

# Chapter 9

## A Graph Theoretic Approach to Atomic Displacements in Fullerenes

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**Abstract** The recently developed idea of analyzing complex networks in terms of node displacement due to vibration (Estrada and Hatano, *Chem Phys Lett* 486:166–170, 2010a) is applied to fullerenes. The fact that the ramafullerenes (fullerenes of Ramanujan graphs) are limited to fullerenes with relatively small number of C atoms is explained from the point of view of the node displacement. The node displacement is also shown to indicate the stability of isomers of C<sub>40</sub> fullerenes. It is suggested from the analysis of local node displacement that instability of fullerenes mainly comes from pentagon-rich areas of the molecules.

### 9.1 Introduction

Most of us have been aware of graphite since we were children. We can remember how useful our pencils were in learning to write and the advantage of deleting our errors simply by using rubber erasers. Fewer, however, have had the opportunity of admiring the bright and perfection of diamond. For people involved in the study of molecular structures, nothing has been more wonderful than contemplating the structure of fullerenes (see Fig. 9.1). The simplicity, elegance and beauty of this molecular structure have captivated many natural scientists and mathematicians in the last decades (Aldersey-Williams 1995). These three allotropes of carbon: graphite, diamond and fullerenes, are examples of how the combinatorial organization of atoms can produce very different structures with remarkable distinct properties (Pierson 1993).

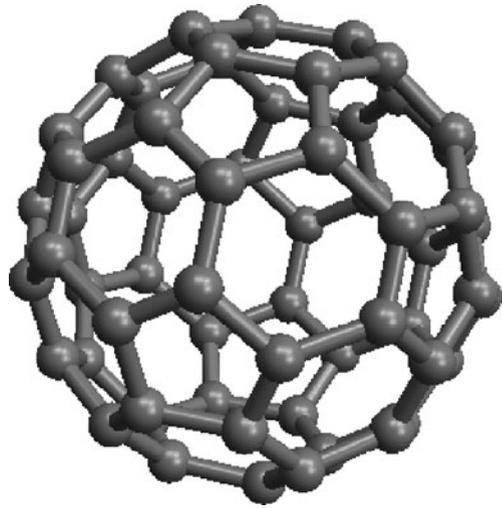
More formally, fullerenes are 3-regular polyhedral graphs. A graph is an object formed by a set of nodes, which are joined together by links or edges. Regular

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**Fig. 9.1** Illustration of the molecular structure of buckminsterfullerene,  $C_{60}$



graphs, in particular, are those having the same number of links per node. In “classical” fullerenes only pentagons and hexagons form the structure, while in the non-traditional ones cycles of other sizes are also allowed. Due to the many interesting mathematical results existing for regular graphs, it is not surprising that many researchers have paid attention to the graph-theoretic properties of fullerenes (Fajtlowitz and Larson 2003; Doslić 2005, 2008; Fowler, 2002, 2003; Manolopoulos et al. 1991; Zhang and Balasubramanian 1993). Many invariants, old and new, have been studied for this family of molecules, and many important conclusions about their structure, stability, function and reactivity have been obtained on the basis of such topological ideas.

Here we propose the study of atomic displacements in fullerenes due to small vibrations in the molecule as a whole. We use a graph-theoretic approach based on physically sounded ideas taken from mechanics. For the first time we show here a connection between some isoperimetric properties of graphs and vibrational properties and we extract important conclusions about the stability of these molecules. We also give a theoretical justification for the empirical evidence that the most stable fullerenes are those displaying the smallest number of adjacent pentagons. What we show here is that such pentagonal isolation confers more vibrational rigidity to the molecule, which is translated in larger stability.

## 9.2 Preliminary Definitions

Let  $G$  be a connected graph without loops or multiple links having  $n$  nodes. Then the adjacency matrix of  $G$ ,  $\mathbf{A}(G) = \mathbf{A}$ , is a square, symmetric matrix of order  $n$ , whose elements  $A_{ij}$  are ones or zeroes if the corresponding nodes are adjacent or

not, respectively. The sum of a row or column of this matrix is known as the degree of corresponding node  $i$  and designated here by  $\delta_i$ . This matrix has  $n$  (not necessarily distinct) real-valued eigenvalues, which are denoted here by  $\lambda_1, \lambda_2, \dots, \lambda_N$ . The  $i$  th component of the  $j$  th eigenvector of the adjacency matrix are designated here by  $\varphi_j(i)$ . Here the eigenvalues are usually labelled in a non-increasing manner:

$$\lambda_1 > \lambda_2 \geq \dots \geq \lambda_n. \quad (9.1)$$

The Laplacian matrix of a graph is defined as  $\mathbf{L} = \mathbf{D} - \mathbf{A}$ , where  $\mathbf{D}$  is the diagonal matrix of degrees  $\delta_i$  and  $\mathbf{A}$  the adjacency matrix of the graph. The eigenvalues of the Laplacian matrix are ordered here as follows:

$$0 = \mu_1 < \mu_2 \leq \dots \leq \mu_{n-1} \leq \mu_n. \quad (9.2)$$

The  $i$  th component of the  $j$  th eigenvector of the Laplacian matrix are designated here by  $U_j(i)$ .

The Moore-Penrose generalised inverse (or the pseudo-inverse)  $\mathbf{L}^+$  of the graph Laplacian  $\mathbf{L}$  has been proved to exist for any connected graphs. Using  $\mathbf{L}^+$  a graph metric known as the resistance distance can be computed. The resistance distance (Klein and Randić 1993) between a pair of nodes can be obtained by using the following formula (Xiao and Gutman 2003):

$$\Omega_{ij} = (\mathbf{L}^+)_{ii} + (\mathbf{L}^+)_{jj} - (\mathbf{L}^+)_{ij} - (\mathbf{L}^+)_{ji} \quad (9.3)$$

for  $i \neq j$ .

### 9.3 Atomic Displacements in Molecules

Let us consider a molecular graph in which atoms represent unit mass balls and bonds are identified with springs of a common spring constant  $k$  (Estrada and Hatano 2010a, b). The vibrational potential energy from the static position of the molecule can be expressed as

$$V(\vec{x}) = \frac{k}{2} \vec{x}^T \mathbf{L} \vec{x}, \quad (9.4)$$

where  $\vec{x}$  is the vector whose  $i$  th entry  $x_i$  is the displacement of the atom  $i$  from its equilibrium position.

Under these assumptions two of the present authors (EE and NH) have derived a topological formula for the mean displacement of a node  $i$  when the molecule is immersed into a thermal bath of inverse temperature  $\beta = 1/k_B T$ , where  $k_B$  is the Boltzmann constant. The procedure followed by Estrada and Hatano (Estrada and Hatano 2010a, b) is sketched below. First we can express the atomic displacements as

$$\Delta x_i \equiv \sqrt{\langle x_i^2 \rangle} = \sqrt{\int x_i^2 P(\vec{x}) d\vec{x}}, \quad (9.5)$$

where  $\langle \dots \rangle$  denotes the thermal average and  $P(\vec{x})$  is the probability distribution of the displacement of the nodes given by the Boltzmann distribution. The normalization factor that appear in the expression of  $P(\vec{x})$  represents the partition function of the molecule and can be expressed as

$$\begin{aligned} Z &= \int d\vec{y} \exp\left(-\frac{\beta k}{2} \vec{y}^T \Lambda \vec{y}\right) \\ &= \prod_{\mu=1}^n \int_{-\infty}^{+\infty} dy_{\mu} \exp\left(-\frac{\beta k}{2} \lambda_{\mu} y_{\mu}^2\right). \end{aligned} \quad (9.6)$$

It is well known that the smallest eigenvalue of the discrete Laplacian matrix is equal to zero,  $\mu_1 = 0$ . This is interpreted in this context as the translational movement of the molecule as a whole, the coherent motion in one direction. Here we remove this motion of the centre of mass and focus on the relative atomic motion only. In this case we obtain the following modified partition function

$$\begin{aligned} \tilde{Z} &= \prod_{\mu=2}^n \int_{-\infty}^{+\infty} dy_{\mu} \exp\left(-\frac{\beta k}{2} \mu_{\mu} y_{\mu}^2\right) \\ &= \prod_{\mu=2}^n \sqrt{\frac{2\pi}{\beta k \mu_{\mu}}}. \end{aligned} \quad (9.7)$$

Then, after some algebraic manipulation we finally arrive at the expression for the topological atomic displacement:

$$\Delta x_i \equiv \sqrt{\langle x_i^2 \rangle} = \sqrt{\sum_{v=2}^n \frac{[U_v(i)]^2}{\beta k \mu_v}}, \quad (9.8)$$

We have also shown that the topological atomic displacements can be obtained directly from the Moore-Penrose generalized inverse of the Laplacian matrix (Estrada and Hatano 2010a, b).

In our previous works we also showed that the Kirchhoff index of a molecule can be expressed as the sum of the squared atomic displacements produced by small molecular vibrations multiplied by the number of atoms in the molecule:

$$Kf = n \sum_{i=1}^n (\Delta x_i)^2 = n^2 \overline{(\Delta x)^2}. \quad (9.9)$$

Furthermore, the sum of resistance distances for a given atom and any other atom in the molecule  $R_i = \sum_{j=1}^n \Omega_{ij}$ , can be expressed in terms of the atomic displacements as

$$R_i = n (\Delta x_i)^2 + \sum_{i=1}^n (\Delta x_i)^2 = n \left[ (\Delta x_i)^2 + \overline{(\Delta x)^2} \right].$$

On the other hand, the mean square displacement of a node  $i$  is given by

$$(\Delta x_i)^2 \equiv \langle x_i^2 \rangle = \int x_i^2 P(\vec{x}) d\vec{x} \quad (9.10)$$

and the correlation between the displacements of nodes  $i$  and  $j$  is given by

$$\langle x_i x_j \rangle = \int x_i x_j P(\vec{x}) d\vec{x}, \quad (9.11)$$

where  $\langle \dots \rangle$  denotes the average with respect to  $P(\vec{x})$ . The function (11) can be represented using the Moore-Penrose generalized Laplacian as follows:

$$\langle x_i x_j \rangle = \frac{1}{\beta k} (\mathbf{L}^+)_{ij}. \quad (9.12)$$

Finally, Eq. (9.11) is followed by the thermal average of the vibrational potential energy Eq. (9.6) in the form

$$\langle V(\vec{x}) \rangle = \frac{1}{2} \sum_{i=1}^n k_i \langle x_i^2 \rangle - \sum_{i,j \in E} \langle x_i x_j \rangle = \frac{1}{\beta k} \sum_{i=1}^n k_i (\mathbf{L}^+)_{ii} - \sum_{i,j \in E} (\mathbf{L}^+)_{ij}. \quad (9.13)$$

## 9.4 Atomic Displacements and Expansion in Regular Graphs

In a regular graph it is known that the following relationship exists between the eigenvalues of the Laplacian and the eigenvalues of the adjacency matrix of a graph (ordered as in Section 9.2):

$$\mu_j = \lambda_1 - \lambda_j.$$

It is also known that for these graphs the eigenvectors of the adjacency and Laplacian matrix coincide. Then it is straightforward to realise that the atomic displacements in molecules whose graphs are regular can be written in terms of the spectra of their adjacency matrix as follow:

$$(\Delta x_i)^2 = \frac{1}{\beta k} \sum_{j=2}^n \frac{[\varphi_j(i)]^2}{\lambda_1 - \lambda_j}. \quad (9.14)$$

Let us consider for the sake of simplicity, the case where  $\beta k \equiv 1$  and let  $\Delta = \lambda_1 - \lambda_2$  be the *spectral gap* of the graph. Then, we can write (10) as follows

$$(\Delta x_i)^2 = \frac{[\phi_2(i)]^2}{\Delta} + \sum_{j=3}^n \frac{\phi_j(i)^2}{\lambda_1 - \lambda_j}. \quad (9.15)$$

Then, the average atomic displacement in a molecule can be expressed as

$$\overline{(\Delta x_i)^2} = \frac{1}{n} \sum_{i=1}^n \left( \frac{[\phi_2(i)]^2}{\Delta} + \sum_{j=3}^n \frac{\phi_j(i)^2}{\lambda_1 - \lambda_j} \right) = \frac{1}{n} \left( \frac{1}{\Delta} + \sum_{j=3}^n \frac{1}{\lambda_1 - \lambda_j} \right). \quad (9.16)$$

Obviously, the first term of the RHS of Eq. (9.15) has the largest contribution to the atomic displacements of a given molecule. Then, for a given regular molecule the magnitude of the atomic displacements due to molecular vibration/oscillations depends very much on the magnitude of the spectral gap. Those molecules having large spectral gaps are expected to display the smallest atomic displacements.

There is a family of graph named good expansion (GE) graphs. A graph is considered to have GE if every subset  $S$  of nodes ( $|S| \leq 1/2 |V|$ ) has a neighborhood that is larger than some “edge expansion ratio”  $h(G)$  multiplied by the number of nodes in  $S$ . A neighborhood of  $S$  is the set of nodes which are linked to the nodes in  $S$ . Formally, for each vertex  $v \in V$  (where  $V$  is the set of nodes in the network), the neighborhood of  $v$ , denoted as  $\Gamma(v)$  is defined as:  $\Gamma(v) = \{u \in V | (u, v) \in E\}$  (where  $E$  is the set of edges in the graph). Then, the neighborhood of a subset  $S \subseteq V$  is defined as the union of the neighborhoods of the nodes in  $S$ :  $\Gamma(S) = \bigcup_{v \in S} \Gamma(v)$  and the network has GE if  $|\Gamma(S)| \geq h(G)|S| \quad \forall S \subseteq V$ .

The edge expansion ratio  $h(G)$  of a graph is defined as (Hoory et al. 2006)

$$h(G) \stackrel{\text{def}}{=} \min_{S \subseteq V, |E(S)| \leq |E|/2} \frac{|E(S, \bar{S})|}{|S|}, \quad (9.17)$$

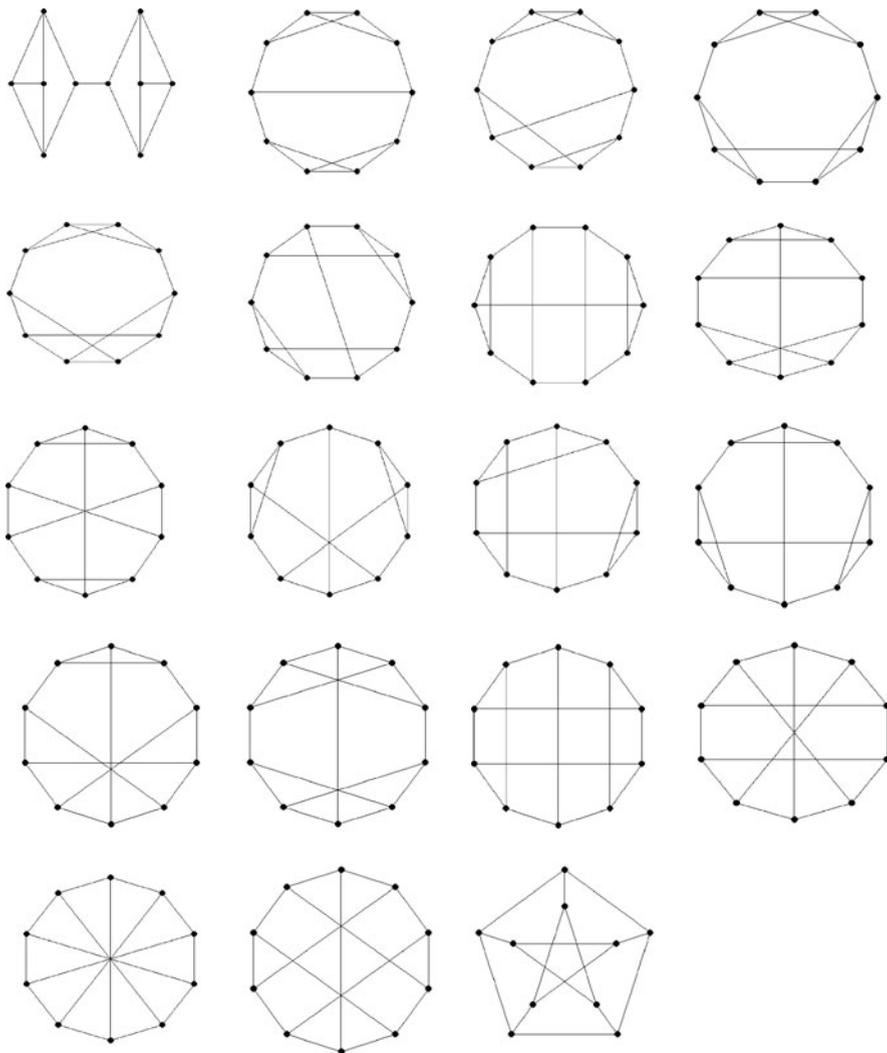
where  $|E(S, \bar{S})|$  denotes the number of links that have one endpoint in  $S$  and another endpoint in  $\bar{S}$ . The connection between good expansion and algebraic graph theory comes from the celebrated Alon-Milman theorem (Alon and Milman 1985), which states that for a finite, connected  $\delta$ -regular graph  $G$ , with spectral gap  $\Delta$ , the expansion constant is bounded as follows:

$$\frac{\Delta}{2} \leq h(G) \leq \sqrt{2\delta\Delta}. \quad (9.18)$$

Accordingly, high expansion necessarily means large spectral gap  $\Delta$ . Consequently, we can resume our results concerning atomic displacements and good expansion as follows:

Among all graphs with  $n$  nodes, those having good expansion properties display the smallest topological displacements for their nodes.

In order to illustrate our results for some artificial graphs we selected the set of all cubic graphs with 10 nodes. These graphs are illustrated in Fig. 9.2



**Fig. 9.2** Illustration of all cubic graphs ( $\delta = 3$ ) with 10 nodes. The last graph depicted is known as the Petersen graph

When we plot the values of the average node displacement  $\overline{(\Delta x_i)^2}$  against the inverse spectral gap  $1/\Delta$  for these 3-regular graphs with 10 nodes we obtain a straight line of slope 0.093 and intercept 0.271 as illustrated in Fig. 9.3. As can be seen the graph displaying the smallest average displacement of nodes in the Petersen graph (last graph in Fig. 9.2), which has the largest spectral gap  $\Delta$  among all cubic graphs of 10 nodes.

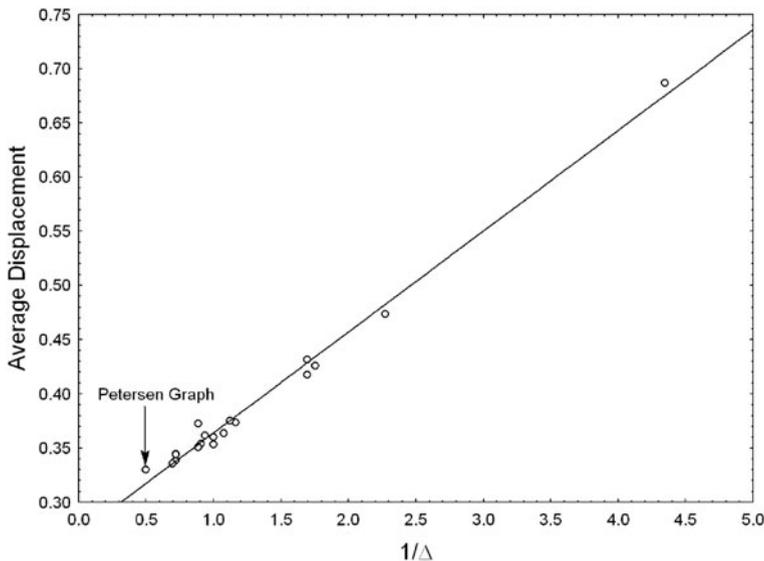


Fig. 9.3 Illustration of the linear regression between the average node displacement and the inverse spectral gap  $1/\Delta$  for the 19 cubic graphs with 10 nodes

### 9.5 Atomic Displacements in Ramafullerenes

A decade ago, Fowler et al. (1999) studied empirically which fullerenes display the property of Ramanujan graphs, or ramafullerenes. The Ramanujan graphs (Lubotzky et al. 1988; Ram Murty 2003) are formally defined as a  $\delta$ -regular graph for which

$$\lambda(G) \leq 2\sqrt{\delta - 1}, \tag{9.19}$$

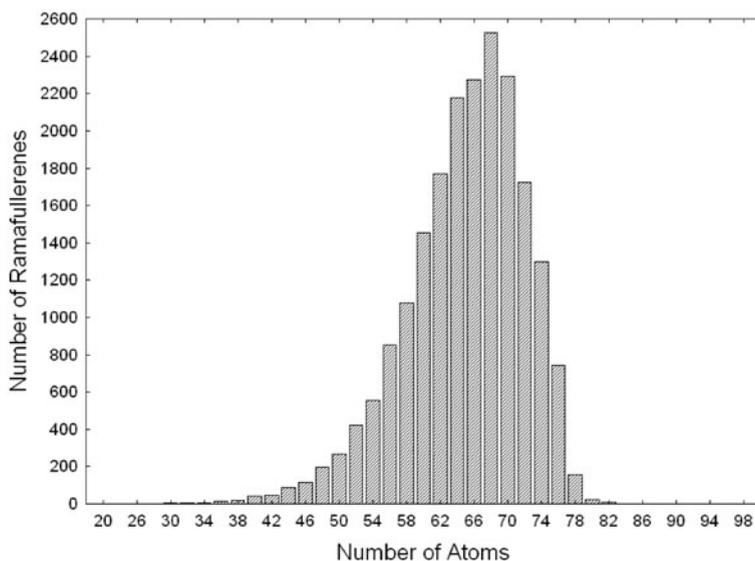
where  $\lambda(G)$  is the maximum of the non-trivial eigenvalues of the graph

$$\lambda(G) = \max_{|\lambda_i| < \delta} |\lambda_i|. \tag{9.20}$$

In the case of fullerenes,  $\lambda(G) \leq 2\sqrt{2}$ . It has been proved that Ramanujan graphs are good expanders. Using the Alon-Boppana theorem (Alon 1986) it can be shown that for a  $\delta$ -regular graph with  $n$  nodes,

$$\lambda_2 \leq \lambda(G) \leq 2\sqrt{\delta - 1}, \quad (9.21)$$

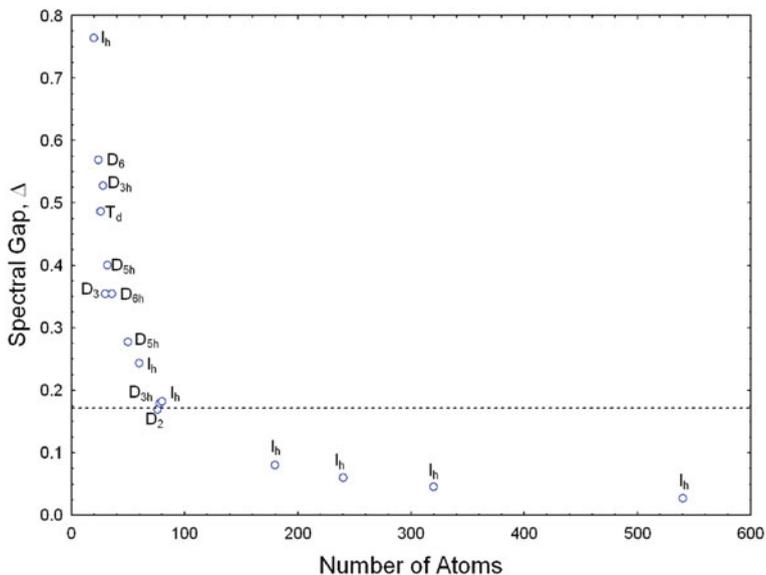
which shows that Ramanujan graphs are good expanders. In the mentioned paper of Fowler et al. (1999) it was found that a relatively large number of ramafullerenes exists among fullerenes having between 50 and 76 atoms. The distribution of ramafullerenes is displayed in Fig. 9.4 for fullerenes having between 20 and 100 atoms. Based on these empirical finding it was conjectured that there is no ramafullerene for  $n > 84$ .



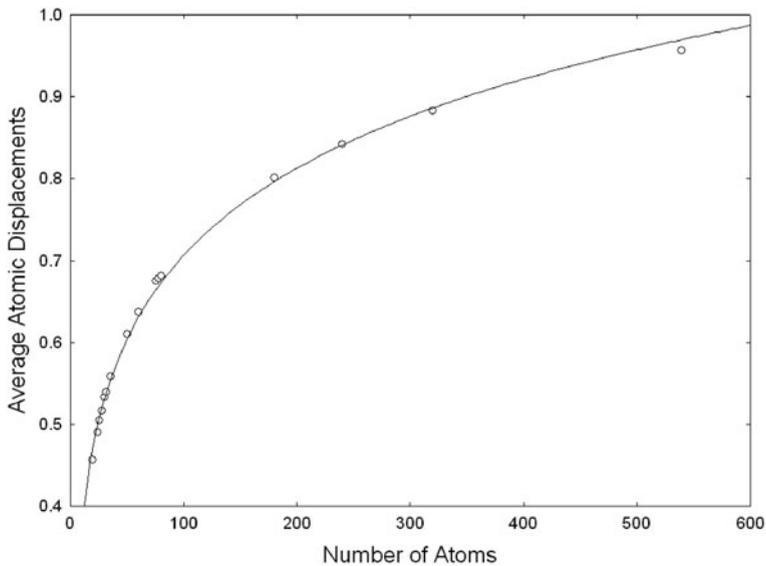
**Fig. 9.4** Distribution of the number of ramafullerenes as a function of the number of atoms (Fowler et al. 1999)

A plausible explanation for this finding is that the spectral gap decays very fast with the number of atoms in the fullerenes. For instance, in Fig. 9.5 we plot the spectral gap of some fullerenes having between 20 and 540 atoms, where we also show the line below which no ramafullerene exists, i.e.,  $\Delta > 3 - 2\sqrt{2}$ .

The immediate implication of this decay of the spectral gap with the number of nodes is that the average atomic displacement  $(\overline{\Delta x_i})^2$  in fullerenes increases as a power law with the number of atoms. This situation is illustrated in Fig. 9.6, where the best fit obtained indicates that  $(\overline{\Delta x_i})^2 \sim n^{0.042}$ .



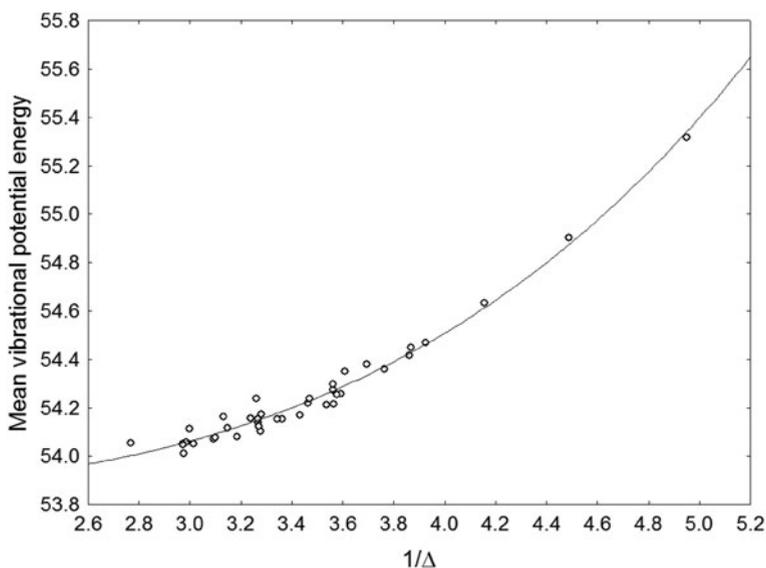
**Fig. 9.5** Decay of the spectral gap as a function of the number of atoms in the fullerenes



**Fig. 9.6** Power law increase of the average atomic displacement as a function of the number of atoms in the fullerenes

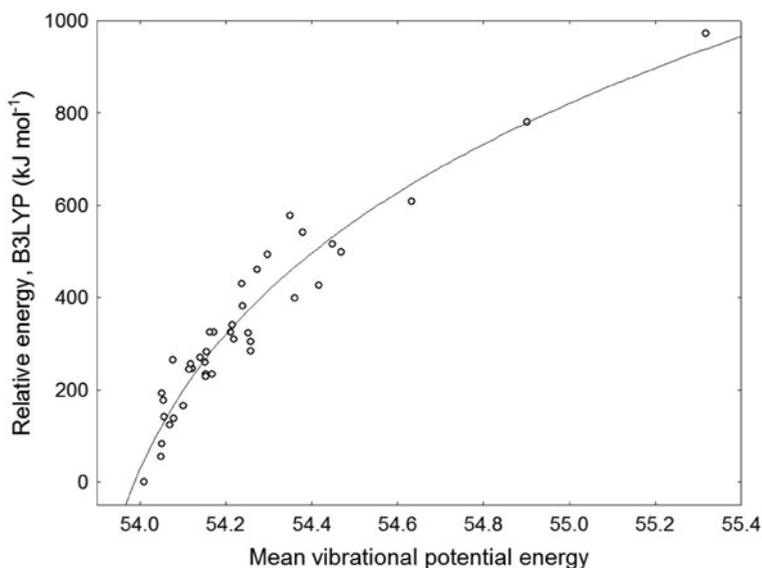
## 9.6 Atomic Displacements in Isomers of Fullerene C<sub>40</sub>

In order to understand in a better way the relation among the spectral gap, the atomic displacements and the energetics of fullerenes we are going to study 40 isomers of C<sub>40</sub>. When plotting the inverse of the spectral gap for these fullerenes versus the vibrational potential (see Fig. 9.7) or the average atomic displacements (graphic not displayed) we observe that the smallest value of  $1/\Delta$ , i.e., the largest spectral gap, corresponds to the fullerene C40:40. Here we denote fullerenes by C40:X, where X corresponds to the labeling given by Fowler and Manolopoulos in their Atlas of Fullerenes (Fowler and Manolopoulos 1995). The smallest vibrational potential, however, corresponds to C40:38 followed by C40:39. The isomer C40:38 has been identified by 11 out of 12 computational methods as the most stable one among C<sub>40</sub> fullerenes (Albertazzi et al. 1999), while C40:39 has been identified as the second most stable by 9 of these methods.



**Fig. 9.7** Increase of the thermal average of the vibrational potential energy as a function of the inverse of the spectral gap in C<sub>40</sub> fullerenes

In Fig. 9.8 we plot the thermal average of the vibrational potential  $\langle V(\vec{x}) \rangle$  of all C<sub>40</sub> isomers versus the relative energy calculated by a hybrid density functional method with a minimal STO-3G basis as reported by Albertazzi et al. (1999). A good correlation exists between both magnitudes with a correlation coefficient  $r = 0.961$  and equation:  $E = 5851.99(-0.4933 + 0.00916 \langle V(\vec{x}) \rangle)^{0.2} - 1532$ . The importance of this relationship goes beyond the possibility of predicting stability of fullerenes. For instance, this relationship indicates a possible cause for the difference in stability of fullerene isomers. That is, the largest the rigidity of

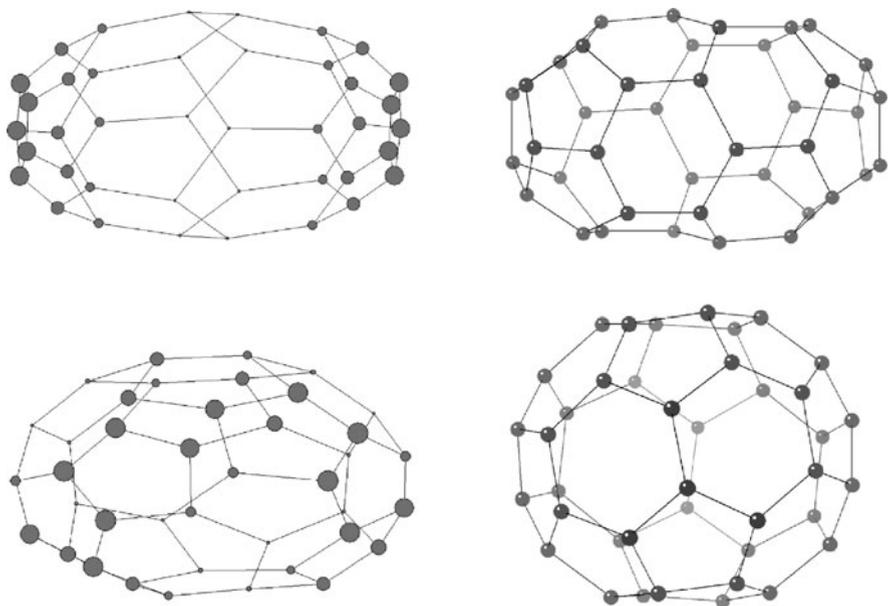


**Fig. 9.8** Relationship between the mean vibrational potential energy  $\langle V(\bar{x}) \rangle$  (Eq. (9.13)) and the relative energy calculated by density functional theory for  $C_{40}$  fullerenes. B3LYP energies are relative to fullerene  $C_{40}:38$  as taken from Albertazzi et al. (1999)

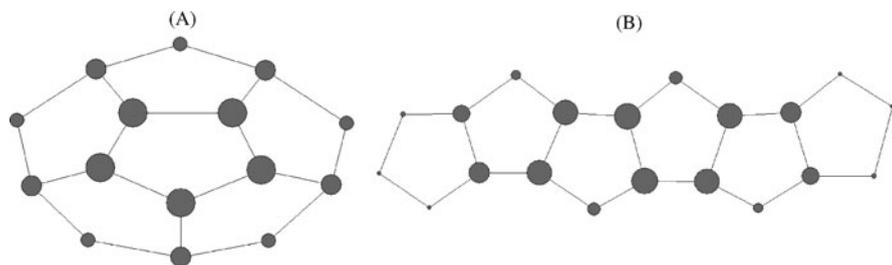
a fullerene the largest its stability. The rigidity here is measured by the average atomic displacements or the thermal average vibrational potential energy.

In agreement with this observation is the fact that the largest atomic displacements in fullerenes are observed for atoms in pentagonal rings. That is, atoms in pentagonal rings display in general more atomic displacements than atoms in hexagonal cycles. Among those atoms in pentagonal rings the ones fusing together show the largest flexibility, i.e., the largest displacements. In Fig. 9.9 we illustrate the atomic displacements for two isomers of  $C_{40}$  with the lowest (*top*) and largest (*bottom*) stability according to B3LYP energies. As can be seen in the least stable  $C_{40}$  isomer ( $C_{40}:1$ ) there are two regions of large flexibility which are located at the left and right part of the figure (top-left image). These two regions are formed completely by fused pentagons in which a central pentagon is surrounded by other six. This central pentagon has the largest flexibility among all cycles in this molecule (see Fig. 9.10a). In the case of the most stable  $C_{40}$  fullerene,  $C_{40}:38$  the largest atomic displacements are observed for the atoms in the very centre of six fused pentagonal rings as can be seen in Fig. 9.10b. Such flexibility decreases as soon as the atoms are far from the centre of this system, which implies that they are in contact with hexagonal rings.

An interesting conclusion that we can extract from these findings is that there is not a plausible geometric explanation for why pentagonal rings are more flexible than hexagonal ones. That is, from geometric intuitive reasoning we could expect that hexagons are more flexible than pentagons. As we have not considered



**Fig. 9.9** Illustration of the atomic displacements (*left graphics*) for the isomers C<sub>40</sub>:1 (*top*) and C<sub>40</sub>:38 (*bottom*) with the lowest and largest stability, respectively, according to B3LYP energies. The graphics at the right hand side are three-dimensional embeddings of these fullerenes. The radii of the nodes in the graphics on the left-hand side are proportional to the atomic displacements

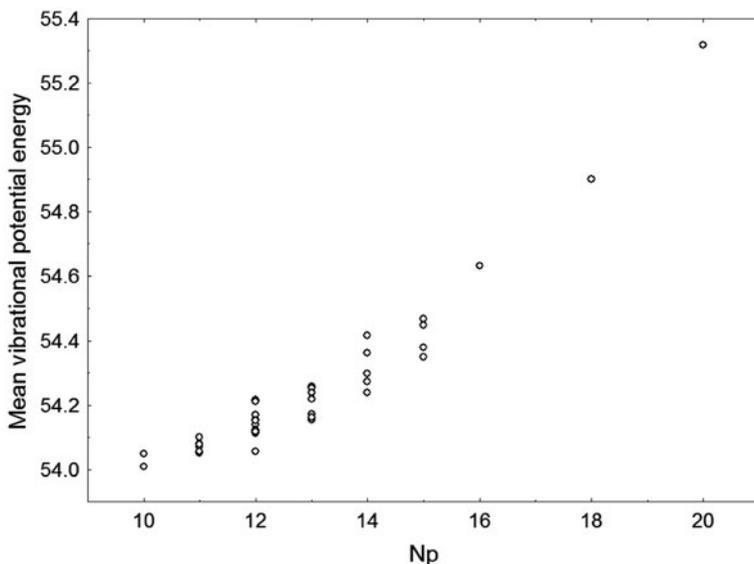


**Fig. 9.10** Illustration of the atomic displacements of fused pentagonal rings in C<sub>40</sub> fullerenes. (a) System of seven fused pentagonal rings in C<sub>40</sub>:1, the least stable C<sub>40</sub> isomer. (b) System of six fused pentagonal rings in C<sub>40</sub>:38, the most stable C<sub>40</sub> isomer. The radii of the nodes in both graphics are proportional to the atomic displacements

any geometric or electronic characteristic of fullerenes in deriving our atomic displacement measures, we can conclude that the cause of the observed differences in flexibility/rigidity between pentagonal and hexagonal rings is a purely topological one.

Finally, we would like to remark that our current findings support the hypothesis that the pentagon adjacency number is a good predictor of the stability of fullerenes. It has been shown in several studies (Balaban et al. 1995; Campbell et al. 1996;

Albertazzi et al. 1999) that the most stable fullerene isomers contain the least number  $N_p$  of adjacent pentagons in their structures. We have observed here that such pentagon isolation confers more rigidity to the fullerenes and this produces larger energy stabilization. However, as we can see in Fig. 9.11 isomers with the same number of adjacent pentagons display different thermal average of the vibrational potential energies, which indicate that not only the adjacency between such rings is important but also the position that certain rings occupy in the structure of the fullerene (see Fig. 9.10).



**Fig. 9.11** Relationship between the thermal average of the vibrational potential energy ( $V(\bar{x})$ ) (Eq. (9.13)) and the number of adjacent pentagons in  $C_{40}$  fullerenes. The values of  $N_p$  are taken from Réti and László (2009)

## 9.7 Conclusions

In the present article, we applied to fullerenes, a recently developed idea of analyzing complex networks in terms of the vibrational potential energy of the atomic displacements. After defining the mean atomic (or node) displacement, we argued that a small atomic displacement means a large spectral gap of the graph (Fig. 9.3), which in turns means that the graph has good expansion.

We demonstrated these relations in fullerenes. Fullerenes with the property of Ramanujan graphs, or ramafullerenes, are good expanders. The ramafullerenes are limited to fullerenes with relatively small numbers of C atoms. We explained this fact from the above two points of view, namely, the spectral gap and the atomic displacement. We demonstrated that as the number of atoms increases, the spectral gap decreases (Fig. 9.5) and the atomic displacement increases (Fig. 9.6).

As another application of the atomic displacement, we examined isomers of fullerenes  $C_{40}$ . We showed that the thermal average of the vibrational potential energy of our simple definition has strong correlation with the energy obtained from elaborate calculation of density functional theory. Since the latter tells us the stability of each isomer, we claim that our vibrational energy also indicates the isomers' stability. We went further and showed that the atomic displacement is generally larger in the area of pentagons than in the area of hexagons. This suggests that the instability of a fullerene isomer is originated in pentagon-rich areas confirming the pentagon isolation rule.

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