	10522	1101
6P1023	1	30	390	2901	13735	43555	94741	142241	146074	99917	43161	10570	1111
6P1024	1	30	390	2902	13753	43695	95364	143978	149172	103394	45496	11412	1235

No.	24	22	20	18	16	14	12	10	8	6	4	2	0
6P2001	1	29	362	2566	11474	33986	68075	92305	83164	47510	15520	2200	0
6P2002	1	29	362	2566	11475	34002	68183	92705	84050	48710	16492	2632	81
6P2003	1	29	362	2565	11457	33871	67666	91482	82297	47298	16018	2700	144
6P2004	1	29	362	2567	11492	34131	68732	94116	86306	50959	17847	3082	144
6P2005	1	29	362	2566	11475	34009	68256	93021	84806	49804	17444	3084	169
6P2006	1	29	362	2566	11475	34009	68256	93024	84827	49867	17543	3165	196
6P2007	1	29	362	2566	11475	34006	68226	92909	84620	49710	17551	3240	225
6P2008	1	29	362	2566	11476	34021	68318	93211	85201	50370	17962	3348	225
6P2009	1	29	362	2567	11493	34145	68820	94432	87007	51938	18684	3481	225
6P2010	1	29	362	2566	11475	34011	68270	93054	84865	49973	17768	3364	256
6P2011	1	29	362	2567	11492	34135	68776	94324	86866	51883	18763	3578	256

Table II-9.

No.	24	22	20	18	16	14	12	10	8	6	4	2	0
6P2012	1	29	362	2567	11493	34146	68827	94456	87097	52198	19072	3745	289
6P2013	1	29	362	2567	11493	34149	68860	94608	87455	52642	19344	3809	289
6P2014	1	29	362	2568	11511	34287	69451	96157	90036	55396	21172	4496	400

No.	23	21	19	17	15	13	11	9	7	5	3	1
6P3001	1	28	335	2257	9499	26179	48121	58858	46787	22897	6151	675
6P3002	1	28	335	2257	9499	26180	48131	58904	46903	23062	6274	711
6P3003	1	28	335	2258	9517	26312	48657	60150	48675	24512	6885	810
6P3004	1	28	335	2258	9516	26302	48607	60004	48441	24326	6828	810

No.	22	20	18	16	14	12	10	8	6	4	2	0
6P4001	1	27	309	1973	7782	19818	33027	35619	23853	8987	1452	0
6P4002	1	27	309	1973	7783	19831	33110	35902	24400	9609	1840	100
6P4003	1	27	309	1974	7800	19953	33580	36968	25864	10796	2360	196

Table III-1.[a]

No.	0	1	2	3
1C0001	1	6	9	2

No.	0	1	2	3	4	5
2C0001	1	11	41	61	31	3

No.	0	1	2	3	4	5	6	7
3C0001	1	16	98	290	429	294	76	4
3C0002	1	16	98	291	435	305	82	5
3P1001	1	15	84	220	273	141	20	

NO.	0	1	2	3	4	5	6	7	8	9
4C0001	1	21	180	814	2096	3092	2497	993	155	5
4C0002	1	21	180	815	2107	3136	2576	1056	175	7
4C0003	1	21	180	816	2117	3173	2638	1102	188	8
4C0004	1	21	180	816	2118	3179	2649	1108	189	8
4C0005	1	21	180	817	2127	3207	2685	1128	198	9
4P1001	1	20	161	673	1569	2031	1363	404	36	
4P2001	1	19	143	547	1132	1244	661	135	6	

a) For 1C0001 one gets $p(G,0)=1$, $p(G,1)=6$, $p(G,2)=9$, and $p(G,3)=2$.

Table III–2, 3.

No.	0	1	2	3	4	5	6	7	8	9	10	11
5C0001	1	26	287	1758	6557	15382	22653	20314	10407	2706	281	6
5C0002	1	26	287	1759	6573	15483	22976	20872	10922	2945	330	9
5C0003	1	26	287	1759	6573	15484	22985	20903	10971	2978	337	10
5C0004	1	26	287	1760	6588	15573	23253	21338	11344	3134	364	11
5C0005	1	26	287	1760	6589	15584	23297	21417	11407	3154	366	11
5C0006	1	26	287	1760	6589	15584	23299	21430	11437	3184	379	12
5C0007	1	26	287	1760	6589	15584	23300	21436	11448	3190	380	12
5C0008	1	26	287	1761	6603	15663	23530	21803	11762	3320	400	13
5C0009	1	26	287	1761	6604	15673	23566	21859	11797	3327	400	13
5C0010	1	26	287	1761	6603	15660	23500	21700	11619	3252	393	13
5C0011	1	26	287	1761	6605	15684	23610	21938	11860	3347	402	13
5C0012	1	26	287	1762	6618	15749	23768	22135	11992	3408	420	14

No.	0	1	2	3	4	5	6	7	8	9	10
5P1001	1	25	263	1520	5285	11378	15041	11701	4909	936	55
5P1002	1	25	263	1521	5298	11444	15207	11921	5063	989	60
5P1003	1	25	263	1521	5299	11454	15245	11986	5109	999	62
5P1004	1	25	263	1521	5299	11454	15244	11984	5115	1012	64
5P1005	1	25	263	1521	5299	11453	15236	11962	5092	1006	64
5P1006	1	25	263	1521	5300	11465	15290	12070	5180	1024	65

No.	0	1	2	3	4	5	6	7	8	9	10
5P2001	1	24	240	1303	4193	8192	9564	6316	2115	289	9
5P2002	1	24	240	1304	4206	8254	9697	6438	2147	284	9
5P2003	1	24	240	1304	4206	8256	9713	6484	2201	308	11

No.	0	1.	2	3	4	5	6	7	8	9
5P3001	1	23	218	1106	3263	5691	5704	3038	726	52

Table III-4, 5.

No.	0	1	2	3	4	5	6	7	8	9	10	11	12	13
6C0001	1	31	419	3247	15962	52024	114157	167919	161973	93213	34836	6374	469	7
6C0002	1	31	419	3248	15983	52207	115019	170315	166003	102270	37185	7099	571	11
6C0003	1	31	419	3248	15983	52208	115033	170394	166234	102640	37498	7223	591	13
6C0004	1	31	419	3249	16003	52374	115778	172366	169383	105624	39093	7660	641	14
6C0005	1	31	419	3249	16004	52390	115879	172689	169941	106139	39332	7709	644	14
6C0006	1	31	419	3249	16003	52375	115791	172435	169574	105914	39324	7744	653	15
6C0007	1	31	419	3249	16004	52391	115893	172767	170163	106478	39596	7800	657	15
6C0008	1	31	419	3249	16004	52390	115882	172722	170079	106419	39626	7870	684	16
6C0009	1	31	419	3249	16004	52390	115882	172722	170080	106425	39637	7876	685	16
6C0010	1	31	419	3249	16004	52391	115895	172790	170264	106697	39847	7948	693	17
6C0011	1	31	419	3249	16004	52391	115896	172801	170308	106776	39910	7968	695	17
6C0012	1	31	419	3250	16023	52542	116550	174485	172945	109242	41207	8306	729	18
6C0013	1	31	419	3250	16024	52557	116638	174742	173336	109536	41300	8313	728	18
6C0014	1	31	419	3250	16024	52557	116639	174751	173367	109585	41333	8320	729	18
6C0015	1	31	419	3250	16025	52573	116740	175074	173925	110100	41572	8369	732	18
6C0016	1	31	419	3250	16024	52557	116641	174773	173460	109779	41545	8437	755	19
6C0017	1	31	419	3250	16024	52557	116642	174783	173496	109835	41580	8444	755	19
6C0018	1	31	419	3250	16025	52573	116742	175096	174017	110288	41773	8480	757	19
6C0019	1	31	419	3250	16025	52573	116743	175107	174061	110367	41836	8500	759	19

No.	0	1	2	3	4	5	6	7	8	9	10	11	12	13
6C0020	1	31	419	3251	16043	52709	117309	176535	176316	112570	43090	8868	805	21
6C0021	1	31	419	3251	16044	52723	117386	176745	176610	112766	43139	8868	805	21
6C0022	1	31	419	3251	16044	52724	117398	176802	176745	112932	43241	8897	807	21
6C0023	1	31	419	3251	16045	52739	117487	177068	177167	113275	43367	8911	807	21
6C0024	1	31	419	3251	16045	52739	117486	177060	177143	113243	43351	8911	807	21
6C0025	1	31	419	3251	16046	52755	117588	177392	177732	113807	43623	8967	811	21
6C0026	1	31	419	3250	16023	52538	116492	174157	172030	107934	40308	8052	705	17
6C0027	1	31	419	3250	16023	52540	116518	174292	172389	108449	40689	8182	730	19
6C0028	1	31	419	3251	16043	52705	117250	176198	175370	111208	42134	8573	767	19
6C0029	1	31	419	3251	16043	52706	117263	176264	175538	111433	42284	8619	780	20
6C0030	1	31	419	3251	16043	52706	117262	176255	175507	111383	42248	8611	780	20
6C0031	1	31	419	3251	16044	52721	117356	176574	176142	112140	42789	8837	820	22
6C0032	1	31	419	3252	16063	52872	118009	178246	178726	114492	43954	9095	840	22
6C0033	1	31	419	3252	16063	52872	118008	178238	178703	114465	43946	9100	842	22
6C0034	1	31	419	3252	16063	52873	118020	178295	178838	114631	44050	9135	847	22
6C0035	1	31	419	3252	16063	52872	118010	178258	178779	114606	44086	9175	854	23
6C0036	1	31	419	3252	16064	52887	118099	178526	179214	114979	44242	9202	855	23
6C0037	1	31	419	3253	16082	53020	118622	179714	180809	116257	44887	9421	892	24

Table III-6, 7.

No.	0	1	2	3	4	5	6	7	8	9	10	11	12
6P1001	1	30	390	2887	13450	41147	83716	112298	96458	50218	14398	1904	77
6P1002	1	30	390	2888	13468	41281	84251	113545	98200	51665	15074	2053	88
6P1003	1	30	390	2888	13469	41296	84342	113830	98684	52094	15253	2086	91
6P1004	1	30	390	2888	13469	41296	84341	113823	98677	52130	15334	2131	96
6P1005	1	30	390	2888	13469	41296	84341	113823	98677	52130	15333	2129	97
6P1006	1	30	390	2888	13469	41295	84328	113758	98520	51944	15239	2117	97
6P1007	1	30	390	2888	13470	41312	84445	114172	99309	52718	15574	2160	97
6P1008	1	30	390	2888	13470	41311	84433	114115	99174	52556	15489	2150	97
6P1009	1	30	390	2888	13470	41311	84434	114126	99219	52640	15560	2175	100
6P1010	1	30	390	2889	13487	41430	84877	115075	100412	53512	15915	2242	104
6P1011	1	30	390	2889	13489	41459	85045	115571	101196	54147	16144	2269	104
6P1012	1	30	390	2889	13487	41429	84864	115012	100276	53398	15916	2268	106
6P1013	1	30	390	2889	13488	41445	84970	115378	100956	54031	16152	2287	107
6P1014	1	30	390	2889	13489	41460	85060	115653	101407	54416	16306	2308	107
6P1015	1	30	390	2889	13488	41445	84968	115362	100914	53993	16151	2295	108
6P1016	1	30	390	2889	13488	41444	84956	115306	100789	53862	16100	2293	108
6P1017	1	30	390	2889	13488	41444	84955	115297	100760	53823	16081	2291	110
6P1018	1	30	390	2889	13488	41443	84943	115241	100633	53682	16016	2285	110
6P1019	1	30	390	2889	13490	41475	85148	115913	101821	54771	16465	2343	110

No.	0	1	2	3	4	5	6	7	8	9	10	11	12
6P1020	1	30	390	2889	13489	41460	85057	115630	101354	54395	16359	2350	112
6P1021	1	30	390	2889	13488	41445	84966	115347	100884	54005	16233	2349	114
6P1022	1	30	390	2889	13489	41460	85058	115639	101383	54435	16382	2358	115
6P1023	1	30	390	2889	13489	41459	85045	115575	101234	54271	16311	2352	115
6P1024	1	30	390	2890	13507	41591	85556	116704	102668	55276	16670	2410	117

No.	0	1	2	3	4	5	6	7	8	9	10	11	12
6P2001	1	29	362	2554	11242	32144	60247	72925	54744	23602	5056	390	0
6P2002	1	29	362	2554	11243	32160	60351	73277	55406	24290	5432	486	9
6P2003	1	29	362	2553	11225	32033	59902	72444	54659	24090	5524	530	12
6P2004	1	29	362	2555	11260	32279	60794	74228	56612	25187	5797	548	12
6P2005	1	29	362	2554	11243	32163	60388	73461	55876	24924	5838	574	13
6P2006	1	29	362	2554	11243	32163	60388	73462	55883	24941	5855	581	14
6P2007	1	29	362	2554	11243	32164	60402	73529	56018	25048	5879	590	15
6P2008	1	29	362	2554	11244	32179	60490	73785	56403	25332	5970	600	15
6P2009	1	29	362	2555	11261	32293	60872	74450	56959	25490	5944	583	15
6P2010	1	29	362	2554	11243	32165	60410	73548	56023	25015	5844	580	16
6P2011	1	29	362	2555	11260	32281	60820	74360	56944	25617	6067	616	16

Table III-8.

No.	0	1	2	3	4	5	6	7	8	9	10	11	12
6P2012	1	29	362	2555	11261	32296	60909	74622	57337	25890	6132	619	17
6P2013	1	29	362	2555	11261	32295	60896	74564	57229	25820	6140	629	17
6P2014	1	29	362	2556	11279	32425	61383	75585	58438	26610	6418	676	20

No.	0	1	2	3	4	5	6	7	8	9	10	11
6P3001	1	28	335	2245	9281	24569	41857	44960	29007	10281	1693	87
6P3002	1	28	335	2245	9281	24570	41869	45014	29119	10388	1736	93
6P3003	1	28	335	2246	9299	24698	42331	45914	30047	10856	1835	102
6P3004	1	28	335	2246	9298	24684	42253	45700	29751	10662	1784	96

No.	0	1	2	3	4	5	6	7	8	9	10	11
6P4001	1	27	309	1961	7578	18426	28127	26079	13659	3491	306	0
6P4002	1	27	309	1961	7579	18441	28218	26354	14086	3817	414	10
6P4003	1	27	309	1962	7596	18557	28624	27126	14866	4202	490	14