

## A Note on the Smallest Eigenvalue of Fullerenes

PATRICK W. FOWLER p.w.fowler@exeter.ac.uk  
*School of Chemistry, University of Exeter,*  
*Stocker Road, Exeter EX4 4QD, UK*

PIERRE HANSEN Pierre.Hansen@gerad.ca  
*GERAD and École des Hautes Études Commerciales, Montréal, Canada*

DRAGAN STEVANOVIĆ\* stevanov@mathematik.uni-bielefeld.de  
*Faculty of Science and Mathematics, University of Niš, Yugoslavia*  
*and*  
*FSP Mathematisierung, Universität Bielefeld, Germany*

November 21, 2002

### Abstract

We prove that amongst all fullerenes the dodecahedron has maximum smallest eigenvalue (equal to  $-\sqrt{5}$ ), followed by the three fullerenes that have all their hexagons disjoint (the unique fullerenes on 24 and 26 vertices, and the tetrahedral fullerene on 28 vertices), for which the smallest eigenvalue is in each case equal to  $-1 - \sqrt{2}$ . We also prove that amongst all IPR fullerenes the icosahedral  $C_{60}$  fullerene has maximum smallest eigenvalue (equal to  $-\phi^2$  where  $\phi$  is the golden ratio  $(1 + \sqrt{5})/2$ ).

## 1 Introduction

Fullerenes have recently attracted much attention both in chemistry and mathematics. From the mathematical point of view, they are 3-regular planar graphs with faces being only pentagons and hexagons. From Euler's formula  $|V| - |E| + |F| = 2$ , where  $V$ ,  $E$  and  $F$  are the sets of vertices, edges and faces, respectively, one can deduce that fullerenes have exactly 12 pentagons. Since they are 3-regular, their largest eigenvalue is equal to 3, and since they are not bipartite, their smallest eigenvalue is larger than  $-3$ . For results on the eigenvalues of regular and bipartite graphs see [5], and for definitions of other terms see [2].

---

\*The third author was supported by the Deutsche Forschungsgemeinschaft (DFG) and the Grant 1389 of the Serbian Ministry of Science, Technology and Development (MNTR).

Recall that the spiral for a fullerene graph is constructed by starting on a face and passing through all other faces exactly once in succession in a tight winding such that each face added to the spiral is in contact with the immediately previous and the earliest still open face [6]. Each successful spiral out of the  $6|V|$  possible spiral starts is denoted by a number made up of twelve 5's and  $(|V|/2 - 10)$  6's for the pentagons and the hexagons, and the *spiral code* for a fullerene is the lexicographical minimum of these numbers. All fullerenes with  $\leq 176$  vertices are known to have spiral codes [3]; all with  $< 100$  vertices have a spiral beginning with a pentagon; the smallest known fullerene graph without a spiral code has 380 vertices [6]. Specific fullerene isomers will be labelled here by  $(a : b)$  where  $a$  is the number of vertices and  $b$  is the position of in the spiral order of general (adjacent-pentagon and isolated-pentagon) fullerenes; for the size range of fullerenes discussed here no ambiguity from technical incompleteness of the spiral construction will arise.

In Section 2 we prove that amongst all fullerenes the dodecahedron has maximum smallest eigenvalue (equal to  $-\sqrt{5}$ ), followed by the unique fullerenes on 24 and 26 vertices and the tetrahedral fullerene on 28 vertices (all with smallest eigenvalue equal to  $-1 - \sqrt{2}$ ). Then in Section 3 we prove that amongst all IPR fullerenes the icosahedral isomer of  $C_{60}$  has maximum smallest eigenvalue (equal to  $-\phi^2$  where  $\phi$  is the golden ratio). Finally, in Section 4 we analyze the correlation between the smallest eigenvalue and the number of pentagon adjacencies in fullerenes.

The fullerenes can be arranged in decreasing order by their smallest eigenvalue. We will call this arrangement the *smallest-eigenvalue order*, but it should be noted that there are nonisomorphic fullerenes with the same smallest eigenvalue, so that the word "order" above is not intended to mean a linear order. In this terminology, the above results state that the dodecahedron is the first fullerene in the smallest-eigenvalue order of fullerenes, followed by the unique fullerenes on 24 and 26 vertices and the tetrahedral fullerene on 28 vertices, and also that the icosahedral  $C_{60}$  fullerene is the first in the smallest-eigenvalue order of IPR fullerenes.

In the proofs, we use the famous Cauchy *interlacing theorem* [5, p.19].

**Theorem 1 (The interlacing theorem)** *Let  $H$  be an induced subgraph of graph  $G$ . If the eigenvalues of  $G$  are  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ , and the eigenvalues of  $H$  are  $\mu_1 \geq \mu_2 \geq \dots \geq \mu_m$ , then  $\lambda_i \geq \mu_i \geq \lambda_{n-m+i}$  for  $i = 1, 2, \dots, m$ .* ■

In fact, we use only  $\mu_m \geq \lambda_n$ .

## 2 Smallest-eigenvalue order of fullerenes

**Theorem 2** *The dodecahedron has maximum smallest eigenvalue amongst all fullerenes.*

**Proof** The eigenvalues (and multiplicities) of the dodecahedral graph [5] are  $+3$  (1),  $+\sqrt{5}$  (3),  $+1$  (5),  $0$  (4),  $-2$  (4),  $-\sqrt{5}$  (3) and the dodecahedron thus has smallest eigenvalue  $\lambda_n \equiv \lambda_{20}$  equal to  $-\sqrt{5} \approx -2.236$ . This eigenvalue occurs with multiplicity 3. The dodecahedron is also the unique fullerene for which all faces are pentagons.

Now, let  $G$  be a fullerene with  $n$  vertices, different from the dodecahedron, and let  $\lambda_n$  denote the smallest eigenvalue of  $G$ . Since  $G$  is different from the dodecahedron, one of its pentagons is adjacent to a hexagon, and then the graph  $H_1$ , depicted in Fig. 1,

must be a subgraph of  $G$ . Moreover,  $H_1$  is an induced subgraph of  $G$ , and since by direct computation the smallest eigenvalue of  $H_1$  is equal to  $-1 - \sqrt{2} \approx -2.414$ , from the interlacing theorem we deduce that  $\lambda_n \leq -1 - \sqrt{2} < -\sqrt{5}$ .

- has an inappropriate length, i.e. it has either less than 5 or more than 6 edges, or
- it has “double” edges, i.e. there exists an edge such that this same face appears on both of its sides.

Suppose that the vertices  $K_1$  and  $K_2$  are joined by an edge  $e$ . The edge  $e$  cannot be placed inside the pentagon containing  $K_1$  and  $K_2$ , otherwise the vertices  $K_1$ ,  $K_2$  and  $M_1$  will form a triangle, which is impossible in a fullerene. Therefore, the edge  $e$  must be placed outside this face, as on Fig. 2. Let  $F_1$  be the face determined by edges  $e$  and  $K_1M_1$ , and let  $F_2$  be the face determined by edges  $e$  and  $K_1N_1$ .

We could also argue in the following way. We see that in the face  $F_2$ , if we go along the edge  $e$  from  $K_1$  to  $K_2$ , then  $F_2$  must also contain edges  $K_2N_2$ ,  $N_2M_5$  and  $M_5L_5$ . On the other hand, if we go along the edge  $e$  from  $K_2$  to  $K_1$ , then  $F_2$  must also contain edges  $K_1N_1$ ,  $N_1M_2$  and  $M_2L_2$ . But then the face  $F_2$  has more than seven edges, which is also a contradiction.

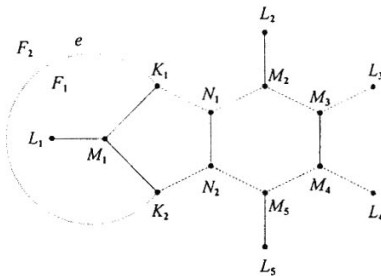


Figure 2: The hypothetical edge between  $K_1$  and  $K_2$ .

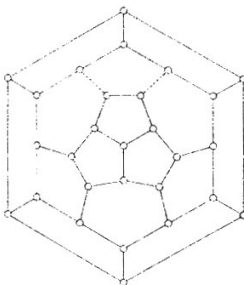


Figure 3: The tetrahedral fullerene on 28 vertices that has isolated hexagons (picture generated by *CaGe* [4]). This is isomer (28 : 2) in the spiral nomenclature.

**Remark** Using a similar proof technique (and a much larger number of cases), it is shown in [7] that amongst all fullerenes the dodecahedron has minimum second largest eigenvalue.

The unique fullerenes on 24 and 26 vertices and the one of the two fullerenes on 28 vertices that is depicted in Fig. 3 all have smallest eigenvalue equal to  $-1 - \sqrt{2} \approx -2.414$ . This eigenvalue occurs with multiplicity 2, 3 and 4 in the 24-, 26- and 28-vertex fullerenes, respectively. For the remaining fullerenes, we can prove the following.

**Theorem 3** *The smallest eigenvalue of a fullerene with at least 28 vertices, which is not isomorphic to the fullerene in Fig. 3, is less than  $-1 - \sqrt{2}$ .*

**Proof** Let  $G$  be a fullerene with at least 28 vertices, which is not isomorphic to a fullerene in Fig. 3. We first prove that  $G$  contains two hexagons sharing an edge.

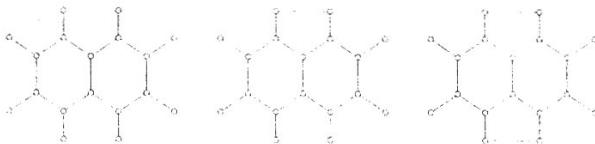


Figure 4: Possible induced subgraphs  $H_{2,1}$ ,  $H_{2,2}$  and  $H_{2,3}$  (in that order).

Suppose the contrary. First of all,  $G$  cannot have exactly 28 vertices. There are exactly two fullerenes with 28 vertices: one of them has two hexagons sharing an edge, and the other one is excluded by an assumption of the theorem.

Therefore, suppose that  $G$  has more than 28 vertices. Now, from Euler's formula and properties of fullerenes cited above, the number  $F_6$  of hexagonal faces of  $G$  satisfies

$$F_6 = 2 - 12 + \frac{3}{2}|V| - |V| = \frac{|V|}{2} - 10.$$

If the hexagons are all disjoint, then as any pentagon can be adjacent to at most two disjoint hexagons, the number of edges common to a hexagon and a pentagon is  $\leq 24$ , so that  $F_6 \leq 4$ , and from the above equality we obtain  $|V| \leq 28$ , which is a contradiction.

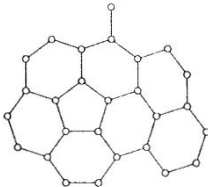
Therefore,  $G$  must contain two hexagons sharing an edge. Now it is not hard to prove, using the same technique as in the proof of Theorem 2, that  $G$  must also contain as an induced subgraph at least one of the graphs  $H_{2,1}$ ,  $H_{2,2}$  and  $H_{2,3}$  depicted in Fig. 4. The smallest eigenvalues of  $H_{2,1}$ ,  $H_{2,2}$  and  $H_{2,3}$  are approximately  $-2.5487$ ,  $-2.5300$  and  $-2.5097$ , respectively. From the interlacing theorem we conclude that the smallest eigenvalue of  $G$  may not be greater than  $-2.5097$ , and thus must be less than  $-1 - \sqrt{2} \approx -2.414$ . ■

From the list of computational results on the fullerenes on at most 100 vertices, it seems that the next three fullerenes in the smallest-eigenvalue order respectively have 32 vertices with  $\lambda_{32} \approx -2.5134$  (32 : 6), 30 vertices with  $\lambda_{30} \approx -2.5218$  (30 : 3), and then comes the non-tetrahedral isomer of  $C_{28}$  (28 : 1) with  $\lambda_{28} \approx -2.5247$ . From the interlacing theorem we see that none of them can contain either  $H_{2,1}$  or  $H_{2,2}$  as an induced subgraph.

### 3 Smallest-eigenvalue order of IPR fullerenes

It is observed in chemistry that fullerenes in which no two pentagons share an edge are typically more stable than other fullerenes. This observation is called the *isolated pentagon rule* [6] and such fullerenes are called IPR fullerenes. An IPR fullerene has at least 60 vertices, since it has 12 disjoint pentagons, and icosahedral  $C_{60}$  is the unique smallest IPR fullerene. Icosahedral  $C_{60}$  is (60:1812) in the full spiral order. This fullerene has many extremal properties, and another one we present here is that it is the first in the smallest-eigenvalue order of IPR fullerenes.

**Theorem 4** *The icosahedral  $C_{60}$  has maximum smallest eigenvalue amongst all IPR fullerenes.*

Figure 5: The induced subgraph  $H_3$ .

**Proof** Let  $G$  be an IPR fullerene with  $n$  vertices, and let  $\lambda_n$  denote the smallest eigenvalue of  $G$ . We show that  $\lambda_n \geq -\phi^2 \approx -2.6180$  (where  $\phi$  is the golden ratio  $\frac{1+\sqrt{5}}{2}$ ) if and only if  $G$  is isomorphic to the icosahedral  $C_{60}$ .

First, the icosahedral  $C_{60}$  has smallest eigenvalue  $\lambda_n \equiv \lambda_{60} = -\phi^2$  and this eigenvalue occurs with multiplicity 3.

Next, suppose that  $\lambda_n \geq -\phi^2$  holds. Let  $P$  be an arbitrary pentagon of  $G$ . Since  $G$  has disjoint pentagons, the first layer of faces around  $P$  consists of five hexagons, and the second layer of faces around  $P$  consists of ten faces, at least five of which are hexagons. If there is a pentagon of  $G$  such that the second layer around it contains at least six hexagons, then it must contain two adjacent hexagons and it is not hard to show, using the technique from Theorem 2, that the graph  $H_3$ , depicted in Fig. 5, must be an induced subgraph of  $G$ . The smallest eigenvalue of  $H_3$  is  $\approx -2.6229$ , and from the interlacing theorem we obtain that  $\lambda_n \leq -2.6229 < -\phi^2$ , which is a contradiction.

Thus, for each pentagon of  $G$  the second layer around it contains exactly five pentagons and five hexagons in alternating order.

Next, we show that each vertex of  $G$  must belong to a pentagon. Suppose that  $v$  is a vertex of  $G$  that does not belong to any pentagon, i.e. the first layer of faces around vertex  $v$  consists of hexagons  $X_1$ ,  $X_2$  and  $X_3$ . If the second layer of faces around  $v$  contains a pentagon  $P$  adjacent to only one of the hexagons  $X_1$ ,  $X_2$  and  $X_3$ , then the other two hexagons are adjacent hexagons in the second layer of faces around pentagon  $P$ , leading to the graph  $H_3$  (Fig. 5) as an induced subgraph of  $G$  and by the interlacing theorem to  $\lambda_n \leq -2.6229 < -\phi^2$ , which is a contradiction.

Thus, the second layer of faces around vertex  $v$  has hexagons as faces adjacent to only one of  $X_1$ ,  $X_2$  and  $X_3$ . The second layer contains three more faces adjacent to two of  $X_1$ ,  $X_2$  and  $X_3$ , which can be either pentagons or hexagons. There are four nonisomorphic possibilities for such second layer, which are shown in Fig. 6, together with their smallest eigenvalues. Since each of these possibilities has smallest eigenvalue smaller than  $-\phi^2$ , we conclude that also  $\lambda_n < -\phi^2$ , which is a contradiction.

From this we conclude that each vertex of  $G$  belongs to a pentagon, and since the pentagons are disjoint in an IPR fullerene, the total number of vertices of  $G$  is equal to 60. As the icosahedral isomer of  $C_{60}$  is the unique IPR fullerene with 60 vertices, we conclude that  $G$  is isomorphic to the icosahedral  $C_{60}$ . ■

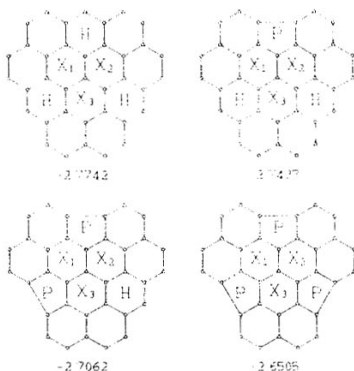


Figure 6: Second layer of a vertex not belonging to a pentagon.

## 4 Empirical observations

The proven bounds give some exact but limited information on  $\lambda_n$  for the class of fullerene graphs. In order to gather some empirical data on the typical behaviour of  $\lambda_n$  in the chemically significant size range, adjacency spectra were calculated numerically for the complete set of 1456598 fullerenes with  $n = 20 + 2k$  vertices ( $k = 0, \dots, 40, k \neq 1$ ) i.e. the whole set of fullerenes from  $C_{20}$  to  $C_{100}$  [6]. Table 1 collects the data on the minimum and maximum values of  $\lambda_n$  at each  $n$  in the range and identifies by their spiral numbers the isomers that realise the extreme values. Figure 7 illustrates the most obvious trend, which is that  $|\lambda_n|$  appears to be a roughly increasing function of  $n$ , with both largest and smallest values at each  $n$  scattered about sublinear, increasing curves. The two curves appear to be diverging, at least for these small vertex counts, as  $n$  and hence the size of the isomer set at  $n$  increases. Deviations from an idealised smooth curve are significant and  $C_{60}$  in particular appears in a pronounced dip on the graph of maximum  $\lambda_n$ . Isolated-pentagon and general fullerenes show the same qualitative pattern (Figures 7a, 7b). The rising form of all curves suggests as a plausible conjecture:

**Conjecture 1** *Amongst all fullerenes with 60 or more vertices, icosahedral  $C_{60}$  (60.1812) has the maximum smallest eigenvalue.*

Examination of the isomers realising the extrema of  $|\lambda_n|$  (Table 1) reveals clear systematic behaviour there too: the fullerene isomers of minimum/maximum smallest eigenvalue tend to appear respectively early and late in the spiral ordering at each  $n$ . Call the number of pentagon-pentagon edges in a fullerene  $n_p$ , the *number of adjacent pentagons*. By construction, the spiral order shows a trend with  $n_p$ ; early spirals include those of isomers with large  $n_p$ , and the late spirals those of isomers with few if any pentagon adjacencies; the trend is not monotonic, as not all pentagon adjacencies are apparent in the form of the spiral itself, some appearing only after it has been wrapped up to assemble the

fullerene. For  $20 \leq n \leq 100$  the isomer of minimum smallest eigenvalue is sometimes first, sometimes second or third in the spiral list (Table 1), and this variation is precisely accounted for by the variation in  $n_p$ , giving rise to the conjecture:

**Conjecture 2** *Amongst all fullerenes with a given number  $n$  of vertices, the one with the minimum smallest eigenvalue has the maximum number of pentagon adjacencies.*

The curve of minimum  $\lambda_n$  (Figure 7(a)) shows local peaks at  $n = 20 + 10k$ ; these correspond to the cylindrical fullerene isomers composed of five-fold symmetric hexagonal barrels capped by two hemi-dodecahedra, which all have  $n_p = 20$  and are local maxima in  $n_p$ .

At the other extreme, the variation of the maximum smallest eigenvalue with the number of pentagon adjacencies is also evident, but less regular. The isomer realising the maximum  $\lambda_n$  is often, but not invariably, one with the minimum achievable number of pentagon adjacencies. Thus, for example, at  $n = 60$ , an isolated-pentagon isomer is possible, and has, as we have seen, the maximum  $\lambda_{60}$ ; however, the sequence for  $n = 70$  is

$\lambda_{70}$	isomer	$n_p$
-2.7269808024	70:8094	1
-2.7288600491	70:7957	2
-2.7307219693	70:7960	2
-2.7312384436	70:8090	2
-2.7320508076	70:8149	0
-2.7322755441	70:8008	2
...	...	...

so that the unique isolated-pentagon isomer comes only fifth in the order, beaten by, amongst others, the unique isomer with a single pair of adjacent pentagons. As Figure 8 shows, however, pentagon adjacency appears to be a qualitative predictor of  $\lambda_n$  within isomer sets.  $n_p$  is known to correlate with total quantum-mechanical energy, in that in particular, if  $n$  is compatible with  $n_p = 0$ , the most thermodynamically stable fullerenes have isolated pentagons, and if  $n$  is not compatible with  $n_p = 0$ , the most stable isomers have the lowest achievable value of  $n_p$  [1]. This could be taken to suggest an admittedly indirect and decidedly approximate chemical significance for  $\lambda_n$ , but the significant quantity is actually  $n_p$ , which correlates well with curvature and other measures of molecular strain. Interestingly, the total quantum-mechanical energy correlates very poorly with the graph-theoretical energy quantity, the Hückel energy (which is defined by a particular sum of adjacency eigenvalues [8]), indicating the chemical fact that the total energy of a fullerene is not predictable from that of the  $\pi$  electrons alone. Correlation of  $\lambda_n$  with chemical quantities is thus not inevitable, and apparent correlations may be artefacts of other factors, but it is worth further exploration as part of the general search for more detailed understanding of the relationship between structure and spectra.

The extrema of  $\lambda_n$  within the subset of IPR isomers (Table 2 and Figure 7b) show a similar pattern to that for the general set, in that again the isomer of minimum smallest eigenvalue usually occurs early in the IPR spiral list, and the isomer of maximum smallest eigenvalue tends to occur late. Here, of course, all isomers have  $n_p = 0$ , and the explanation of the trend would have to be sought in more detailed consideration of properties of the graph, perhaps in the hexagon-neighbour signature [6].



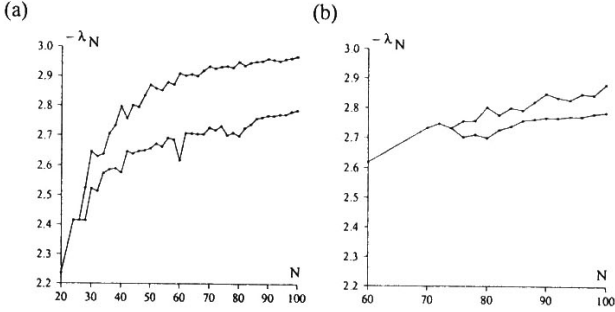


Figure 7: Extreme values of the smallest adjacency eigenvalue plotted against the number of vertices for the fullerene graphs (a) in the complete set of general fullerenes  $C_{20}$  to  $C_{100}$ , (b) the complete set of isolated-pentagon fullerenes  $C_{60}$  to  $C_{100}$ .

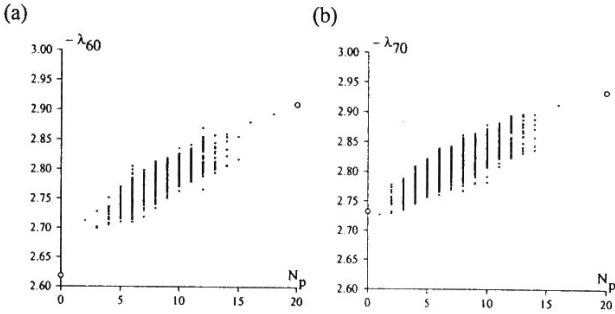


Figure 8: Scatterplot of the absolute value of the smallest adjacency eigenvalue against the number of pentagon adjacencies for (a) the 1812 isomers of  $C_{60}$ , (b) the 8149 isomers of  $C_{70}$ . The two open circles at  $n_p = 0$  denote the unique  $C_{60}$  and  $C_{70}$  isolated-pentagon isomers and the two at  $n_p = 20$ , denote the unique hemi-dodecahedrally capped cylindrical isomers.

$n$	$\max \lambda_n$	Isomer	$n_p$	$\min \lambda_n$	Isomer	$n_p$
20	-2.236068	1/1	30	-2.236068	1	30
24	-2.414214	1/1	24	-2.414214	1	24
26	-2.414214	1/1	21	-2.414214	1	21
28	-2.414214	2/2	18	-2.524691	1	20
30	-2.521832	3/3	17	-2.645751	1	20
32	-2.513447	6/6	15	-2.629652	2	18
34	-2.573159	5/6	14	-2.637939	1	17
36	-2.585043	14/15	12	-2.705728	2	18
38	-2.589475	16/17	12(11)	-2.732051	2	18
40	-2.575743	39/40	10	-2.797933	1	20
42	-2.646254	39/45	10	-2.756268	1	16
44	-2.639857	73/89	12(9)	-2.801961	2	18
46	-2.647517	99/116	8	-2.795500	1	16
48	-2.650113	171/199	7	-2.833649	2	18
50	-2.657091	264/271	6(5)	-2.869855	1	20
52	-2.672404	422/437	5	-2.858362	2	18
54	-2.662571	540/580	4	-2.851571	1	16
56	-2.691636	864/924	4	-2.879385	3	18
58	-2.687044	571/1205	6(3)	-2.871320	1	16
60	-2.618034	1812/1812	0	-2.909313	1	20
62	-2.707865	1982/2385	4(3)	-2.902113	2	18
64	-2.707403	2983/3465	3(2)	-2.906836	2	18
66	-2.705324	4059/4478	4(2)	-2.900987	1	16
68	-2.704639	6073/6332	2	-2.918986	3	16
70	-2.726981	8094/8149	1(0)	-2.933236	1	20
72	-2.717527	10611/11190	2(0)	-2.926573	2	18
74	-2.731567	14246/14246	0	-2.931852	2	18
76	-2.701718	19151/19151	0	-2.934178	2	18
78	-2.709956	24109/24109	0	-2.929473	1	16
80	-2.699315	31924/31924	0	-2.948816	1	20
82	-2.725371	39717/39718	0	-2.936288	1	16
84	-2.737860	51587/51592	0	-2.946237	2	18
86	-2.757238	63757/63761	0	-2.949856	2	18
88	-2.761926	81737/81738	0	-2.951063	2	18
90	-2.767001	99915/99918	0	-2.959522	1	20
92	-2.766015	126409/126409 <sup>1</sup>	0	-2.956295	3	18
94	-2.770599	153469/153493	0	-2.951747	1	16
96	-2.771209	191815/191839	0	-2.958956	2	18
98	-2.780413	230980/231017	0	-2.961571	2	18
100	-2.784995	285895/285914	0	-2.967192	1	20

Table 1: Maximum and minimum values of  $\lambda_n$  for general fullerenes in the range  $C_{20}$ - $C_{100}$ . At each value of  $n$  are shown the maximum value of  $\lambda_n$ , the isomer that achieves it (denoted by  $a/b$ , where  $a$  is its position in the spiral order of the total of  $b$  isomers), the value of  $n_p$ , the number of pentagon adjacencies for that isomer (with the minimum value for  $n_p$  achievable at that value of  $n$  also shown in brackets), the minimum value of  $\lambda_n$ , the isomer achieving it, and the value of  $n_p$  for that isomer.

$n$	$\max \lambda_n$	Isomer	$\min \lambda_n$	Isomer
60	-2.618034	1/1	-2.618034	1
70	-2.732051	1/1	-2.732051	1
72	-2.746680	1/1	-2.746680	1
74	-2.731567	1/1	-2.731567	1
76	-2.701718	2/2	-2.754959	1
78	-2.709956	5/5	-2.755980	4
80	-2.699315	7/7	-2.801938	1
82	-2.725371	8/9	-2.776052	1
84	-2.737860	19/24	-2.799899	1
86	-2.757238	15/19	-2.792331	3
88	-2.761926	34/35	-2.819541	1
90	-2.767001	43/46	-2.847759	1
92	-2.766015	86/86 <sup>2</sup>	-2.834159	1
94	-2.770599	110/134	-2.826574	3
96	-2.771209	163/187	-2.847306	1
98	-2.780413	222/259	-2.843414	66
100	-2.784995	432/450	-2.879385	1

Table 2: Maximum and minimum values of  $\lambda_n$  for isolated-pentagon fullerenes in the range C<sub>60</sub>-C<sub>100</sub>. At each value of  $n$  are shown the maximum value of  $\lambda_n$ , the isomer that achieves it (denoted by its position in the IPR spiral order  $a/b$ , in the total of  $b$  IPR isomers), and then the equivalent data for minimum value of  $\lambda_n$ .

## References

- [1] E. Albertazzi, C. Domene, P.W. Fowler, T. Heine, G. Seifert, C. Van Alsenoy, F. Zerbetto, *Pentagon adjacency as a determinant of fullerene stability*, Phys. Chem. Chem. Phys. 1 (1999), 2913–2918.
- [2] C. Berge, *Graphs and hypergraphs*, North-Holland, Amsterdam, 1973.
- [3] G. Brinkmann, A.W.M. Dress, *Penthex puzzles—A reliable and efficient top-down approach to fullerene-structure enumeration*, Adv. Appl. Math. 21 (3) (1998), 473–480.
- [4] G. Brinkmann, O.D. Friedrichs, A. Dress, T. Harmuth, *CaGe - a Virtual Environment for Studying Some Special Classes of Large Molecules*, MATCH Commun. Math. Chem. 36 (1997), 233–237.  
see also <http://www.mathematik.uni-bielefeld.de/~CaGe/>
- [5] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs - Theory and Application*, Johann Ambrosius Barth Verlag, Heidelberg-Leipzig, 1995.
- [6] P.W. Fowler and D.E. Manolopoulos, *An Atlas of Fullerenes*, Oxford University Press, 1995.
- [7] D. Stevanović, G. Caporossi, *On the separator of fullerenes*, Les Cahiers du GERAD G-2001-55, submitted.
- [8] A. Streitwieser, *Molecular orbital theory for organic chemists*, Wiley, New York, 1961.