

# Strain Energies Due to Nonplanar Distortion of Fullerenes and Their Dependence on Structural Motifs

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Accurate strain energies due to nonplanar distortion of 114 isolated pentagon rule (IPR) fullerenes with 60–102 carbon atoms have been calculated based on B3LYP/6-31G(d) optimized structures. The calculated values of strain energy due to nonplanar distortion ( $E_{np}$ ) are reproduced by three simple schemes based upon counts of 8, 16, and 30 distinct structural motifs composed of hexagons and pentagons. Using  $C_{180}$  ( $I_h$ ) and  $C_N$  ( $I_h$ ) ( $N$  is very large) as test molecules, the intrinsic limitations of the motif model based on six-membered rings (6-MRs) as the central unit have been discussed. On the basis of the relationship between the contributions of motifs to  $E_{np}$  and the number of five-membered rings (5-MRs) in motifs, we found that IPR fullerenes with dispersed 5-MRs present smaller nonplanar distortions.

## 1. Introduction

It is well-known that fullerenes contain large strain energies ( $E_S$ ), which are mainly due to nonplanar distortion. For instance, in a previous study of  $C_{60}$ , the total strain energy was estimated to be approximately 100% of the heat of formation.<sup>1</sup> The  $E_S$  due to nonplanar distortion was estimated to be 78% of the excess energy of the carbon atoms relative to graphite.<sup>2</sup> Moreover, the strain energies due to nonplanar distortion ( $E_{np}$ ) and in-plane bond-angle bending ( $E_{ba}$ ) have been identified as two major sources of destabilization for carbon clusters.<sup>3</sup> In addition to stability,<sup>4–6</sup> the chemical reactivity<sup>2,7</sup> and magnetic properties<sup>8</sup> of fullerenes have also shown strong correlation with nonplanar distortion. Hence, the investigation of strain energies induced by nonplanar distortion is fundamentally significant for understanding the stability and reactivity of fullerenes. The accurate calculation of strain energy due to nonplanar distortion can be carried out based on optimized structures by high-level quantum chemical calculations. However, it is very computationally expensive for such large systems. Moreover, the number of possible fullerene cages grows very rapidly with the number of carbon atoms, increasing from 1812 for  $C_{60}$  to 1 207 119 for  $C_{116}$ .<sup>9,10</sup> Even semiempirical methods are too expensive as pre-screening tools for fullerenes with hundreds of thousands of isolated pentagon rule (IPR) structures.<sup>11</sup> Hence, it is highly desirable to develop effective and simple methods to estimate the strain energy of fullerenes based simply on their geometries.

Fortunately, Cioslowski et al.<sup>11</sup> and Yu et al.<sup>12</sup> have shown that thermodynamic parameters of polycyclic aromatic hydrocarbons (PAHs) and fullerenes can be readily estimated within a few kilocalories per mole by simple schemes based upon counts of distinct structural motifs. First a series of molecules are selected and optimized quantum mechanically at a high level. Then, the calculated values are fitted by a set of parameters

(each parameter corresponding to one motif). In fact, before Cioslowski, Fowler et al. optimized the 1812 fullerene structural isomers of  $C_{60}$  formed by 12 pentagons and 20 hexagons and studied the correlations of total energy with many structural motifs.<sup>13</sup> Their results are reasonable in terms of the curved nature of fullerene molecules: pentagons should be isolated to avoid sharp local curvature; moreover, hexagon triples are costly because they enforce local planarity and hence imply high curvature in another part of the fullerene surface, but hexagon–pentagon–hexagon triples allow the surface to distribute steric strain by warping.<sup>13</sup> In a similar way, this methodology was applied to the study of the standard heats of formation ( $\Delta H_f^0$ ) of fullerenes by Cioslowski et al.<sup>11</sup> Due to the absence of abutting pentagons, hexagons in fullerenes possess only five distinct first neighborhoods and this arrangement of rings gives rise to 30 possible structural motifs.<sup>11</sup> Furthermore, the values of  $\Delta H_f^0$  calculated from B3LYP/6-31G(d) can be reproduced within 3 kcal/mol by a simple scheme based upon counts of these motifs. These successes in the estimation of thermodynamic parameters of PAHs and fullerenes stimulated us to think whether the strain energies due to nonplanar distortion of fullerenes can be estimated simply by some basic motifs. In the present work, the values of  $E_{np}$  of 114 IPR fullerenes with 60–102 carbon atoms have been calculated based on B3LYP/6-31G(d) optimized structures and then they were reproduced within several kilocalories per mole by three simple schemes based upon counts of 8, 16, and 30 distinct structural motifs. The three groups of motifs were tested by  $C_{180}$  ( $I_h$ ) and  $C_N$  ( $I_h$ ) and their applicability for large fullerenes is discussed. On the basis of the contributions of different motifs to  $E_{np}$ , the nonplanar distortions of fullerenes and their geometries were discussed.

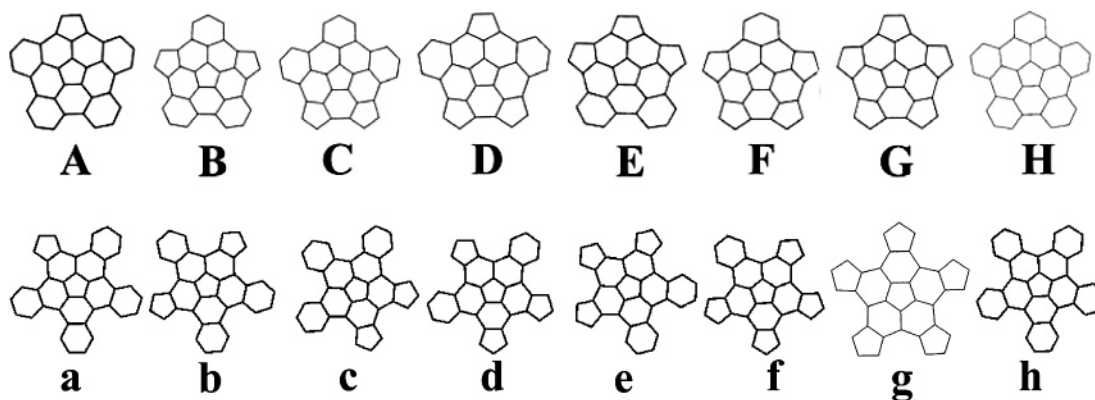
## 2. Computational Methods

Strain energies are very difficult to compute because it is complicated to separate the strain energy from the loss of aromaticity and other effects. Normally, strain energies are defined based on some standard structures, such as a graphite surface for aromatic hydrocarbons. When some structural

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**Figure 1.** Motifs of IPR fullerenes. **A–H** and **a–h** denote the possible configurations of the second and third neighborhoods of the central 5-MR, respectively. **A–H** are labeled as Motif Model I, and **A–H** and **a–h** as Motif Model II.

parameters deviate from the standard values, strain energies are introduced. Hence strain energies are defined based on the types of structural distortions, such as  $E_{np}$  and  $E_{ba}$ , which stand for the strain energies due to nonplanar distortions and bond-angle bending away from the  $sp^2$  ideal, respectively. Basically, different strain energies are calculated based on a force field. For aromatic hydrocarbons, the set of force constants developed by Cyvin et al.<sup>14</sup> have been widely and successfully used for fullerenes<sup>1–3,15</sup> and carbon nanotubes.<sup>16</sup> Following Cyvin,<sup>14,15</sup>  $E_{np} = \sum (1/2)k(D\gamma)^2$ , where the sum is over vertexes, the force constant,  $k$ , is equal to 0.15 mdyne/Å, and the bond length,  $D$ , is 1.4 Å. For small deflection angles ( $\theta_{\sigma\pi} - (\pi/2)$ ), the expression of  $E_{np}$  can be simplified with an approximate curvature conservation,<sup>1</sup>  $E_{np} = (9/2)kD^2 \sum (\theta_{\sigma\pi} - (\pi/2))^2$ , where  $\theta_{\sigma\pi}$  is the common angle made by the  $\pi$ -orbital axis vector and the  $\sigma$  bond based on the theory of the  $\pi$ -Orbital Axis Vector (POAV),<sup>17</sup> which can provide a very logical and natural bridge between  $\sigma$ – $\pi$  separability assumed in planar conjugated systems and the realistic condition of  $\pi$ -bonding in nonplanar geometries.<sup>18</sup> Following Haddon,<sup>2</sup> for fullerenes,  $E_{np}$  can be further simplified by an approximate hybridization conservation as

$$E_{np} = 100 \sum \frac{m}{m+1} \quad (1)$$

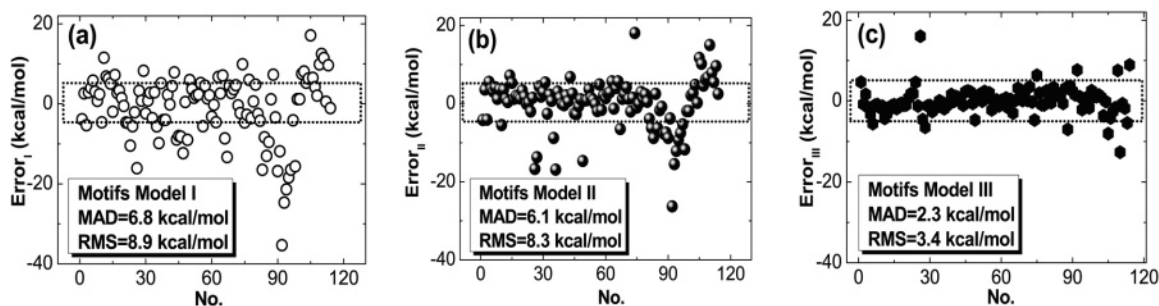
In eq 1,  $m/(m+1)$  denotes the fractional hybridization of the atomic  $\pi$  orbitals ( $s^m p$ ) based on the POAV theory.<sup>17–19</sup> The parameter  $m$  can be directly obtained from the atomic coordinates by using the POAV package. In our calculations, 114 IPR fullerenes optimized at the level of B3LYP/6-31G(d) were obtained from Cioslowski<sup>11</sup> and the POAV analysis in the present work was carried out with the POAV package<sup>17–19</sup> provided by Prof. R. C. Haddon. The validity of eq 1 was previously confirmed in ref 2. It is cautiously pointed out that, as we mentioned above, the absolute value of the strain energy is normally not of interest and also very difficult to calculate accurately from a force field or its simplified expression. However, it is still possible to obtain insight into the strain energy due to the nonplanar distortion and relative stability of different IPR fullerenes, as illustrated in the following.

### 3. Results and Discussion

Strain energies of  $E_{np}$  for 114 IPR fullerenes are listed in the Supporting Information (Table S1). To specify IPR fullerenes with the same molecular formula and symmetry, a bold number, ranging from 1 to 114, has been assigned to each molecule and written in front of the molecule in the table. For instance,  $C_{60}$  takes the number of **1**, **2** for  $C_{70}$ , **3** for  $C_{72}$ , and so on. From

Table S1, the values of  $E_{np}$  obtained for the various IPR fullerenes were significantly different. Moreover,  $E_{np}$  seemed to be independent of the number of carbon atoms, which is different from their standard heats of formation.<sup>11</sup> It is very interesting that, although **44**: $C_{84}$  ( $D_2$ ) and **24**: $C_{84}$  ( $D_2$ ) have the same symmetry and the same number of carbon atoms, the values of  $E_{np}$  change from 498.5 kcal/mol for **44** to 542.0 kcal/mol for **24**, which indicates that some other factors, rather than the symmetry and the number of carbon atoms, determine the nonplanar distortion of fullerenes. Previously, Schmalz et al. suggested that, for cages of fullerenes,  $E_{np}$  remains constant ( $E_{np} = 19.97$  eV = 460.5 kcal/mol).<sup>1</sup> As shown in Table S1, however, our results were clearly higher than theirs, since Schmalz et al. assumed that the sum of the squares of the POAV angles should be nearly constant for spheroidal clusters,  $\sum \theta_i^2 \approx 4\pi/(3\sqrt{3}) = 2.418$ . Also Bakowies et al.<sup>3</sup> made the same assumptions. However, according to the ab initio optimization of fullerenes at the level of B3LYP/6-31G(d), this assumption is not strictly satisfied since some IPR structures deviate from a spheroidal shape; moreover, based on the optimized structures and POAV analysis, it was found that the nonplanar distortion of fullerenes strongly depends on the distribution of five-membered rings (5-MRs). Hence,  $E_{np}$  is quantitatively related to basic motifs in fullerenes, as described below.

A typical character of the motifs proposed by Cioslowski et al. was that one six-membered rings (6-MR) was selected as the central ring.<sup>11</sup> Considering that the number of 6-MRs will increase monotonically with the molecular size, the counts of motifs and the terms predicted by these motifs represent a size effect. This approach is suitable for the prediction of the standard heats of formation of fullerenes since the values of  $\Delta H_f^\circ$  do increase with the molecular size, as shown by Cioslowski et al.<sup>11</sup> However, the molecular size shown in this approach will be a shortage for the prediction of those parameters which do not present the molecular size effect, such as the nonplanar strain energies of fullerenes. Thus, in the present work, 5-MRs were selected as the central units of the motifs, as shown in Figure 1. Theoretically, to completely describe the chemical environment of central 5-MR, there could be eight possible configurations for the first neighbors: 66666, 66665, 66655, 66565, 66555, 65655, 65555, and 55555, where 5 and 6 denote 5-MRs and 6-MRs, respectively. For instance, 55555 corresponds to a 5-MR surrounded by five 5-MRs, such as that in  $C_{20}$ . However, the first neighbors of all IPR fullerenes investigated here are 66666. Similarly, there are eight possible configurations for the second neighbors (**A–H**) and eight for the third (**a–h**), as shown in Figure 1. Theoretically, there should be 64 possible compound nodes for the second and third neighbor configurations. Here it



**Figure 2.** Errors defined by eq 3: (a, b, and c) are Error<sub>I</sub>, Error<sub>II</sub>, and Error<sub>III</sub>, respectively.

is assumed that the contribution of the second neighbors is independent of the third neighbors. Motifs A–H were designated as Motif Model I, and 16 motifs (A–H, a–h) as Motif Model II, for the sake of conciseness. Previously, the standard heats of formation ( $\Delta H_f^0$ ) for the IPR fullerenes investigated here were calculated and reproduced within 3 kcal/mol, using 30 structural motifs by Cioslowski et al.<sup>11</sup> Hence, the structural motifs proposed by Cioslowski et al. are considered here and designated as Motif Model III, and the motif structural schemes of Motif Model III can be found elsewhere.<sup>11</sup> To understand the nonplanar distortion of IPR fullerenes, values of  $E_{np}$  in Table S1 (Supporting Information) were estimated based on the above three models by

$$E_{np}^I = \sum_i N_i E_{np}^i + \frac{x}{n} \quad (i = \mathbf{A}, \dots, \mathbf{H}) \quad (2.1)$$

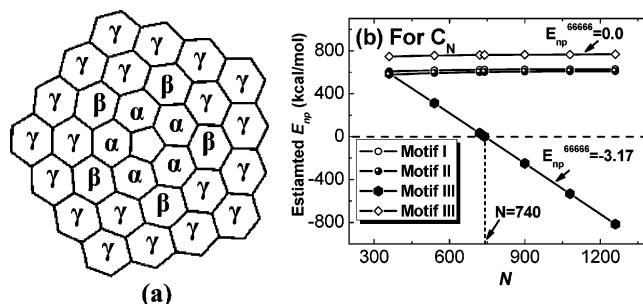
$$E_{np}^{II} = \sum_i N_i E_{np}^i + \frac{x}{n} \quad (i = \mathbf{A}, \dots, \mathbf{H}, \mathbf{a}, \dots, \mathbf{h}) \quad (2.2)$$

$$E_{np}^{III} = \sum_{i=1}^{30} N_i E_{np}^i - \frac{x}{N - y} \quad (2.3)$$

where A, ..., H and a, ..., h denote motifs shown in Figure 1,  $N_i$  and  $E_{np}^i$  are the number of each motif and their contribution to  $E_{np}$ , respectively,  $N$  and  $n$  are the numbers of carbon atoms and 6-MRs in the molecules, and  $x$  and  $y$  are fitted parameters. Here  $x/n$  and  $x/(N - y)$  describe the effect of the molecular size on the nonplanar distortion. Equation 2.3 takes a similar form to that used for the estimation of  $\Delta H_f^0$ .<sup>11</sup> The superscripts I, II, and III denote the models used in the estimation of  $E_{np}$ .

The values of  $E_{np}$  in Table S1 were fitted by eqs 2.1–2.3 based on the least-squares theory, and three sets of parameters were produced for Motif Model I, II, and III, respectively. For Motif Model I,  $E_{np}^i = 53.54, 53.86, 56.05, 56.89, 57.35, 58.39, 60.56$ , and  $53.12$  kcal/mol for  $i = \mathbf{A}, \mathbf{B}, \dots, \mathbf{H}$ , respectively, and  $x = -4933.21$  kcal/mol. For Motif Model II,  $E_{np}^i = 59.37, 63.13, 63.59, 68.33, 67.87, 71.92, 77.01$ , and  $55.27$  kcal/mol for  $i = \mathbf{A}, \mathbf{B}, \dots, \mathbf{H}$ , respectively;  $E_{np}^i = -0.04, 1.87, 2.01, 1.77, 4.74, 5.92, 6.72$ , and  $-3.27$  kcal/mol for  $i = \mathbf{a}, \mathbf{b}, \dots, \mathbf{h}$ , respectively, and  $x = -8104.91$  kcal/mol. And for Motif Model III,  $E_{np}^i = -3.17, -36.91, 89.54, -68.02, -67.05, 215.52, 56.76, -110.21, 343.90, 181.15, 180.18, 468.82, 755.78, 49.83, 27.86, 17.61, -27.23, -4.90, 145.55, 4.71, 100.92, -48.64, 54.97, -78.35, 81.45, 36.16, 76.15, 62.95, 49.17$ , and  $84.54$  kcal/mol for  $i = 1, 2, \dots, 30$ , respectively, and  $x = 1.11 \times 10^5$  kcal/mol,  $y = -31.59$ . The errors are described by

$$\text{Error}_j = E_{np}^j - E_{np}^{\text{cal}} \quad (j = \text{I, II, and III}) \quad (3)$$

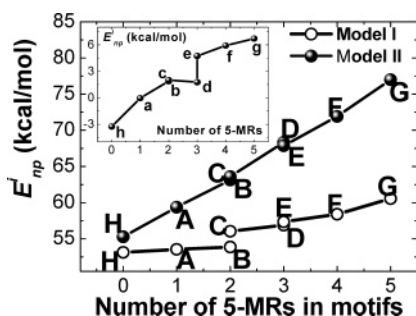


**Figure 3.** (a) 6-MRs around the central 5-MR are designated based on Motif Model III:  $\alpha$ , 6666;  $\beta$ , 666665; and  $\gamma$ , 666666. (b) Estimated  $E_{np}$  for model molecules  $C_N$  from eq 4.1–4.3, based on Motif Model I, II, and III.  $E_{np}^{66666}$  is in units of kcal/mol.

$E_{np}^j$  and  $E_{np}^{\text{cal}}$  are estimated by Motif Models and calculated based on the coordinates optimized at the level of B3LYP/6-31G(d). The goodness of fitting was also described by the mean absolute deviation (MAD) and the root-mean-square error (RMS). Panels a–c of Figure 2 illustrate the error distributions with MAD and RMS for estimated values of  $E_{np}$  from eq 2.1 to (2.3). As shown in Figure 2, the quality of fitting is  $I < II < III$  from the values of MAD and RMS.

The purpose of developing motifs is to estimate the values of  $E_{np}$  of fullerenes with hundreds of carbon atoms; hence, the validity of the motifs should be tested by very large molecules if the parameters developed here are universal. Using  $C_{180}$  ( $I_h$ ) as an example,  $E_{np}$  was 539.1 kcal/mol, using eq 1 based on the coordinates from B3LYP/6-31G(d).<sup>11</sup> Using Motif Models I, II, and III, the structure of  $C_{180}$  ( $I_h$ ) can be described by  $12\mathbf{H}$ ,  $12\mathbf{H} + 12\mathbf{h}$ , and  $20 \times 656565 + 60 \times 666666$ , respectively. Here 656565 and 666666 denote motifs defined by Cioslowski et al. and the details about their definitions can be found elsewhere.<sup>11</sup> On the basis of the above fitted parameters,  $E_{np}^I = 575.8$ ,  $E_{np}^{II} = 522.8$ , and  $E_{np}^{III} = 261.3$  kcal/mol for  $C_{180}$  ( $I_h$ ). Clearly, Motif Model II produced the best estimation for  $C_{180}$  ( $I_h$ ). In addition, the result of  $E_{np}^{III}$  was surprisingly poor even though there were 32 parameters, which were many more than those of Motif Models I (8 motifs) and II (16 motifs). To further illustrate the intrinsic limitations of Motif Model III, a model molecule  $C_N$  ( $I_h$ ) was designed: there were only 5- and 6-MRs in  $C_N$ , moreover, 5-MRs in fullerenes  $C_N$  distribute so far away from each other that each 5-MR would have almost no effect on the nearest 5-MR; hence, the environment of each 5-MR can be described by Figure 3a. Mathematically, the number of 6-MR can be expressed by  $n = (N - 20)/2$  if there are only 5- and 6-MRs in  $C_N$ . On the basis of Motif Model III, 6-MRs around the central 5-MR were designated as  $\alpha$  6666,  $\beta$  666665, and  $\gamma$  666666, as shown in Figure 3a. Therefore, the structure of  $C_N$  can be described by  $12\mathbf{H}$ ,  $12\mathbf{H} + 12\mathbf{h}$ ,  $12 \times (5 \times 6666 + 5 \times 666665 + 5 \times 666666) + (n - 12 \times 15) \times 666666$ , based on Motif Models I, II, and III. Thus, the values of  $E_{np}$





**Figure 4.**  $E_{np}^i$  ( $i = A, \dots, H, a, \dots, h$ ) versus the number of 5-MRs in each motif.

for  $C_N$  can be estimated by Motif Models I, II, and III as

$$E_{np}^I = 12 \times 53.12 - 4933.21/n \quad (4.1)$$

$$E_{np}^{II} = 12 \times 55.27 + 12 \times (-3.27) - 8104.91/n \quad (4.2)$$

$$E_{np}^{III} = 60 \times 49.83 + 60 \times (-36.91) + (n - 120) \times (-3.17) - 11097/(N + 31.59) \quad (4.3)$$

For the model molecule  $C_N$ , the relationships between  $E_{np}$  and  $N$  described by eq 4.1–4.3 are illustrated in Figure 3b. Clearly, Motif Models I and II gave stable results around 600 kcal/mol, while Motif Model III gave negative results for  $E_{np}$  when  $N > 740$ , which is obviously wrong. The invalidity of Motif Model III is due to the definition which uses a 6-MR as the central unit. According to the Euler law, the number of 5-MRs in fullerenes composed of 5- and 6-MRs maintains a constant value of 12. Then the number of 6-MRs,  $n$ , increases monotonically with the increment of  $N$ , as described by  $n = (N - 20)/2$ . Hence, the contribution of 666666,  $E_{np}^{666666}$ , will dominate the value of  $E_{np}$  and produce a negative value for large  $C_N$  since its contribution from the above is  $-3.17$  kcal/mol. To avoid the estimated  $E_{np}$  from Motif Model III decreasing or increasing (if  $E_{np}^{666666}$  takes a positive value) monotonically,  $E_{np}^{666666}$  must take the value of 0.0 kcal/mol, which produced values as large as 740 to 770 kcal/mol, as shown in Figure 3b. According to the symmetry, the model molecule  $C_N$  should be a stable configuration, suggesting that the high values of  $E_{np}$  which were calculated based on Motif Model III with  $E_{np}^{666666} = 0.0$  kcal/mol are completely wrong. Therefore, Motif Model III is not valid for the estimation of  $E_{np}$ , although it produces very good results for the estimation of the standard heats of formation of fullerenes and also gave good estimation of  $E_{np}$  for 114 IPR fullerenes investigated here. The success of the estimation of  $E_{np}$  presented in Figure 2c may be due to the increment of the employed parameters.

Figure 4 illustrates the relationship between the contributions of motifs,  $E_{np}^i$  ( $i = A, \dots, H, a, \dots, h$ ) and the number of 5-MRs in the respective motifs. For Motif Model I,  $E_{np}^H < E_{np}^A < E_{np}^B < E_{np}^C < E_{np}^D < E_{np}^E < E_{np}^F < E_{np}^G$ , suggesting that  $E_{np}^i$  increases monotonically with the increment of the number of 5-MRs. For Motif Model II, the above conclusion is satisfied for A–H as well,  $E_{np}^H < E_{np}^A < E_{np}^B < E_{np}^C < E_{np}^D < E_{np}^E < E_{np}^F < E_{np}^G$ . For motifs of a–h in Motif Model II,  $E_{np}^h < E_{np}^a < E_{np}^d < E_{np}^b < E_{np}^c < E_{np}^e < E_{np}^f < E_{np}^g$ , as shown in the inset of Figure 4; exceptionally, the contribution of d is slightly smaller than that of b and c. For motifs with the same number of 5-MRs, such as D and E, B and C, b and c, and d and e, motifs with dispersive distributions of 5-MRs have smaller contributions to  $E_{np}$  except for D and E. The above two exceptions (d and D

and E) may be due to the limitation of sample molecules employed in the above fitting. Since the number of 5-MRs in motifs indicates the concentration of 5-MRs, the nonplanar distortion of fullerenes increases with the concentration of 5-MRs.

#### 4. Conclusion

In conclusion, accurate strain energies due to nonplanar distortions ( $E_{np}$ ) of 114 IPR fullerenes containing 60 to 102 carbon atoms were calculated based on the structures optimized at the level of B3LYP/6-31G(d). The calculated values of  $E_{np}$  have been reproduced within several kilocalories per mole by three simple schemes based on counts of 8, 16, and 30 distinct motifs. With use of  $C_{180}$  and  $C_N$  ( $I_h$ ) as test molecules, it was found that Motif Model III becomes invalid when  $C_N$  is extended to very large molecules. For Motif Models I and II, the relationship between the contributions of motifs to  $E_{np}$  and the number of 5-MRs in motifs suggests that IPR fullerenes with dispersed 5-MRs present smaller nonplanar distortions. The findings presented in this work will be very useful for the quantitative estimation of  $E_{np}$  and understanding the formation, stability, and reactivity of IPR fullerenes. For instance, based on these results, fragments with the motif G have high nonplanar distortion, and thus they should exhibit high reactivity.

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**Supporting Information Available:** Table S1 lists the values of  $E_{np}$ . This material is available free of charge via the Internet at <http://pubs.acs.org>.

#### References and Notes

- Schmalz, T. G.; Seitz, W. A.; Klein, D. J.; Hite, G. E. *J. Am. Chem. Soc.* **1988**, *110*, 1113.
- Haddon, R. C. *Science* **1993**, *261*, 1545.
- Bakowies, D.; Thiel, W. *J. Am. Chem. Soc.* **1991**, *113*, 3704.
- Austin, S. J.; Fowler, P. W.; Manolopoulos, D. E.; Orlandi, G.; Zerbetto, F. *J. Phys. Chem.* **1995**, *99*, 8076.
- Kiyobayashi, T.; Yamamoto, K. *Rev. Heteroat. Chem.* **1998**, *18*, 231.
- Ivanciuc, O.; Babic, D.; Balaban, A. T. *Fullerene Sci. Technol.* **1999**, *7*, 1.
- Nunzi, F.; Sgamellotti, A. *Organometallics* **2002**, *21*, 2219.
- Meier, M. S.; Spielmann, H. P.; Bergosh, R. G.; Tetreau, M. C. *J. Org. Chem.* **2003**, *68*, 7867.
- Brinkmann, G.; Dress, A. W. M. *Adv. Appl. Math.* **1998**, *21*, 473.
- Achiba, Y.; Fowler, P. W.; Mitchell, D.; Zerbetto, F. *J. Phys. Chem. A* **1998**, *102*, 6835.
- Cioslowski, J.; Rao, N.; Moncrieff, D. *J. Am. Chem. Soc.* **2000**, *122*, 8265.
- Yu, J.; Sumathi, R.; Green, W. H., Jr. *J. Am. Chem. Soc.* **2004**, *126*, 12685.
- Austin, S. J.; Fowler, P. W.; Manolopoulos, D. E.; Orlandi, G.; Zerbetto, F. *J. Phys. Chem.* **1995**, *99*, 8076.
- Cyvin, B. N.; Neerland, G.; Brunvoll, J.; Cyvin, S. J. *Z. Naturforsch., A: Phys. Sci.* **1980**, *35*, 731.
- Cyvin, S. J.; Brendsdal, E.; Cyvin, B. N.; Brunvoll, J. *Chem. Phys. Lett.* **1988**, *143*, 377.
- Sun, C. H.; Finnerty, J. J.; Lu, G. Q.; Cheng, H. M. *J. Phys. Chem. B* **2005**, *109*, 12406.
- Haddon, R. C.; Scott, L. T. *Pure Appl. Chem.* **1986**, *58*, 137.
- Haddon, R. C. *J. Phys. Chem.* **1987**, *91*, 3719.
- Haddon, R. C. *J. Am. Chem. Soc.* **1986**, *108*, 2837.