

Relating the shape of a molecule and its reactivity – Haddon's curvature and the pyramidalization angle

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The supporting information presents an exploration of the C_n fullerenes data base available at <http://www.nanotube.msu.edu/fullerene/fullerene-isomers.html>.

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1 Geometry of a molecule: the representation problem

In this section, we precise our notations for molecules and the classical representation of a given molecule. We also formulated the Haddon's representation problem which was the first interest of R. C. Haddon [1].

1.1 Assumption on the description of a molecule

A molecule M is a structural assembly of N atoms denoted by A_i , $i = 1, \dots, N$. By structural assembly we mean that each atoms A_i of M is related to another atom of M by a bond whose nature is not further precised for the moment. In the following we look for a molecule in the following way:

1. Each atoms is represented in \mathbb{R}^3 by the position of the atoms nuclei also denoted by A_i . We denote by $\mathcal{A} = (A_i)_{i=1, \dots, N}$.
2. A set of real number $R_{i,j}$ indicating if an interaction between A_i and A_j exists: $R_{i,j} = 0$ if no interaction exists and $R_{i,j} = 1$ otherwise. We call matrix of connection and we denote by \mathcal{R} the matrix $\mathcal{R} = (R_{i,j})_{1 \leq i, j \leq N}$.
3. Two atoms A_i and A_j such that $A_{i,j} = 1$ are called **adjacent**.

A molecule is then encoded as $M = (\mathcal{A}, \mathcal{R})$. Of course, we have $R_{i,j} = R_{j,i}$ and the matrix of connection is a real symmetric matrix.

Remark 1 *The previous view point on a molecule can be encoded in a pure abstract way as a **graph** (Appendix A [2]) and the matrix \mathcal{R} corresponds to the **adjacency matrix** of the graph associated to the molecule.*

1.2 Skeleton of a molecule

It is not easy with the previous definition of a molecule to imagine the shape of a given molecule and many authors have decided to introduce a pure geometrical object supporting all these information introducing the notion of **skeleton** for a molecule.

Definition 1 *The skeleton of a molecule $M = (\mathcal{A}, \mathcal{R})$ is the geometrical object obtain by drawing a segment between the atoms A_i and A_j if $R_{i,j} = 1$. We denote by $S(M)$ the skeleton of M .*

The skeleton of a molecule is clearly the initial geometrical picture that one has looking for a molecule.

In some cases, the skeleton of a molecule looks like a polygonal curve or a polyhedron. This is for example the case of the fullerene C_{32} .

Remark 2 *It must be pointed out that the length of the bonds between atoms are fixed by the data of the molecule as atoms are associated to a given **position** in \mathbb{R}^3 . In the contrary, a typical graph of a molecule does not contain any metric information on the bonds between atoms.*

A skeleton of a molecule will be most of the time a **polygonal curve** or a **polyhedral surface** of \mathbb{R}^3 . These objects can be studied with the tool of **discrete differential geometry** (see for example [3]). We introduce some terminology which will be of some help in the following:

Let $M = (\mathcal{A}, \mathcal{R})$ be molecule and $S(M)$ its skeleton.

1. An atom $A \in \mathcal{A}$ is a **vertex** of $S(M)$.
2. A bond between two vertex A_i and A_j of $S(M)$ will be called an **edge** of $S(M)$.

We denote by E the set of edges of $S(M)$. We will use the two terminology vertex or atom equivalently.

Definition 2 *Let M be a molecule and $S(M)$ its skeleton. Let $A \in \mathcal{A}$. We call **star** of A and we denote by $\star(A)$ the set of vertex B connected to A by an edge.*

The **degree** or **valence** of an atom $A \in S(M)$ is the number of atoms connected to A (then the cardinal of $\star(A)$).

Remark 3 *The definition of $\star(A)$ is a different in the book of P. Romon [3] as it corresponds to the set of edges connected to A and the set of faces containing A .*

1.3 Solid structure of a molecule

Another common way to represent molecules is to associate to its skeleton a solid representation. We discuss this type of representation as it leads to some difficulties for some molecules.

Let $M = (\mathcal{A}, \mathcal{R})$ be a molecule and $S(M)$ its skeleton. In some cases, we can identify particular structures in $S(M)$ which are called **cycles**.

Definition 3 (Cycles) A finite set of atoms $A_{i_j} \in \mathcal{A}$, $j = 1, \dots, m$ is called a cycle if A_{i_j} and $A_{i_{j+1}}$ are adjacent and A_{i_m} is adjacent with A_{i_1} .

The image of a cycle by the mapping S is a closed polygonal curve in \mathbb{R}^3 . As an example, a graphene is made of cycles which correspond to hexagones and fullerene are made of pentagonal and hexagonal cycles. If all the atoms of a given cycle belong to the same plane, one can replace all cycles by a solid tile corresponding to the plane polygon. We then obtain a solid representation of the molecule leading to the classical picture of a fullerene as a soccer ball or a graphene as a plane.

However, the polygonal curve C is **in general a skew polygon** meaning that the curve is not contained in a fixed plane. As a consequence, one **can not replace the polygonal curve by a solid plane tile**. An idea to "fill" all the closed chains of a given

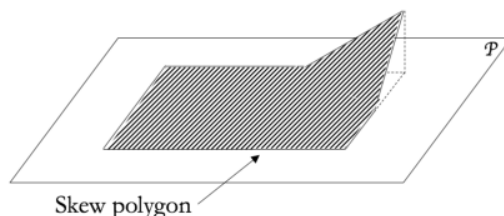


Figure S1: A skew polygon.

molecule is to bypass the planarity condition using a triangulation. A triangulation is a finite set of triangles T_i , $j = 1, \dots, p$ such that $\bigcup_{i=1}^p T_i = C$ and $T_i \cap T_j$ is reduced to a point or an edge. A triangulation is not unique or canonical.

Replacing each triangles by a solid plane tile leads to a "solid" representation of a molecule. However, this representation is very delicate to manipulate from the chemical point of view as we modify the number of vertices: some of these vertices correspond to real atoms and some other are only "virtual".

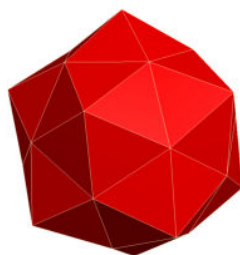


Figure S2: A possible triangulation of the C_{20} .

1.4 Skeleton representation versus continuous representation

Some skeleton presentations can have very nice shapes which make them very close to continuous surfaces or curves. This is the case for example with the skeleton of the C_{60} fullerene which looks like a sphere or the graphene which looks like a plane.

Definition 4 A molecule $M = (\mathcal{A}, \mathcal{R})$ is said to admit a continuous representation of dimension 1 or 2 if there exists a (smooth) submanifold $\mathcal{S} \subset \mathbb{R}^3$ of dimension 1 or 2 such that $A_i \in \mathcal{M}$ for all $i = 1, \dots, N$ and \mathcal{M} is homeomorphic to a solid representation of M .

As an example, the butadiene C_4H_6 has no continuous representation. Indeed, if so, then it must be of dimension 1. However, the structure of the molecule implies that we have an intersection of two 1 dimensional curves in order to take into account the hydrogen atoms. As a consequence, this can not be a submanifold. If one restrict only on the structure attached to the carbon atoms then it admits a continuous 1-dimensional representation. The fullerene however admits a two dimensional one. Indeed, a solid representation is given by a polyhedron and is homeomorphic to a sphere.

It must be noted that in some cases, one makes the reverse construction starting from a continuous surface and putting atoms on it respecting some classical physical constraints like the fact that the distance between two atoms can not be too small.

2 Tabulated value of $P_{yr}(A)$

The following table gives an overview of numerical values of $P_{yr}(A)$, the hybridization coefficients c_π and λ_π , the hybridization numbers m and n as a function of the angle θ as define on figure 2 of the article. In that case, we reminds that $P_{yr}(A) = \pi - \theta$.

The last column gives the hybridization, from the equations:

$$s^{\lambda_\pi^2} p_{x,y}^{n-3m} p_z^{c_\pi^2} \quad (1)$$

for the $\sigma - orbitals(h_i)$ and

$$s^{c_\pi^2} p_z^{\lambda_\pi^2} \quad (2)$$

for the $\pi - orbitals(h_\pi)$.

θ	$P_{yr}(A)$	c_π^2	λ_π^2	m	n	Hybridization
90.0	0.0	0.000	1.000	0.000	2.000	$(s^{1.000} p_{x,y}^{2.000} p_z^{0.000})_\sigma (s^{0.000} p_z^{1.000})_\pi$
92.0	2.0	0.002	0.998	0.002	2.007	$(s^{0.998} p_{x,y}^{2.000} p_z^{0.002})_\sigma (s^{0.002} p_z^{0.998})_\pi$
94.0	4.0	0.010	0.990	0.010	2.030	$(s^{0.990} p_{x,y}^{2.000} p_z^{0.010})_\sigma (s^{0.010} p_z^{0.990})_\pi$
96.0	6.0	0.022	0.978	0.023	2.068	$(s^{0.978} p_{x,y}^{2.000} p_z^{0.022})_\sigma (s^{0.022} p_z^{0.978})_\pi$
98.0	8.0	0.040	0.960	0.041	2.123	$(s^{0.960} p_{x,y}^{2.000} p_z^{0.040})_\sigma (s^{0.040} p_z^{0.960})_\pi$
100.0	10.0	0.062	0.938	0.066	2.199	$(s^{0.938} p_{x,y}^{2.000} p_z^{0.062})_\sigma (s^{0.062} p_z^{0.938})_\pi$
102.0	12.0	0.090	0.910	0.099	2.298	$(s^{0.910} p_{x,y}^{2.000} p_z^{0.090})_\sigma (s^{0.090} p_z^{0.910})_\pi$
104.0	14.0	0.124	0.876	0.142	2.426	$(s^{0.876} p_{x,y}^{2.000} p_z^{0.124})_\sigma (s^{0.124} p_z^{0.876})_\pi$
106.0	16.0	0.164	0.836	0.197	2.590	$(s^{0.836} p_{x,y}^{2.000} p_z^{0.164})_\sigma (s^{0.164} p_z^{0.836})_\pi$
107.0	17.0	0.187	0.813	0.230	2.690	$(s^{0.813} p_{x,y}^{2.000} p_z^{0.187})_\sigma (s^{0.187} p_z^{0.813})_\pi$
108.0	18.0	0.211	0.789	0.268	2.803	$(s^{0.789} p_{x,y}^{2.000} p_z^{0.211})_\sigma (s^{0.211} p_z^{0.789})_\pi$
109.0	19.0	0.237	0.763	0.311	2.932	$(s^{0.763} p_{x,y}^{2.000} p_z^{0.237})_\sigma (s^{0.237} p_z^{0.763})_\pi$
109.5	19.5	0.250	0.750	0.333	3.000	$(s^{0.750} p_{x,y}^{2.000} p_z^{0.250})_\sigma (s^{0.250} p_z^{0.750})_\pi$
110.0	20.0	0.265	0.735	0.360	3.081	$(s^{0.735} p_{x,y}^{2.000} p_z^{0.265})_\sigma (s^{0.265} p_z^{0.735})_\pi$
112.0	22.0	0.326	0.674	0.485	3.454	$(s^{0.674} p_{x,y}^{2.000} p_z^{0.326})_\sigma (s^{0.326} p_z^{0.674})_\pi$
114.0	24.0	0.396	0.604	0.657	3.971	$(s^{0.604} p_{x,y}^{2.000} p_z^{0.396})_\sigma (s^{0.396} p_z^{0.604})_\pi$
116.0	26.0	0.476	0.524	0.908	4.723	$(s^{0.524} p_{x,y}^{2.000} p_z^{0.476})_\sigma (s^{0.476} p_z^{0.524})_\pi$

3 Global analysis

3.1 Shape analysis

This part completes the elements presented in part II (B. 8. b.) and part V (B.). The information mentioned provide an analysis of the shape of the C_n isomers. To do that, we compute the mean and standard deviation of the pyramidalization angle for each isomer.

Table S1 presents the average and standard deviation of the pyramidalization angle of the isomers with 180 or more atoms. These isomers are the most spherical ones.

Table S1: Average and standard deviation of the pyramidalization angle (in degrees) of isomers with more than 100 atoms.

Compound	# Atom	$\langle Pyr(A) \rangle$	$\sigma_{Pyr(A)}$
C_{180}	180	6.68	0.11
C_{240}	240	5.78	0.05
C_{260}	260	5.56	0.11
C_{320}	320	5.02	0.19
C_{500}	500	4.03	0.35
C_{540}	540	3.89	0.33
C_{720}	720	3.38	0.52

On the contrary, table IV in the article, lists the isomers that present the largest deviation standard of the pyramidalization angle ($\sigma_{Pyr(A)} > 4.5^\circ$).

The various figures associated with this section are in the paper: figures 5, 16, tables III, IV.

4 Atomic analysis

4.1 Full analysis

Here we present an overview of the range of variation and the correlations between the geometrical descriptors defined in the article. The data base contains 2487 isomers between 20 and 720 atoms and the total number of atoms is 181794. First, table S2, shows statistical descriptors of the geometrical quantities.

Table S2: Statistical descriptors of the angular defect (degrees), $Pyr(A)$, the pyramidalization angle (degrees), the spherical curvature $\kappa(A)$, the hybridization coefficients c_π^2 and λ_π^2 , the hybridization numbers m and n , and the hybridization.

	$Pyr(A)$	Angular defect	Spherical curvature	c_π^2	λ_π^2	m	n	Hybridization
mean	10.49	10.42	0.262	0.074	0.926	0.084	2.252	$(s^{0.926} p_{x,y}^{2.000} p_z^{0.074})_\sigma (s^{0.074} p_z^{0.926})_\pi$
std	2.83	6.04	0.072	0.048	0.048	0.067	0.201	$(s^{0.048} p_{x,y}^{0.000} p_z^{0.048})_\sigma (s^{0.048} p_z^{0.048})_\pi$
min	2.60	0.61	0.065	0.004	0.485	0.004	2.012	$(s^{0.485} p_{x,y}^{2.000} p_z^{0.004})_\sigma (s^{0.004} p_z^{0.485})_\pi$
25%	8.72	6.84	0.217	0.047	0.918	0.049	2.148	$(s^{0.918} p_{x,y}^{2.001} p_z^{0.047})_\sigma (s^{0.047} p_z^{0.918})_\pi$
50%	9.80	8.59	0.246	0.060	0.940	0.063	2.190	$(s^{0.940} p_{x,y}^{2.001} p_z^{0.060})_\sigma (s^{0.060} p_z^{0.940})_\pi$
75%	11.45	11.64	0.288	0.082	0.953	0.089	2.268	$(s^{0.953} p_{x,y}^{2.001} p_z^{0.082})_\sigma (s^{0.082} p_z^{0.953})_\pi$
max	26.90	59.67	0.637	0.515	0.996	1.061	5.184	$(s^{0.996} p_{x,y}^{2.001} p_z^{0.515})_\sigma (s^{0.515} p_z^{0.996})_\pi$

This section is associated to figure 18 part V (B. 3.) in the article which shows the pairwise relationship between $Pyr(A)$, the angular defect, the spherical curvature and the hybridization on the whole isomers of the data base.

Figure S3 presents pairwise relationships, considering all isomers in the database, between a complete set of quantities: $Pyr(A)$, the angular defect, the spherical curvature, the hybridization coefficients c_π^2 and λ_π^2 , the hybridization numbers m and n and the hybridization. As previously in the paper, the isomers are separated in three classes: *small* isomers, *medium* isomers and *large* isomers corresponding to isomers with less than 60 atoms, less than 100 atoms and larger than 100 atoms respectively. Figure S4 is exactly the same but only for isomers smaller than 60 atoms.

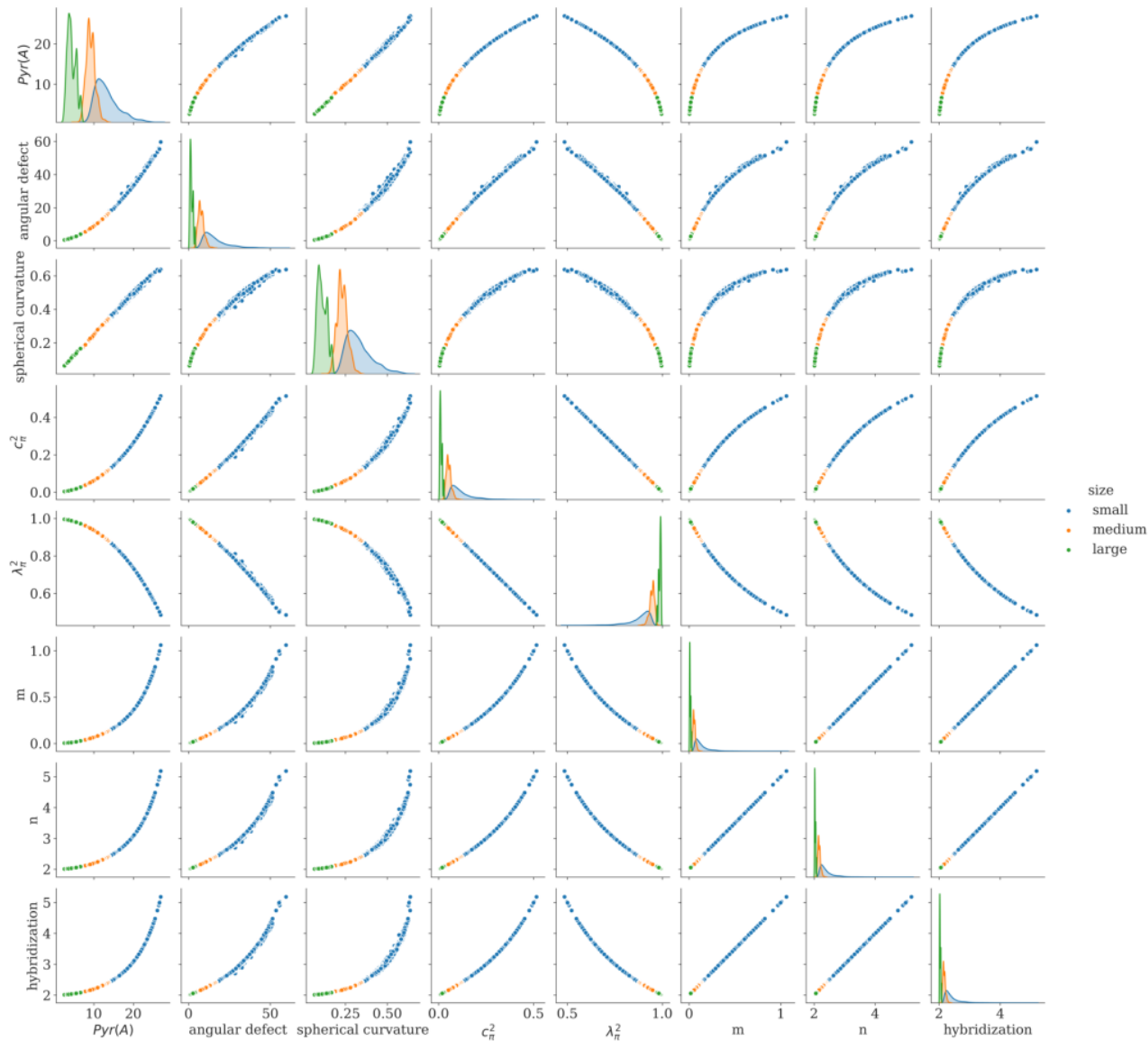


Figure S3: Pairwise relationships between the pyramidalization angle $Pyr(A)$, the angular defect, the spherical curvature, the hybridization coefficients c_π^2 and λ_π^2 , the hybridization numbers m and n and the hybridization on the whole isomers of the data base. Size *small*, *medium* and *large* correspond to isomers with less than 60 atoms, less than 100 atoms and larger than 100 atoms respectively.

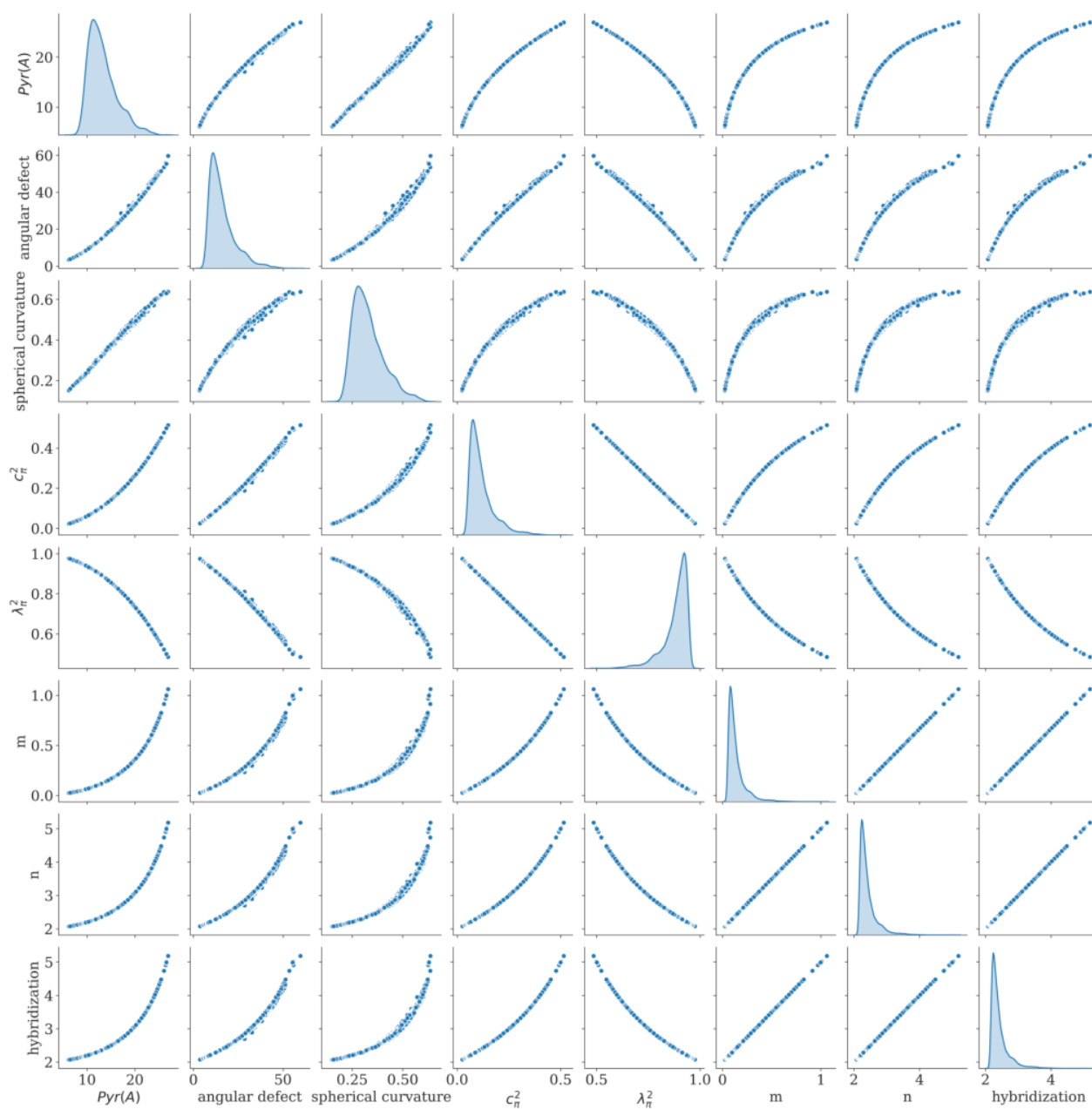


Figure S4: Pairwise relationships between the pyramidalization angle $Pyr(A)$, the angular defect, the spherical curvature, the hybridization coefficients c_{π}^2 and λ_{π}^2 , the hybridization numbers m and n and the hybridization on isomers with less than 60 atoms.

Figures S5 and S6 are the same as figure 18 shows that there is a clear relation between the pyramidalization angle, the angular defect and the spherical curvature, it may be enough to consider only one geometrical parameters, $Pyr(A)$ and to look at its relationship with electronic descriptors, the hybridization coefficients c_{π}^2 and λ_{π}^2 , the hybridization numbers m and n and the hybridization.

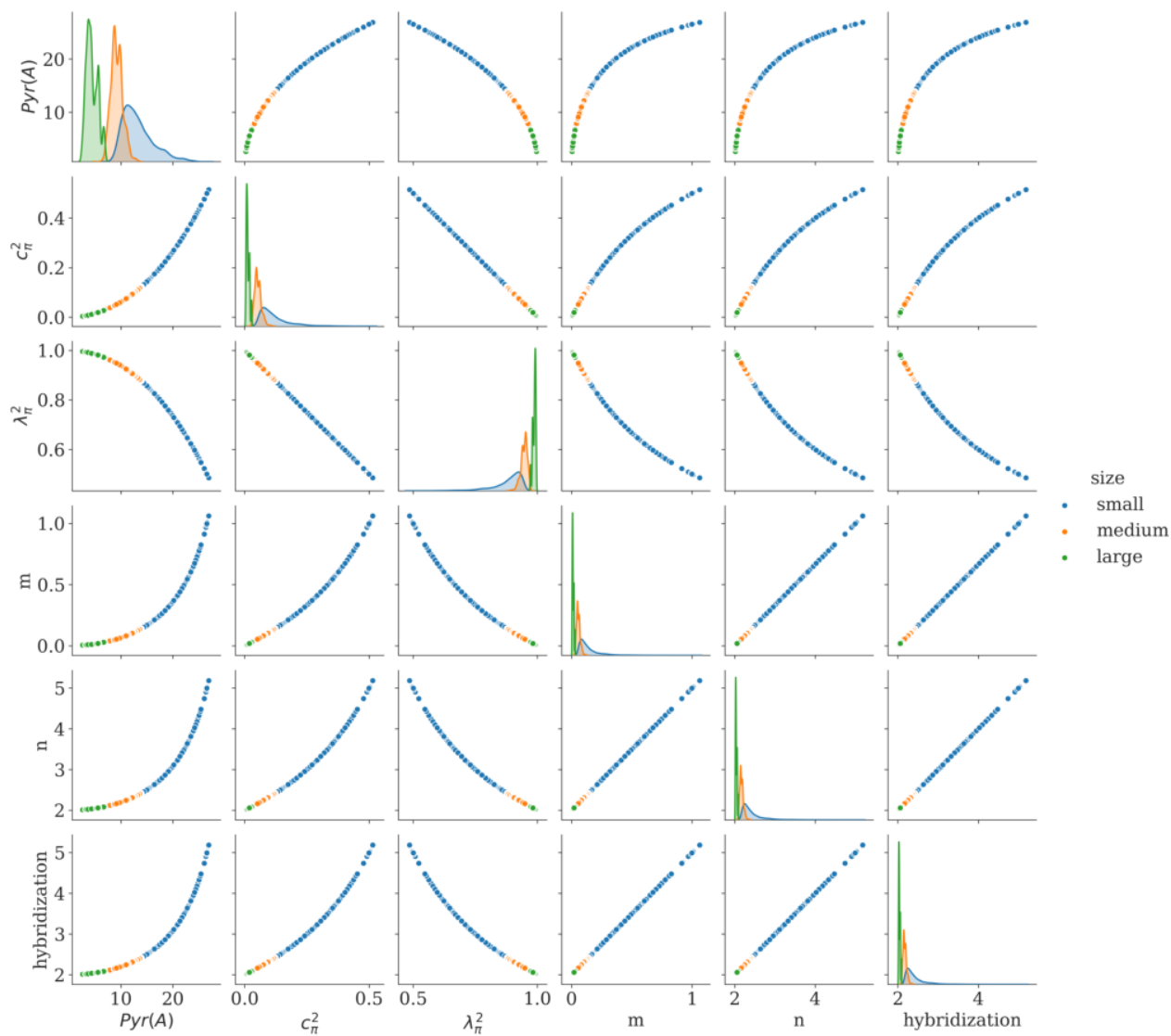


Figure S5: Pairwise relationships between the pyramidalization angle $Pyr(A)$, the hybridization coefficients c_{π}^2 and λ_{π}^2 , the hybridization numbers m and n and the hybridization on the whole isomers of the data base. Size *small*, *medium* and *large* correspond to isomers with less than 60 atoms, less than 100 atoms and larger than 100 atoms respectively.

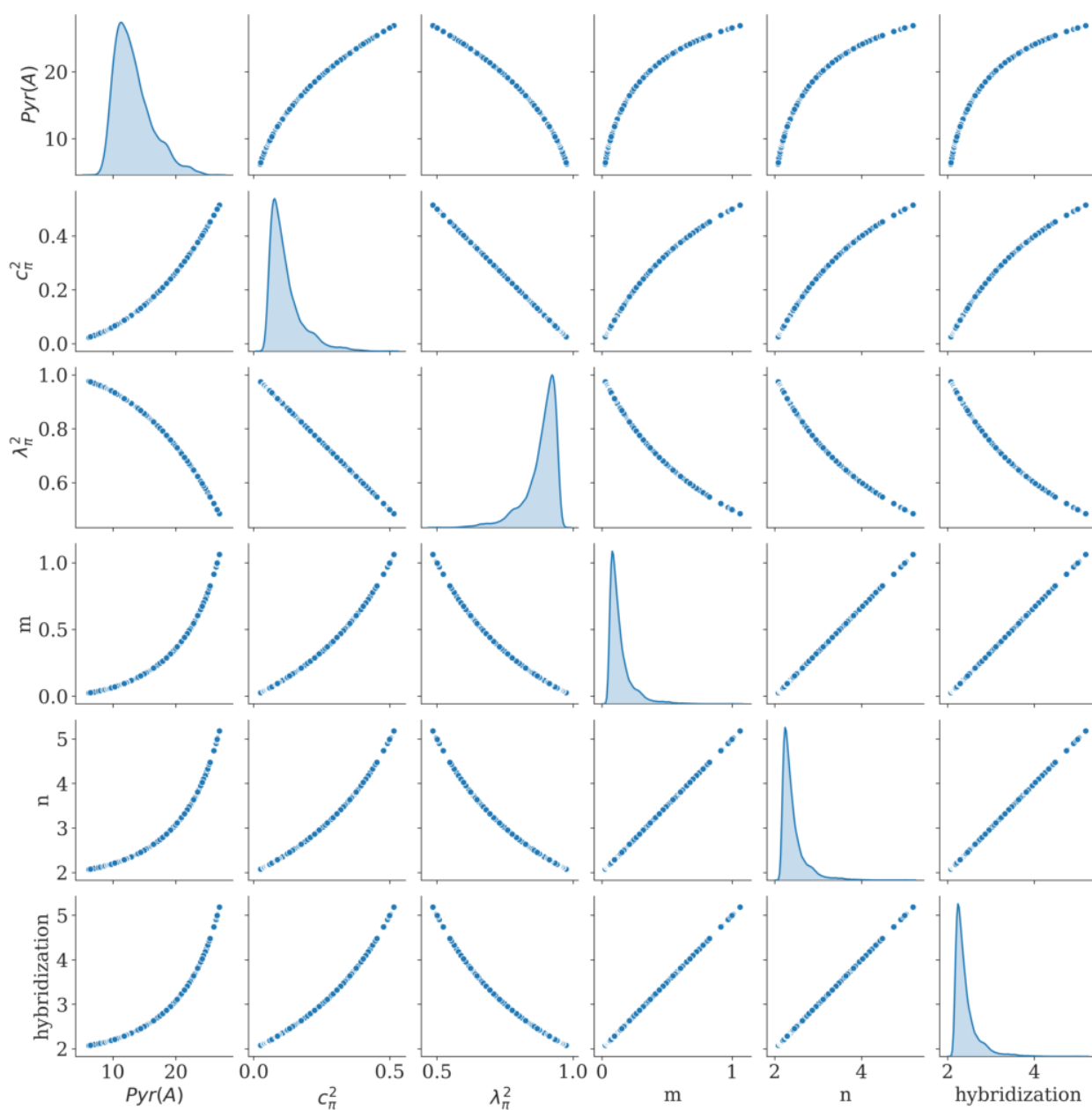


Figure S6: Pairwise relationships between the pyramidalization angle $Pyr(A)$, the hybridization coefficients c_{π}^2 and λ_{π}^2 , the hybridization numbers m and n and the hybridization on isomers with less than 60 atoms.

4.2 C_{60} isomer

The data in the tables S3 and S4 concern the C_{60} isomer and are given as reference for further comparison. One can see that the results of the geometrical optimization leads to a higher symmetrical structure with a small dispersion of the geometrical quantities. Moreover, the C_{60} isomer is close to a spherical shape and presents a shape anisotropy close to zero.

Table S3: Statistical data for the C_{60} isomer before and after the geometrical optimization.

Structure	$Pyr(A)$		Angular defect		Spherical curvature	
	Initial	Optimized	Initial	Optimized	Initial	Optimized
mean	11.64	11.64	12.00	12.00	0.290	0.281
std	0.22	0.01	0.45	0.01	0.006	0.000
min	11.21	11.63	11.17	11.97	0.280	0.281
25%	11.46	11.64	11.64	11.99	0.286	0.281
50%	11.60	11.64	11.92	12.00	0.290	0.281
75%	11.81	11.65	12.35	12.01	0.295	0.282
max	12.13	11.66	13.01	12.03	0.303	0.282

Structure	c_π^2		λ_π^2		m		n	
	Initial	Optimized	Initial	Optimized	Initial	Optimized	Initial	Optimized
mean	0.085	0.085	0.915	0.915	0.093	0.093	2.278	2.278
std	0.003	0.000	0.003	0.000	0.004	0.000	0.012	0.000
min	0.079	0.085	0.908	0.915	0.085	0.092	2.256	2.277
25%	0.082	0.085	0.913	0.915	0.090	0.093	2.269	2.278
50%	0.084	0.085	0.916	0.915	0.092	0.093	2.276	2.278
75%	0.087	0.085	0.918	0.915	0.096	0.093	2.288	2.279
max	0.092	0.085	0.921	0.915	0.102	0.093	2.305	2.279

Table S4: Hybridization following the statistical data for C_{60} before and after the geometrical optimization

Hybridization	
Initial	Optimized
$(s^{0.915} p_{x,y}^{1.999} p_z^{0.085})_\sigma (s^{0.085} p_z^{0.915})_\pi$	$(s^{0.915} p_{x,y}^{1.999} p_z^{0.085})_\sigma (s^{0.085} p_z^{0.915})_\pi$
$(s^{0.003} p_{x,y}^{0.000} p_z^{0.003})_\sigma (s^{0.003} p_z^{0.003})_\pi$	$(s^{0.000} p_{x,y}^{0.000} p_z^{0.000})_\sigma (s^{0.000} p_z^{0.000})_\pi$
$(s^{0.908} p_{x,y}^{2.001} p_z^{0.079})_\sigma (s^{0.079} p_z^{0.908})_\pi$	$(s^{0.915} p_{x,y}^{2.001} p_z^{0.085})_\sigma (s^{0.085} p_z^{0.915})_\pi$
$(s^{0.913} p_{x,y}^{1.999} p_z^{0.082})_\sigma (s^{0.082} p_z^{0.913})_\pi$	$(s^{0.915} p_{x,y}^{1.999} p_z^{0.085})_\sigma (s^{0.085} p_z^{0.915})_\pi$
$(s^{0.916} p_{x,y}^{2.000} p_z^{0.084})_\sigma (s^{0.084} p_z^{0.916})_\pi$	$(s^{0.915} p_{x,y}^{1.999} p_z^{0.085})_\sigma (s^{0.085} p_z^{0.915})_\pi$
$(s^{0.918} p_{x,y}^{2.000} p_z^{0.087})_\sigma (s^{0.087} p_z^{0.918})_\pi$	$(s^{0.915} p_{x,y}^{2.000} p_z^{0.085})_\sigma (s^{0.085} p_z^{0.915})_\pi$
$(s^{0.921} p_{x,y}^{1.999} p_z^{0.092})_\sigma (s^{0.092} p_z^{0.921})_\pi$	$(s^{0.915} p_{x,y}^{2.000} p_z^{0.085})_\sigma (s^{0.085} p_z^{0.915})_\pi$

4.3 C_{32} isomers

4.3.1 Statistics

The statistical descriptors of the geometrical quantities for the six isomers of the C_{32} family after a geometrical optimization are presented and discussed in the article in part V (C. figures 19, 20 and table V).

Table S5 presents the mean quantities grouped by isomers after the geometrical relaxation.

Table S5: Mean of the geometrical and hybridization quantities grouped by isomers of the C_{32} family after a geometrical optimization.

	$Pyr(A)$	Angular defect	Spherical curvature	c_{π}^2	λ_{π}^2	m	n	Hybridization	ΔE (kcal/mol)
D_3 (6)	16.24	22.86	0.387	0.171	0.829	0.208	2.623	$(s^{0.829} p_{x,y}^{1.999} p_z^{0.171})_{\sigma} (s^{0.171} p_z^{0.829})_{\pi}$	0.0
C_2 (4)	16.35	23.25	0.389	0.175	0.825	0.216	2.647	$(s^{0.825} p_{x,y}^{1.999} p_z^{0.175})_{\sigma} (s^{0.175} p_z^{0.825})_{\pi}$	25.9
C_2 (1)	16.46	23.70	0.391	0.181	0.819	0.229	2.687	$(s^{0.819} p_{x,y}^{2.000} p_z^{0.181})_{\sigma} (s^{0.181} p_z^{0.819})_{\pi}$	54.2
D_2 (2)	16.56	24.02	0.393	0.184	0.816	0.235	2.705	$(s^{0.816} p_{x,y}^{2.000} p_z^{0.184})_{\sigma} (s^{0.184} p_z^{0.816})_{\pi}$	64.8
D_{3d} (3)	16.58	24.14	0.394	0.186	0.814	0.249	2.748	$(s^{0.814} p_{x,y}^{2.001} p_z^{0.186})_{\sigma} (s^{0.186} p_z^{0.814})_{\pi}$	73.4
D_{3h} (5)	16.54	24.04	0.393	0.184	0.816	0.235	2.705	$(s^{0.816} p_{x,y}^{2.000} p_z^{0.184})_{\sigma} (s^{0.184} p_z^{0.816})_{\pi}$	78.0
I_h (0)	11.64	12.00	0.281	0.085	0.915	0.093	2.278	$(s^{0.915} p_{x,y}^{1.999} p_z^{0.085})_{\sigma} (s^{0.085} p_z^{0.915})_{\pi}$	

4.3.2 Graphical analysis

In the paper, figures 19 and 20 present the distributions of the pyramidalization angle and the hybridization of the atoms in C_{32} isomers before (initial) and after (optimized) a geometrical optimization using quantum chemistry, respectively. From these figures, one can see that the geometrical optimization leads to increase the symmetry of the systems. Moreover, these isomers present globally higher pyramidalization angle than the C_{60} isomer. This is due to the small size of the systems. Looking at the relative energies between isomers, the most stable isomers is not the one which shows the lowest pyramidalization angle nor the one with the higher symmetry. However, the relative stability of the isomers seems to be linked to the width of the pyramidalization angle distributions and thus to the heterogeneity of the structures.

Figures S7 and S8 present the pairwise relationships between $Pyr(A)$, the angular defect, the spherical curvature and the hybridization for the six C_{32} isomers.

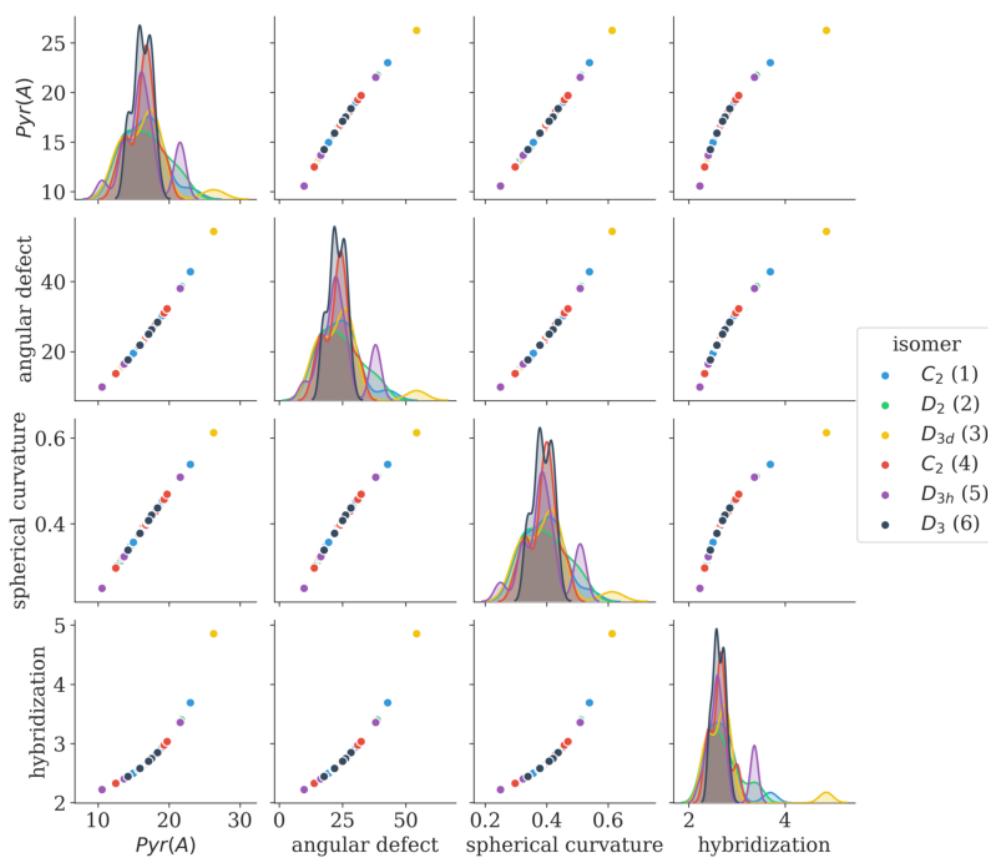


Figure S7: Pairwise relationships between $Pyr(A)$, the angular defect and the spherical curvature for the six C_{32} isomers considering only optimized structures.

ù

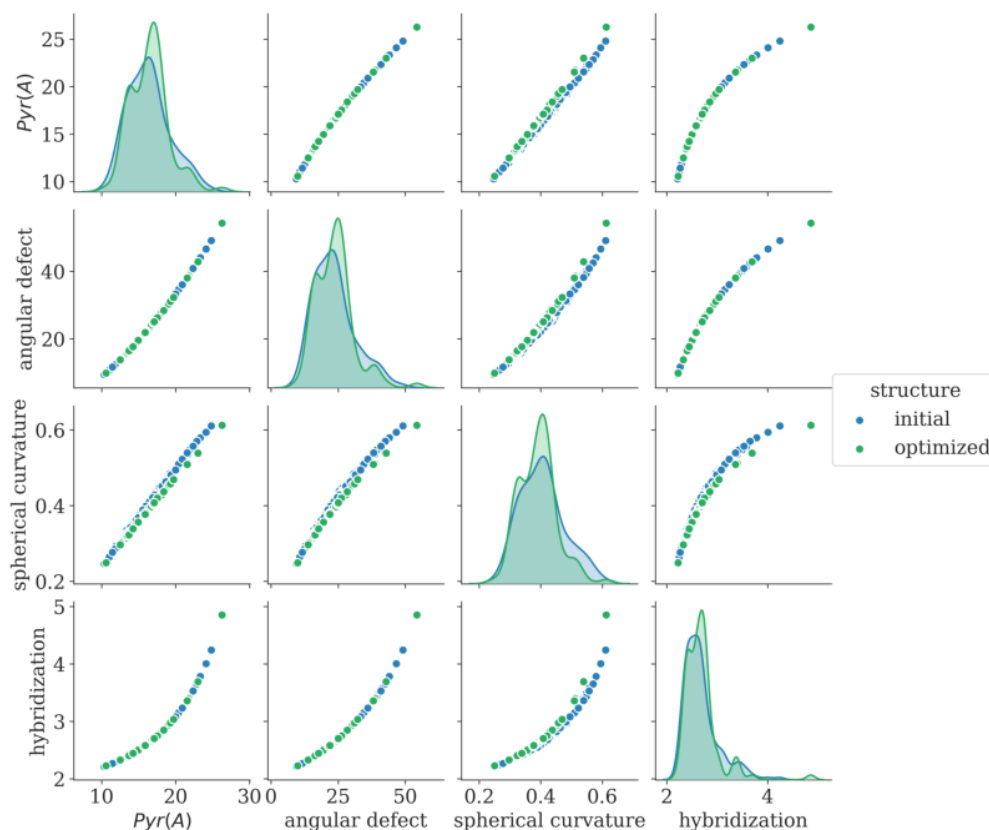


Figure S8: Pairwise relationships between $Pyr(A)$, the angular defect and the spherical curvature for the six C_{32} isomers and comparing optimized and initial structures.

4.4 C_{40} isomers

4.4.1 Statistics

Table S6 provides statistical descriptors of the geometrical quantities for the isomers of the C_{40} family after a geometrical optimization.

Table S6: Statistical descriptors of isomers of the C_{40} family.

	$Pyr(A)$	Angular defect	Spherical curvature	c_π^2	λ_π^2	m	n	Hybridization
mean	14.73	19.45	0.352	0.145	0.855	0.177	2.531	$(s^{0.855} p_{x,y}^{2.000} p_z^{0.145}) \sigma (s^{0.145} p_z^{0.855}) \pi$
std	2.96	7.40	0.070	0.063	0.063	0.096	0.289	$(s^{0.063} p_{x,y}^{0.000} p_z^{0.063}) \sigma (s^{0.063} p_z^{0.063}) \pi$
min	8.26	6.09	0.196	0.042	0.578	0.044	2.132	$(s^{0.578} p_{x,y}^{2.000} p_z^{0.042}) \sigma (s^{0.042} p_z^{0.578}) \pi$
25%	12.61	14.02	0.302	0.100	0.820	0.111	2.334	$(s^{0.820} p_{x,y}^{2.001} p_z^{0.100}) \sigma (s^{0.100} p_z^{0.820}) \pi$
50%	14.43	18.19	0.346	0.132	0.868	0.153	2.458	$(s^{0.868} p_{x,y}^{1.999} p_z^{0.132}) \sigma (s^{0.132} p_z^{0.868}) \pi$
75%	16.70	23.96	0.399	0.180	0.900	0.219	2.658	$(s^{0.900} p_{x,y}^{2.001} p_z^{0.180}) \sigma (s^{0.180} p_z^{0.900}) \pi$
max	24.67	48.60	0.579	0.422	0.958	0.730	4.189	$(s^{0.958} p_{x,y}^{1.999} p_z^{0.422}) \sigma (s^{0.422} p_z^{0.958}) \pi$

Table S7 presents the mean quantities grouped by isomers after the geometrical relaxation.

Table S7: Mean of the geometrical quantities grouped by isomers of the C₄₀ family.

	<i>Pyr(A)</i>	Angular defect	Spherical curvature	c_{π}^2	λ_{π}^2	<i>m</i>	<i>n</i>	Hybridization	ΔE (kcal/mol)
<i>D</i> ₂ (38)	14.46	18.39	0.346	0.135	0.865	0.157	2.470	$(s^{0.865} p_{x,y}^{1.999} p_z^{0.135})_{\sigma} (s^{0.135} p_z^{0.865})_{\pi}$	0.0
<i>D</i> _{5d} (39)	14.49	18.61	0.347	0.137	0.863	0.160	2.480	$(s^{0.863} p_{x,y}^{2.000} p_z^{0.137})_{\sigma} (s^{0.137} p_z^{0.863})_{\pi}$	10.2
<i>C</i> _s (31)	14.54	18.67	0.348	0.137	0.863	0.162	2.485	$(s^{0.863} p_{x,y}^{1.999} p_z^{0.137})_{\sigma} (s^{0.137} p_z^{0.863})_{\pi}$	16.1
<i>C</i> ₂ (29)	14.55	18.77	0.348	0.139	0.861	0.164	2.492	$(s^{0.861} p_{x,y}^{2.000} p_z^{0.139})_{\sigma} (s^{0.139} p_z^{0.861})_{\pi}$	21.6
<i>C</i> ₁ (26)	14.56	18.82	0.348	0.139	0.861	0.165	2.495	$(s^{0.861} p_{x,y}^{2.000} p_z^{0.139})_{\sigma} (s^{0.139} p_z^{0.861})_{\pi}$	23.9
<i>C</i> _s (24)	14.56	18.87	0.349	0.140	0.860	0.167	2.500	$(s^{0.860} p_{x,y}^{1.999} p_z^{0.140})_{\sigma} (s^{0.140} p_z^{0.860})_{\pi}$	28.5
<i>C</i> _{2v} (37)	14.53	18.68	0.348	0.137	0.863	0.161	2.482	$(s^{0.863} p_{x,y}^{1.999} p_z^{0.137})_{\sigma} (s^{0.137} p_z^{0.863})_{\pi}$	29.7
<i>T</i> _d (40)	14.58	18.82	0.349	0.139	0.861	0.164	2.493	$(s^{0.861} p_{x,y}^{2.001} p_z^{0.139})_{\sigma} (s^{0.139} p_z^{0.861})_{\pi}$	36.9
<i>C</i> ₂ (36)	14.53	18.75	0.348	0.138	0.862	0.163	2.488	$(s^{0.862} p_{x,y}^{1.999} p_z^{0.138})_{\sigma} (s^{0.138} p_z^{0.862})_{\pi}$	39.2
<i>C</i> ₂ (25)	14.66	19.18	0.351	0.143	0.857	0.171	2.513	$(s^{0.857} p_{x,y}^{2.000} p_z^{0.143})_{\sigma} (s^{0.143} p_z^{0.857})_{\pi}$	41.7
<i>C</i> ₁ (22)	14.64	19.13	0.350	0.142	0.858	0.172	2.515	$(s^{0.858} p_{x,y}^{1.999} p_z^{0.142})_{\sigma} (s^{0.142} p_z^{0.858})_{\pi}$	42.1
<i>C</i> _s (14)	14.64	19.17	0.350	0.143	0.857	0.174	2.521	$(s^{0.857} p_{x,y}^{1.999} p_z^{0.143})_{\sigma} (s^{0.143} p_z^{0.857})_{\pi}$	42.3
<i>C</i> ₂ (21)	14.68	19.25	0.351	0.143	0.857	0.173	2.520	$(s^{0.857} p_{x,y}^{2.001} p_z^{0.143})_{\sigma} (s^{0.143} p_z^{0.857})_{\pi}$	43.1
<i>C</i> ₂ (27)	14.61	19.04	0.350	0.141	0.859	0.169	2.507	$(s^{0.859} p_{x,y}^{2.000} p_z^{0.141})_{\sigma} (s^{0.141} p_z^{0.859})_{\pi}$	44.5
<i>C</i> ₃ (30)	14.65	19.21	0.350	0.143	0.857	0.175	2.525	$(s^{0.857} p_{x,y}^{2.018} p_z^{0.143})_{\sigma} (s^{0.143} p_z^{0.857})_{\pi}$	44.5
<i>C</i> ₂ (35)	14.56	18.91	0.349	0.140	0.860	0.166	2.497	$(s^{0.860} p_{x,y}^{1.999} p_z^{0.140})_{\sigma} (s^{0.140} p_z^{0.860})_{\pi}$	48.8
<i>C</i> ₁ (34)	14.63	19.13	0.350	0.142	0.858	0.170	2.509	$(s^{0.858} p_{x,y}^{1.999} p_z^{0.142})_{\sigma} (s^{0.142} p_z^{0.858})_{\pi}$	49.6
<i>C</i> _s (28)	14.65	19.22	0.350	0.143	0.857	0.170	2.511	$(s^{0.857} p_{x,y}^{2.001} p_z^{0.143})_{\sigma} (s^{0.143} p_z^{0.857})_{\pi}$	51.2
<i>C</i> ₂ (15)	14.65	19.19	0.350	0.143	0.857	0.171	2.513	$(s^{0.857} p_{x,y}^{2.000} p_z^{0.143})_{\sigma} (s^{0.143} p_z^{0.857})_{\pi}$	51.4
<i>C</i> ₁ (17)	14.69	19.32	0.351	0.144	0.856	0.176	2.528	$(s^{0.856} p_{x,y}^{2.000} p_z^{0.144})_{\sigma} (s^{0.144} p_z^{0.856})_{\pi}$	54.2
<i>C</i> ₁ (10)	14.73	19.44	0.352	0.145	0.855	0.177	2.532	$(s^{0.855} p_{x,y}^{2.000} p_z^{0.145})_{\sigma} (s^{0.145} p_z^{0.855})_{\pi}$	56.0
<i>C</i> _s (13)	14.73	19.47	0.352	0.145	0.855	0.177	2.532	$(s^{0.855} p_{x,y}^{2.001} p_z^{0.145})_{\sigma} (s^{0.145} p_z^{0.855})_{\pi}$	61.3
<i>C</i> ₂ (16)	14.71	19.40	0.352	0.145	0.855	0.178	2.533	$(s^{0.855} p_{x,y}^{2.001} p_z^{0.145})_{\sigma} (s^{0.145} p_z^{0.855})_{\pi}$	61.5
<i>C</i> ₁ (12)	14.72	19.43	0.352	0.145	0.855	0.176	2.527	$(s^{0.854} p_{x,y}^{1.999} p_z^{0.146})_{\sigma} (s^{0.146} p_z^{0.854})_{\pi}$	61.5
<i>C</i> ₂ (9)	14.73	19.45	0.352	0.146	0.854	0.180	2.539	$(s^{0.857} p_{x,y}^{1.999} p_z^{0.143})_{\sigma} (s^{0.143} p_z^{0.857})_{\pi}$	61.6
<i>C</i> _{3v} (20)	14.65	19.19	0.350	0.143	0.857	0.173	2.518	$(s^{0.852} p_{x,y}^{1.999} p_z^{0.148})_{\sigma} (s^{0.148} p_z^{0.852})_{\pi}$	62.6
<i>C</i> ₂ (19)	14.71	19.58	0.351	0.148	0.852	0.187	2.561	$(s^{0.854} p_{x,y}^{2.000} p_z^{0.146})_{\sigma} (s^{0.146} p_z^{0.854})_{\pi}$	65.7
<i>C</i> ₂ (23)	14.74	19.58	0.353	0.146	0.854	0.176	2.529	$(s^{0.851} p_{x,y}^{2.001} p_z^{0.149})_{\sigma} (s^{0.149} p_z^{0.851})_{\pi}$	73.5
<i>C</i> ₁ (6)	14.84	19.83	0.354	0.149	0.851	0.186	2.557	$(s^{0.851} p_{x,y}^{1.999} p_z^{0.149})_{\sigma} (s^{0.149} p_z^{0.851})_{\pi}$	75.7
<i>C</i> ₂ (18)	14.81	19.82	0.354	0.149	0.851	0.181	2.544	$(s^{0.850} p_{x,y}^{2.001} p_z^{0.150})_{\sigma} (s^{0.150} p_z^{0.850})_{\pi}$	84.9
<i>C</i> _s (5)	14.86	19.90	0.355	0.150	0.850	0.187	2.562	$(s^{0.846} p_{x,y}^{2.001} p_z^{0.154})_{\sigma} (s^{0.154} p_z^{0.846})_{\pi}$	85.8
<i>C</i> _{2v} (8)	14.94	20.26	0.356	0.154	0.846	0.198	2.594	$(s^{0.851} p_{x,y}^{2.000} p_z^{0.149})_{\sigma} (s^{0.149} p_z^{0.851})_{\pi}$	94.4
<i>D</i> _{2h} (33)	14.84	19.94	0.354	0.149	0.851	0.183	2.548	$(s^{0.848} p_{x,y}^{1.999} p_z^{0.152})_{\sigma} (s^{0.152} p_z^{0.848})_{\pi}$	96.8
<i>C</i> ₁ (4)	14.94	20.18	0.356	0.152	0.848	0.190	2.570	$(s^{0.848} p_{x,y}^{2.000} p_z^{0.152})_{\sigma} (s^{0.152} p_z^{0.848})_{\pi}$	102.8
<i>C</i> _s (7)	14.92	20.18	0.356	0.152	0.848	0.189	2.566	$(s^{0.848} p_{x,y}^{1.999} p_z^{0.152})_{\sigma} (s^{0.152} p_z^{0.848})_{\pi}$	106.3
<i>C</i> ₂ (11)	14.91	20.17	0.356	0.152	0.848	0.189	2.566	$(s^{0.845} p_{x,y}^{1.999} p_z^{0.155})_{\sigma} (s^{0.155} p_z^{0.845})_{\pi}$	116.3
<i>C</i> ₂ (2)	15.04	20.49	0.359	0.155	0.845	0.193	2.580	$(s^{0.838} p_{x,y}^{2.001} p_z^{0.162})_{\sigma} (s^{0.162} p_z^{0.838})_{\pi}$	122.6
<i>D</i> ₂ (3)	15.25	21.16	0.363	0.162	0.838	0.210	2.631	$(s^{0.838} p_{x,y}^{2.001} p_z^{0.162})_{\sigma} (s^{0.162} p_z^{0.838})_{\pi}$	157.7
<i>D</i> _{5d} (1)	15.48	21.90	0.368	0.170	0.830	0.222	2.667	$(s^{0.830} p_{x,y}^{2.001} p_z^{0.170})_{\sigma} (s^{0.170} p_z^{0.830})_{\pi}$	204.1
<i>C</i> ₆₀	11.64	12.00	0.281	0.085	0.915	0.093	2.278	$(s^{0.915} p_{x,y}^{1.999} p_z^{0.085})_{\sigma} (s^{0.085} p_z^{0.915})_{\pi}$	

4.4.2 Graphical analysis

Figures S9 and S10 show the distributions of the pyramidalization angle and the hybridization of the atoms in C_{40} isomers before (initial) and after (optimized) a geometrical optimization using quantum chemistry, respectively. As previously observed concerning the C_{32} isomers, the energy seems to be linked to the width of the pyramidalization angle distribution.

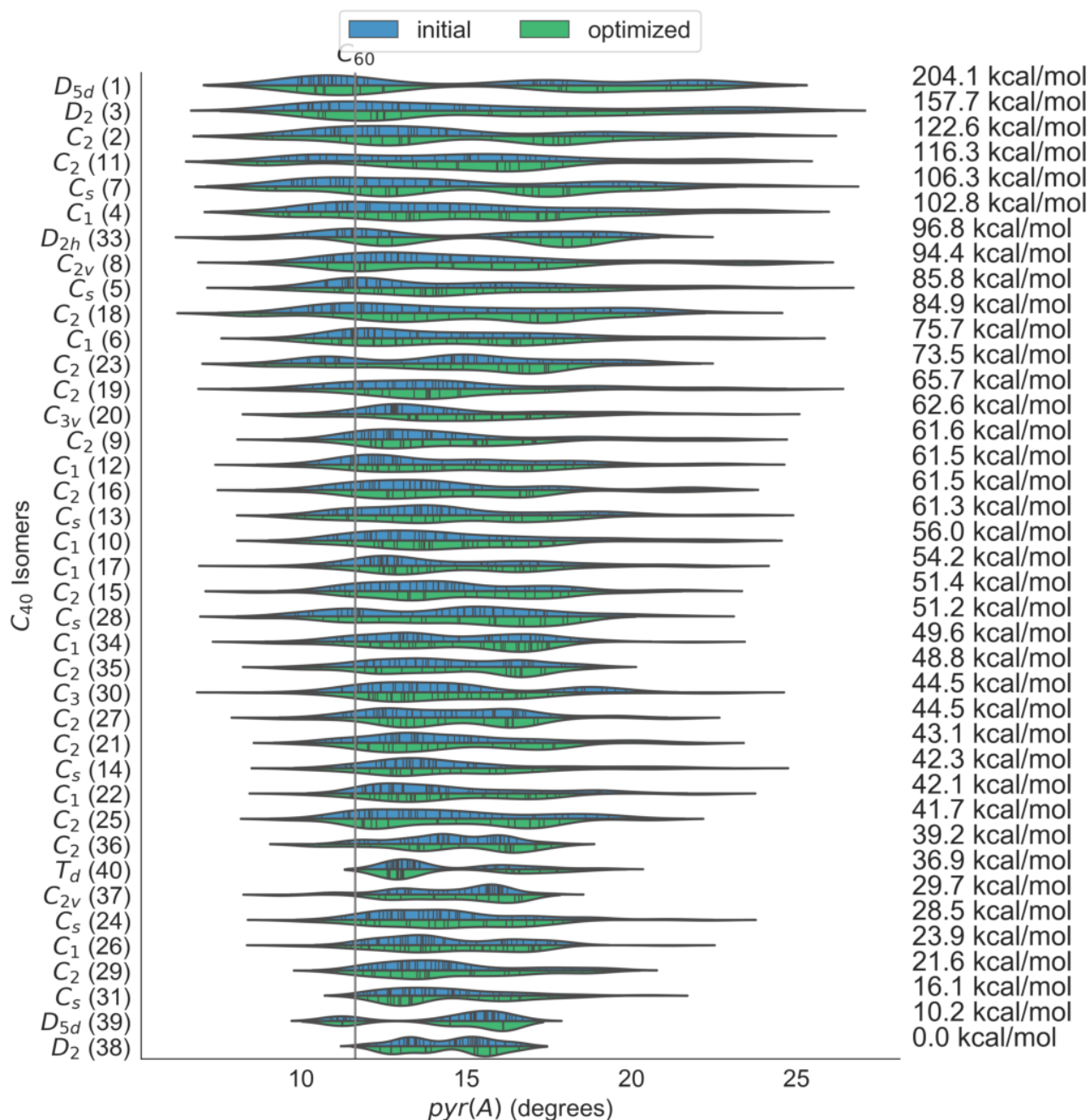


Figure S9: Pyramidalization angle distributions of the C_{40} isomers before and after the geometrical optimization. The vertical line shows the value of the pyramidalization angle of the C_{60} isomer. The energies are relative to the most stable isomer.

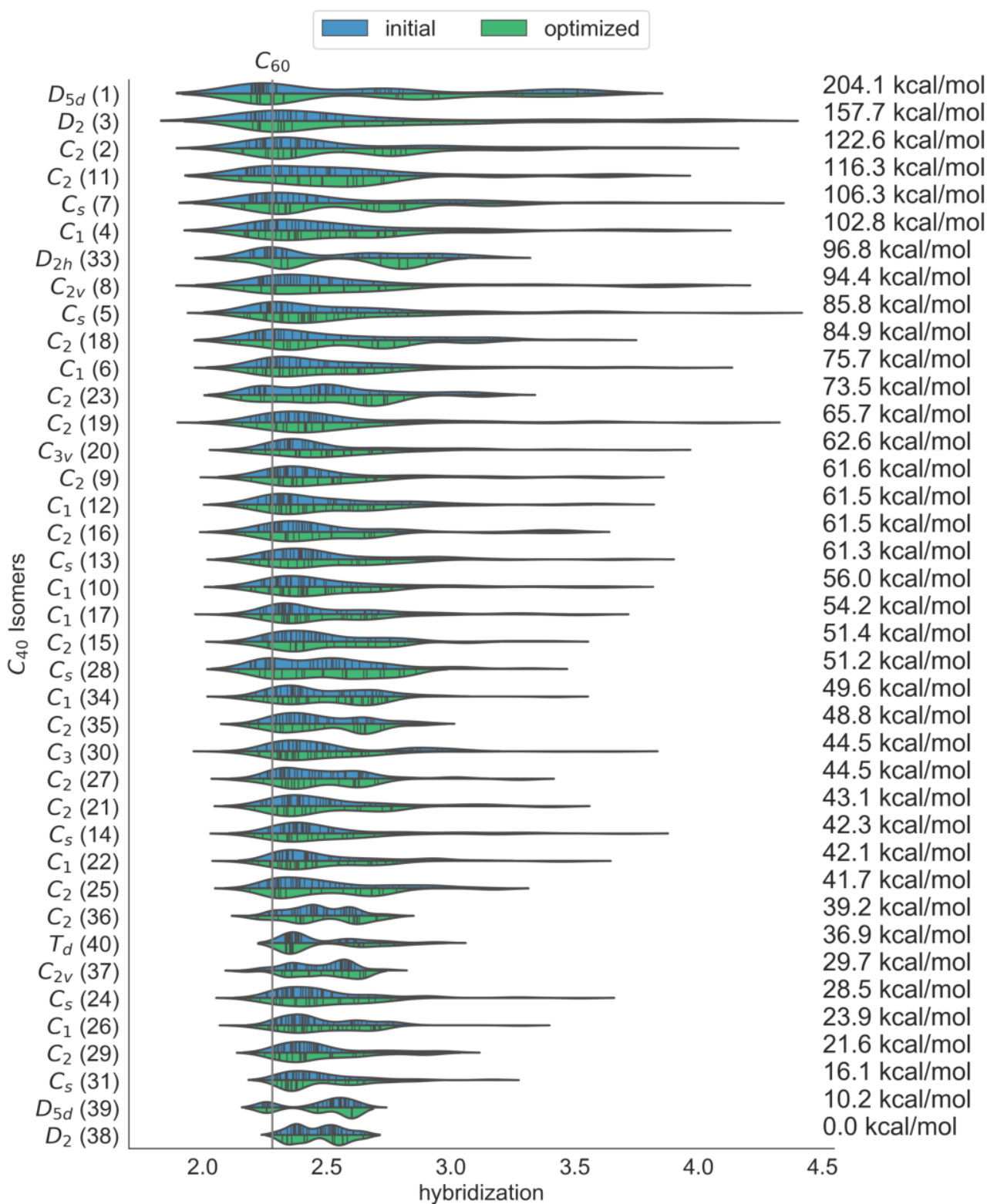


Figure S10: Hybridization of the C_{40} isomers before and after the geometrical optimization. The vertical line shows the value of the pyramidalization angle of the C_{60} isomer. The energies are relative to the most stable isomer.

Figure S11 presents the pairwise relationships between $Pyr(A)$, the angular defect, the spherical curvature and the hybridization for the C_{40} isomers.

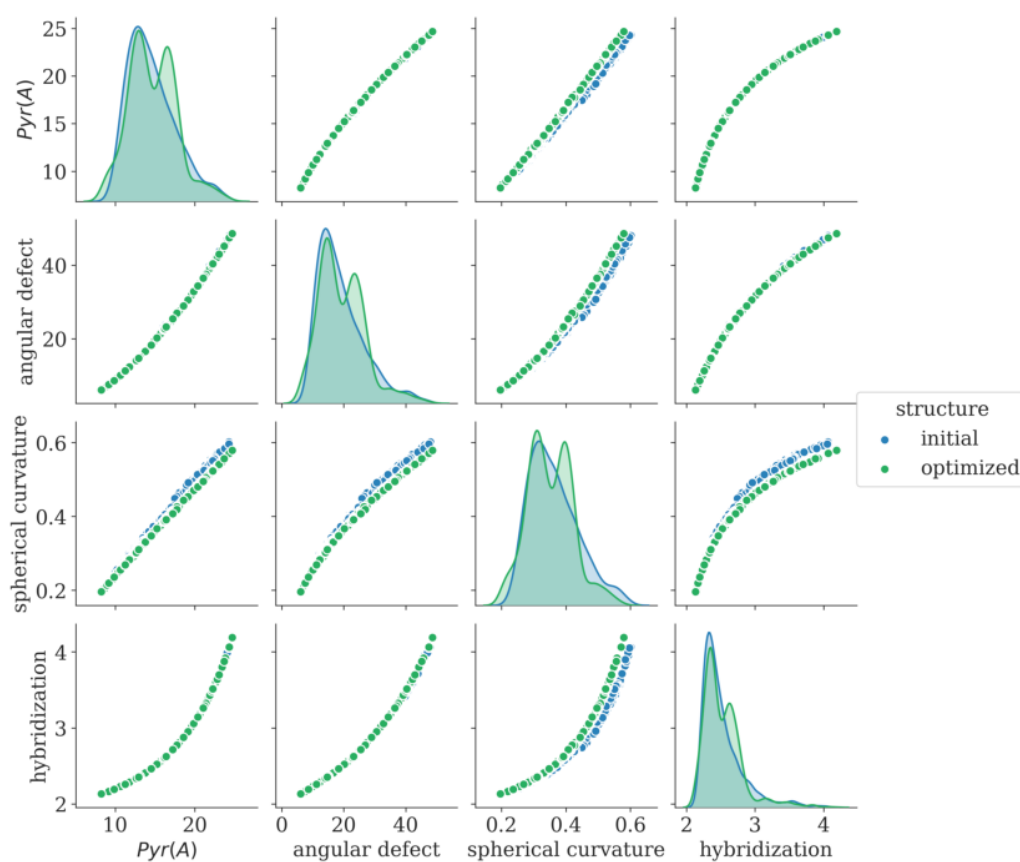


Figure S11: Pairwise relationships between $pyr(A)$, the angular defect and the spherical curvature for the six C_{40} isomers and comparing optimized and initial structures.

4.5 C_{80} isomers

4.5.1 Statistics

Table S8 presents statistical descriptors of the geometrical quantities for the six isomers of the C_{80} family after a geometrical optimization.

Table S8: Statistical descriptors of isomers of the C₈₀ family.

	Pyr(A)	Angular defect	Spherical curvature	c_{π}^2	λ_{π}^2	m	n	Hybridization
mean	10.16	9.40	0.246	0.066	0.934	0.071	2.213	$(s^{0.934} p_{x,y}^{2.000} p_z^{0.066})_{\sigma} (s^{0.066} p_z^{0.934})_{\pi}$
std	1.57	2.65	0.038	0.019	0.019	0.022	0.065	$(s^{0.019} p_{x,y}^{0.000} p_z^{0.019})_{\sigma} (s^{0.019} p_z^{0.019})_{\pi}$
min	5.74	2.96	0.137	0.020	0.903	0.021	2.062	$(s^{0.903} p_{x,y}^{1.999} p_z^{0.020})_{\sigma} (s^{0.020} p_z^{0.903})_{\pi}$
25%	9.08	7.40	0.220	0.051	0.918	0.054	2.162	$(s^{0.918} p_{x,y}^{2.000} p_z^{0.051})_{\sigma} (s^{0.051} p_z^{0.918})_{\pi}$
50%	10.59	9.97	0.256	0.070	0.930	0.075	2.225	$(s^{0.930} p_{x,y}^{2.000} p_z^{0.070})_{\sigma} (s^{0.070} p_z^{0.930})_{\pi}$
75%	11.47	11.66	0.278	0.082	0.949	0.090	2.269	$(s^{0.949} p_{x,y}^{1.999} p_z^{0.082})_{\sigma} (s^{0.082} p_z^{0.949})_{\pi}$
max	12.39	13.55	0.300	0.097	0.980	0.107	2.320	$(s^{0.980} p_{x,y}^{1.999} p_z^{0.097})_{\sigma} (s^{0.097} p_z^{0.980})_{\pi}$

Table S9 shows the mean quantities grouped by isomers after the geometrical relaxation.

Table S9: Mean of the geometrical quantities grouped by isomers of the C₈₀ family.

	pyr(A)	Angular defect	Spherical curvature	c_{π}^2	λ_{π}^2	m	n	Hybridization	ΔE (kcal/mol)
D_2 (2)	10.20	9.57	0.247	0.067	0.933	0.073	2.218	$(s^{0.933} p_{x,y}^{1.999} p_z^{0.067})_{\sigma} (s^{0.067} p_z^{0.933})_{\pi}$	0.0
D_{5d} (1)	10.23	9.61	0.248	0.068	0.932	0.073	2.219	$(s^{0.932} p_{x,y}^{2.000} p_z^{0.068})_{\sigma} (s^{0.068} p_z^{0.932})_{\pi}$	0.8
C_{2v} (3)	10.14	9.35	0.246	0.066	0.934	0.071	2.212	$(s^{0.934} p_{x,y}^{1.999} p_z^{0.066})_{\sigma} (s^{0.066} p_z^{0.934})_{\pi}$	4.2
D_3 (4)	10.18	9.49	0.247	0.067	0.933	0.072	2.216	$(s^{0.933} p_{x,y}^{2.000} p_z^{0.067})_{\sigma} (s^{0.067} p_z^{0.933})_{\pi}$	9.3
C_{2v} (5)	10.12	9.25	0.245	0.065	0.935	0.069	2.208	$(s^{0.935} p_{x,y}^{2.001} p_z^{0.065})_{\sigma} (s^{0.065} p_z^{0.935})_{\pi}$	9.9
D_{5h} (6)	10.09	9.15	0.244	0.064	0.936	0.068	2.205	$(s^{0.936} p_{x,y}^{2.001} p_z^{0.064})_{\sigma} (s^{0.064} p_z^{0.936})_{\pi}$	12.7
C_{60}	11.64	12.00	0.281	0.085	0.915	0.093	2.278	$(s^{0.915} p_{x,y}^{1.999} p_z^{0.085})_{\sigma} (s^{0.085} p_z^{0.915})_{\pi}$	

4.5.2 Graphical analysis

Figures S12 and S13 represent the distributions of the pyramidalization angle and the hybridization of the atoms in C₈₀ isomers before (initial) and after (optimized) a geometrical optimization using quantum chemistry, respectively. The pyramidalization angles of C₈₀ isomers are lower than C₆₀ isomer, corresponding to a larger system closer to a flat geometry. Contrary to C₄₀ and C₃₂ isomers, the energies of C₈₀ isomers increase when the width of the pyramidalization angle distributions increase.

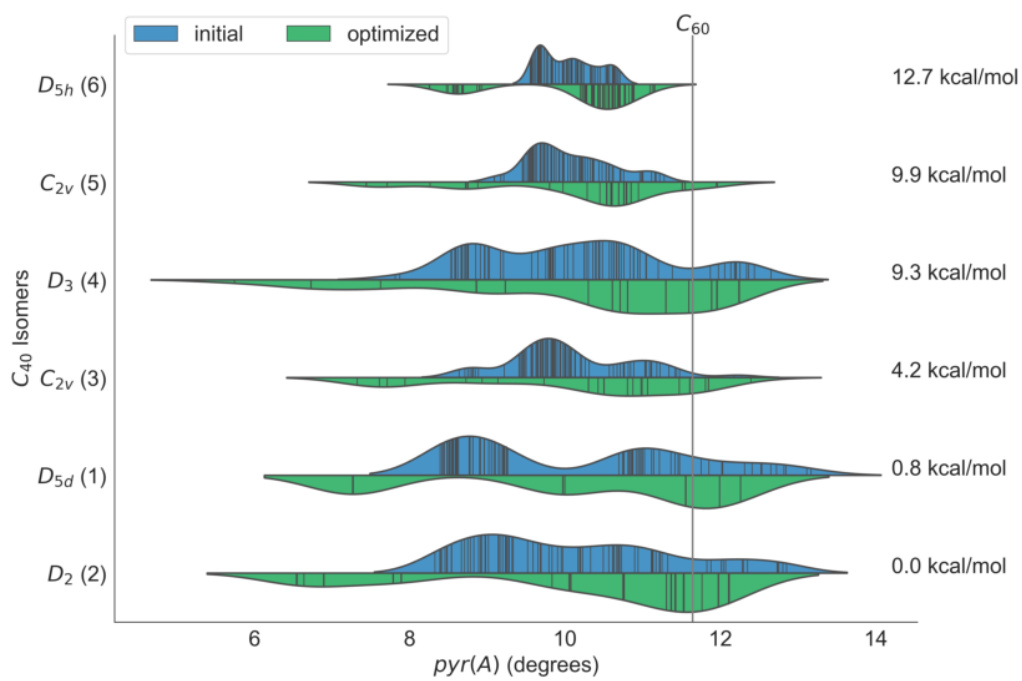


Figure S12: Pyramidization angle distributions of the C_{80} isomers before and after the geometrical optimization. The vertical line shows the value of the pyramidization angle of the C_{60} isomer.

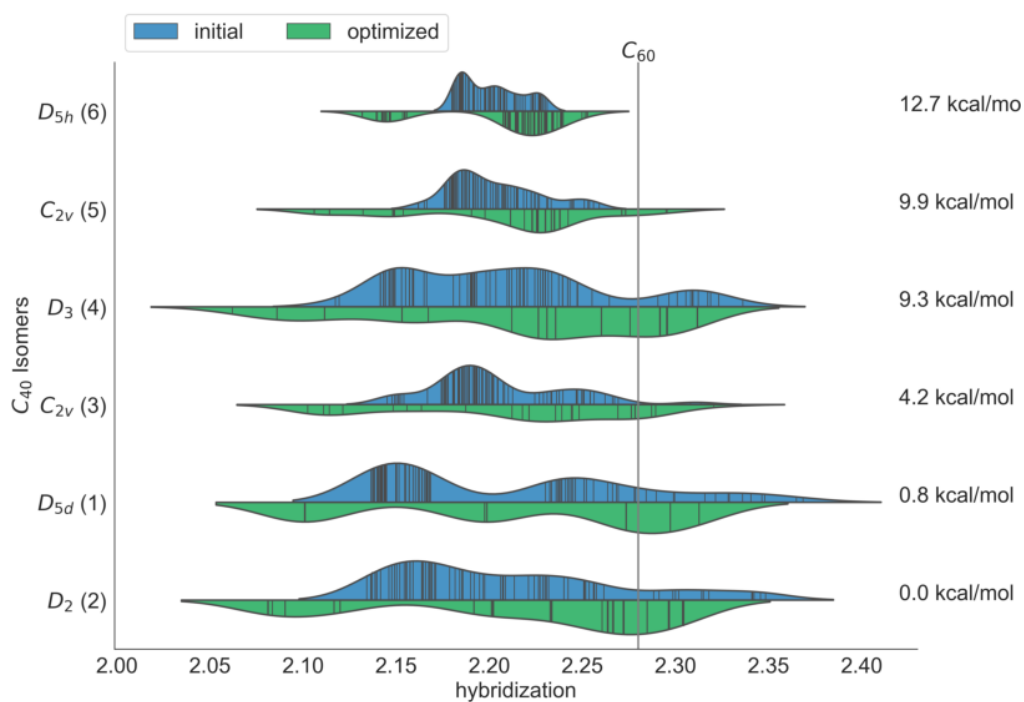


Figure S13: Pyramidalization angle distributions of the C_{80} isomers before and after the geometrical optimization. The vertical line shows the value of the pyramidalization angle of the C_{60} isomer.

Figures S14 and S15 refer to the pairwise relationships between $P_{yr}(A)$, the angular defect and the spherical curvature for the six C_{80} isomers.

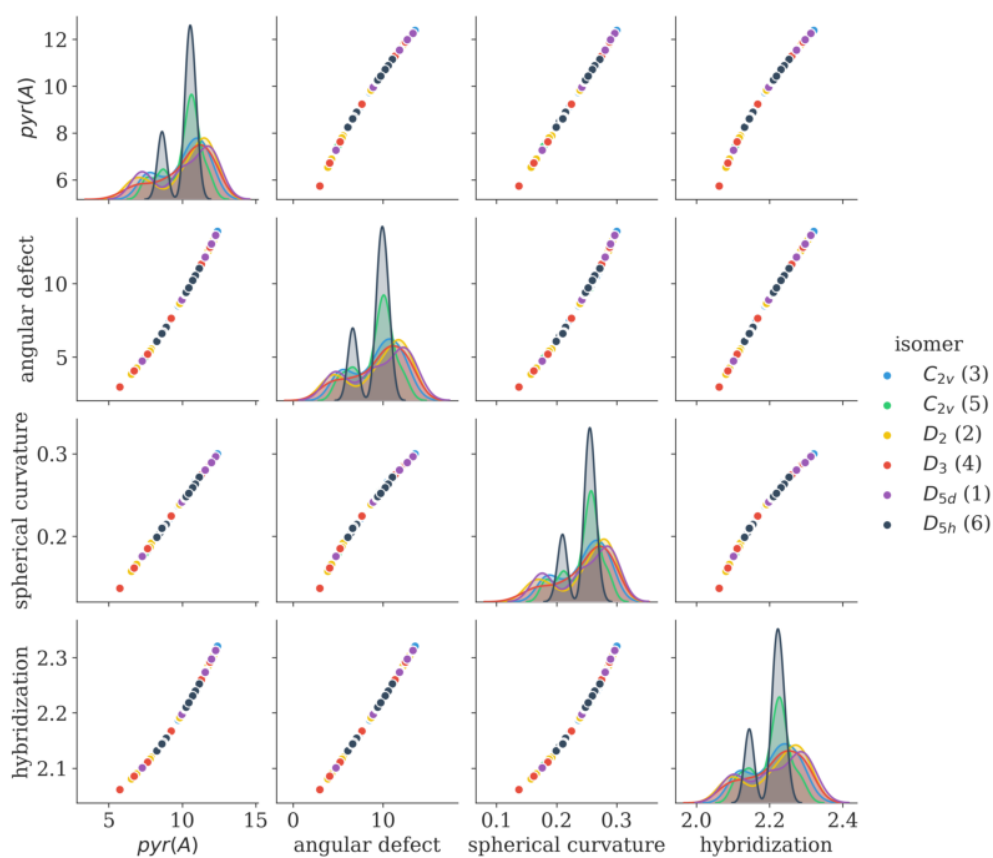


Figure S14: Pairwise relationships between $P_{yr}(A)$, the angular defect and the spherical curvature for the six C_{80} isomers considering only optimized structures.

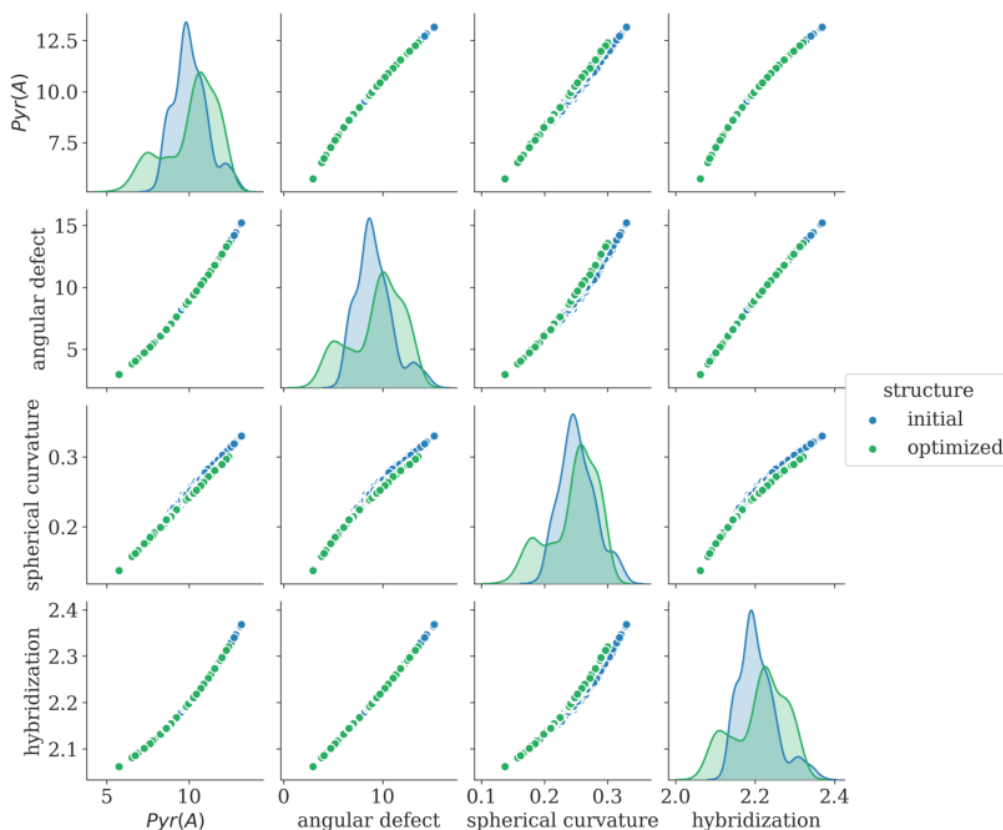


Figure S15: Pairwise relationships between $Pyr(A)$, the angular defect and the spherical curvature for the six C_{80} isomers and comparing optimized and initial structures.

5 Elasticity and curvature energy

Here the idea is to link $Pyr(A)$ to the energy of the isomers. Starting from a planar system, we assume that an increase of $Pyr(A)$ increases the energy. This is classically the way planar system are stabilized in classical force-field using specific terms in the energy for improper torsion. Two main strategies can be found in the most common force fields: a quadratic energy term:

$$E_{improper} = k(\phi - \phi_o)^2 \quad (3)$$

or a Fourier serie as used for dihedral angles:

$$E_{improper} = k[1 - \cos(\phi - \phi_o)] \quad (4)$$

In figure S16 we consider the C_{40} isomers family and we compute the deformation energy using equation (3), as a sum over the pyramidalization angles on the atoms of an isomer:

$$E_{deformation} = \sum_{i, atoms} k(Pyr(A)_i - Pyr(A)_o) \quad (5)$$

with $Pyr(A)_o = 0$.

Figure S16 presents the correlation between the deformation energy computed using $Pyr(A)$ and the energy obtained from quantum chemistry calculations. A clear relationship is obtained that let imagine a way to compute the deformation energy using $Pyr(A)$.

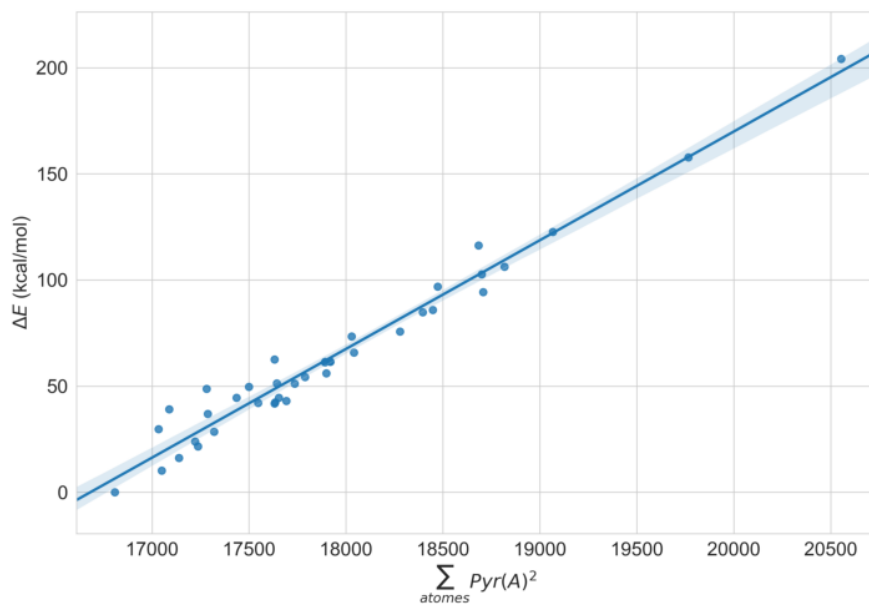


Figure S16: Correlation between deformation energy and the pyramidalization angle.

The slope of the line is $0.051 \text{ kcal.mol}^{-1}.\text{degrees}^{-2}$ and the determination coefficient is $r^2 = 0.9659$.

Actually these energies can be related to the curvature energies computed on a continuum model in Guan *et al.* [4] (paper associated to the data base of fullerenes).

6 Computational details

The various calculations carried out in this paper are based on the xyz coordinates presented in the following. The cartographies and the others figures of the article are generated from the data presented in the section.

6.1 Coordinates of C_{32}

Coordinates of C_{32} symmetry : $C_2 - 1, C_2 - 4, D_2 - 2$.

Table S10: Coordinates xyz of C_{32}

C_{32}	$C_2 - 1$			$C_2 - 4$			$D_2 - 2$		
	x	y	z	x	y	z	x	y	z
C1	2.70450	1.16090	-0.14630	-0.54160	-2.13380	-1.18140	-1.26580	-1.98300	0.58440
C2	1.61930	1.72490	-0.79330	-1.79600	-1.65730	-0.98130	1.26920	-1.93930	-0.53550
C3	2.34210	1.02670	1.14620	-0.04200	-2.54900	0.03870	0.14550	-1.64880	-1.30890
C4	-0.68690	2.16170	-0.13790	1.20920	-2.19700	0.4232	-1.14720	-1.79840	-0.80190
C5	0.67160	2.15830	0.14350	2.11530	-1.54930	-0.39980	-2.33050	-1.22630	0.97980
C6	1.13120	1.62110	1.35570	-2.09400	-1.62750	0.35020	-2.99990	-0.66660	-0.06350
C7	-1.12620	1.61730	-1.36160	-2.57700	-0.36030	0.57720	-2.18990	-0.94290	-1.16620
C8	2.18930	-0.29660	1.44190	-1.92630	0.42630	1.51860	-1.81700	-0.23410	1.75170
C9	2.60030	-1.02320	0.30830	-0.95710	-2.07950	0.99160	-0.48650	-0.52530	2.03250
C10	1.69600	-1.92290	-0.19620	0.23190	-1.26320	1.88050	0.47570	0.49700	2.01930
C11	0.90620	-0.50390	1.98300	0.69530	0.05620	2.08850	-2.20200	0.97630	1.18460
C12	0.12220	-1.59750	1.56110	-1.77800	1.64730	0.95550	-1.15730	1.82880	0.82040
C13	0.54170	-2.30400	0.42410	-0.52280	2.10880	1.16360	0.13420	1.69810	1.33170
C14	-1.24920	-1.42110	1.42490	-0.04490	2.57360	-0.05530	-3.02000	0.69460	0.07960
C15	-1.14420	0.87570	1.76820	0.21620	1.14940	1.87930	1.80770	0.21720	1.73220
C16	0.23640	0.76950	1.99930	-2.12180	1.64320	-0.36440	2.34030	1.21110	0.95290
C17	-1.94980	-0.25730	1.64140	-2.61090	0.37680	-0.62490	1.26520	1.95870	0.56770
C18	-1.66430	1.74280	0.78410	-1.96890	-0.43390	-1.55270	2.20500	-0.99860	1.19570
C19	-0.09100	-1.59790	-1.56070	-0.97880	2.09440	-0.99570	1.16360	-1.87680	0.86630
C20	1.28590	-1.43250	-1.43730	-0.26490	1.25190	-1.86550	-0.12960	-1.74330	1.36950
C21	-0.88350	-0.49650	-1.94680	-0.72660	-0.06710	-2.09930	3.00320	-0.68590	0.08780
C22	-0.53680	-2.31180	-0.43120	1.96290	0.40160	-1.43280	3.01670	0.68430	-0.09250
C23	2.86830	-0.07630	-0.68260	1.52910	-0.92100	-1.53770	2.33090	-1.20160	-0.95790
C24	1.95680	-0.25610	-1.68950	0.18370	-1.16260	-1.89620	1.83380	-0.21860	-1.76700
C25	-0.22440	0.77640	-2.02190	1.06760	1.43120	-1.52140	-0.13780	1.67190	-1.33120
C26	1.15680	0.87900	-1.82970	2.74490	0.56560	-0.30850	1.16220	1.82610	-0.82950
C27	-1.68540	-1.92300	0.20100	2.11170	1.57380	0.40050	2.22230	0.99150	-1.19480
C28	-2.59620	-1.01150	-0.27630	1.22500	2.24920	-0.41240	-1.28660	1.94140	-0.57470
C29	-2.15060	-0.27480	-1.38400	1.11800	-1.43290	1.57690	-2.36790	1.22340	-0.98650
C30	-2.92050	-0.05510	0.68110	2.04170	-0.41380	1.49490	0.49500	-0.48560	-2.06760
C31	-2.77280	1.19710	0.15410	1.57300	0.90180	1.54280	-0.50060	0.50820	-2.08510
C32	-2.34930	1.05370	-1.12100	2.77750	-0.60000	0.34900	-1.83440	0.24950	-1.79200

Coordinates of C_{32} symmetry : $D_3 - 6, D_{3d} - 3, D_{3h} - 5.$

C_{32}	$D_3 - 6$			$D_{3d} - 3$			$D_{3h} - 5$		
	x	y	z	x	y	z	x	y	z
C1	-2.80970	0.00660	0.00420	-1.83520	-0.54660	1.70120	1.59180	1.68580	-1.07190
C2	-2.36070	-1.23590	-0.40000	0.59900	0.85180	1.82150	0.52220	2.42230	-0.67840
C3	-1.65970	0.29290	-1.85150	-0.59730	1.44760	1.40410	-0.75910	2.19970	-1.07340
C4	-2.34300	0.96830	-0.86850	-1.83170	0.82280	1.53000	1.36400	0.43560	-1.69220
C5	0.30950	-2.19190	-0.67180	1.82120	1.18290	1.26230	-0.28990	-1.36740	-1.66390
C6	-0.31290	-1.51150	-1.75980	-2.66670	-1.03880	0.72200	0.00820	0.01690	-1.95890
C7	-1.63140	-1.06190	-1.57240	-3.22720	-0.00660	-0.00360	-1.04880	0.96500	-1.69070
C8	-1.62750	1.87720	-0.11290	-2.67360	1.15350	0.50540	0.65440	-2.22000	-1.04750
C9	-0.39170	0.67230	-2.20510	-1.83830	-1.80880	-0.04560	-2.47770	1.36550	0.00590
C10	0.31340	1.68720	-1.55120	-0.60790	-2.03350	0.55700	-1.58980	2.36500	0.00770
C11	-0.31350	2.27610	-0.42060	0.60380	-2.08480	-0.15230	-2.34500	-0.74510	-0.67030
C12	0.42330	-0.44450	-2.30340	-1.83310	-1.21260	-1.30680	-2.23960	0.54190	-1.07900
C13	-1.69440	1.45930	1.21160	-0.60200	-0.90320	-1.86070	-1.50470	-1.74750	-1.04510
C14	-2.38510	0.26960	1.28610	0.60450	-1.48310	-1.44930	-0.76090	2.22390	1.09400
C15	-1.64990	-0.82840	1.70750	-2.65710	-0.10890	-1.23430	0.53190	2.46150	0.71440
C16	-0.41540	1.58120	1.69840	1.84460	-1.75180	0.37680	1.60640	1.70450	1.06160
C17	0.30760	0.51020	2.24510	2.69490	-1.14650	-0.52030	-2.28900	0.53670	1.08820
C18	-0.32880	-0.76380	2.19740	1.83120	-0.84190	-1.54960	-1.06710	0.97000	1.67000
C19	0.40800	2.21740	0.77790	1.82000	-0.96010	1.52000	2.44610	1.47300	-0.00340
C20	-0.40410	-2.24810	0.53710	0.59080	-0.56300	2.02450	2.84460	0.20700	-0.02140
C21	-1.67510	-1.76560	0.66290	-0.61110	-1.21130	1.73320	-0.01340	0.00640	1.90650
C22	1.65190	-1.56860	1.02280	2.65370	0.08990	1.20460	1.34770	0.43730	1.63730
C23	0.40130	-1.76050	1.53680	3.25630	0.00500	-0.02360	2.28720	-0.45210	1.06680
C24	2.34010	-0.39360	1.20290	2.68950	1.05340	-0.71160	1.84110	-1.66460	-0.67660
C25	1.61210	0.65820	1.74960	-0.60450	0.52680	-1.96530	2.29010	-0.45190	-1.09130
C26	2.82430	-0.01110	-0.02340	0.59250	1.18630	-1.65620	0.66890	-2.23810	1.07000
C27	2.35910	1.27400	-0.25100	1.81840	0.53870	-1.65370	1.85800	-1.69310	0.71360
C28	1.68330	1.72110	0.85520	-1.84010	0.95940	-1.49020	-2.40430	-0.77220	0.72000
C29	1.62230	1.17570	-1.43090	0.61460	2.08540	-0.54410	-1.55690	-1.78220	1.06720
C30	1.64070	-1.84510	-0.34250	-0.61430	2.14100	0.15160	-0.31960	-1.38620	1.63330
C31	2.39850	-0.87970	-1.00880	-1.85490	1.81190	-0.38880	-1.24890	-2.61130	0.00450
C32	1.70240	-0.13100	-1.91930	1.85470	1.85090	0.04440	0.04690	-2.88040	0.00560

6.2 Coordinates of C_{40}

Coordinates of C_{40} symmetry : $C_1 - 4, C_1 - 6, C_1 - 10$.

Table S11: Coordinates xyz of C_{40}

C_{40}	$C_1 - 4$			$C_1 - 6$			$C_1 - 10$		
	x	y	z	x	y	z	x	y	z
C1	3.38010	-0.45200	0.87630	-0.19360	-2.07170	1.26420	-1.13690	-2.06130	1.14140
C2	2.33510	-1.17130	1.36690	-1.43260	-2.09340	0.68640	-2.34030	-1.39180	1.19640
C3	1.82050	0.90190	1.79980	-2.46900	-1.33700	1.19130	0.00490	-1.67270	1.80800
C4	2.99130	0.84850	1.04340	0.91350	-2.36080	0.53450	1.42150	-2.24440	-0.00560
C5	0.79480	1.78940	1.54110	-3.34780	-1.03650	0.19660	1.31560	-1.90840	1.36100
C6	-0.31430	-1.88590	1.28570	-2.67180	-1.30370	-0.95570	-0.01610	-0.35810	2.34100
C7	0.00190	-0.74550	2.07660	-2.60550	-0.11950	-1.63550	-1.13800	0.48870	2.13950
C8	1.37460	-0.41640	2.03050	0.90710	-2.23980	-0.85030	-2.35880	-0.05870	1.64470
C9	0.85090	2.41560	0.26290	-0.29850	-1.81340	-1.45130	-0.73490	1.75720	1.60270
C10	1.81590	1.99050	-0.63060	-1.51050	-2.01620	-0.73680	1.29820	0.04670	2.25250
C11	2.99470	1.38860	-0.22910	-3.67260	0.28120	0.21810	1.66720	1.27300	1.74090
C12	-0.43660	2.55730	-0.08950	-3.28430	0.85740	-0.94900	0.61390	2.05430	1.30130
C13	-2.48460	1.89420	0.38420	-2.05560	1.80450	0.59200	3.13430	-0.30600	1.04300
C14	-1.31570	2.30330	0.91390	-2.80900	0.78630	1.17270	2.16430	-0.90630	1.79770
C15	-3.18070	0.81200	0.82450	-0.78150	2.04920	1.02040	3.33410	-0.67970	-0.26500
C16	-2.61620	-1.26700	0.97840	-2.33670	1.80700	-0.77340	2.39290	-1.58250	-0.74060
C17	-2.36680	-0.04900	1.60120	-0.15660	1.23700	1.98740	-1.50340	2.23560	0.56010
C18	-1.54170	-2.03610	0.75390	-0.75560	-0.00320	2.30370	-2.62980	1.65070	0.12190
C19	-1.04490	0.26100	2.10340	-2.09070	-0.18540	1.88420	-3.21660	0.57970	0.72190
C20	-0.56680	1.57530	1.82080	0.20300	-1.04930	2.15450	-3.56710	-0.32640	-0.25190
C21	3.32290	0.37750	-1.08900	1.18950	1.38240	1.79520	-2.37290	1.34560	-1.19270
C22	1.29340	1.20570	-1.70320	2.15440	0.39970	1.85970	-2.85480	0.09090	-1.37450
C23	2.20630	0.19010	-1.83570	1.60600	-0.88660	1.97870	-3.06270	-1.52100	0.04500
C24	3.60400	-0.77690	-0.42810	0.24800	2.44620	0.14380	2.11950	-1.90250	-0.85470
C25	2.60430	-1.66620	-0.75590	1.46330	2.21720	0.75460	0.25000	-2.30830	-0.77230
C26	0.58570	-2.35870	0.31310	2.90890	-1.49370	0.03860	-1.00270	-2.40530	-0.22460
C27	1.89700	-2.03310	0.37340	2.04900	-1.81020	1.03980	0.45650	-1.43270	-1.87140
C28	-0.94630	1.97940	-1.25010	3.49640	-0.24780	-0.04190	-1.90690	-0.85390	-1.76650
C29	-0.09410	1.05790	-1.90410	3.10230	0.72350	0.86540	-0.58800	-0.51290	-2.19220
C30	-0.62810	-0.30150	-2.04230	3.09810	0.23550	-1.27330	-1.10410	1.75680	-1.54630
C31	0.33480	-1.37360	-1.77140	2.51040	1.44800	-1.14360	1.24280	1.17200	-1.92680
C32	1.71860	-1.09680	-1.70810	2.60670	1.81830	0.16020	-0.15190	0.89550	-2.15020
C33	-0.17700	-2.36970	-0.87780	-1.19730	1.60250	-1.55440	2.79870	1.04980	0.97280
C34	-2.24220	1.67430	-0.94810	1.23520	1.40370	-1.74910	2.83090	1.48190	-0.34230
C35	-2.84120	0.51650	-1.26690	0.08910	2.04690	-1.22410	1.67170	2.04280	-0.86320
C36	-2.02710	-0.51870	-1.73130	2.14640	-1.69400	-1.11970	0.64800	2.49760	-0.04960
C37	-3.67440	0.08010	-0.24780	2.24090	-0.58860	-1.89410	-0.63690	2.48740	-0.45260
C38	-3.40600	-1.22330	-0.15070	1.06760	0.05990	-2.23320	3.20230	0.40750	-1.08970
C39	-2.52120	-1.68590	-1.11460	-0.21420	-0.53940	-2.17560	2.22380	0.18960	-2.00780
C40	-1.50330	-2.38880	-0.56980	-1.35400	0.28560	-2.07660	1.76920	-1.06870	-1.84740

Coordinates of C_{40} symmetry : $C_1 - 12, C_1 - 17, C_1 - 22.$

C_{40}	$C_1 - 12$			$C_1 - 17$			$C_1 - 22$		
	x	y	z	x	y	z	x	y	z
C1	1.12650	-2.30130	0.74520	-3.17640	-0.76050	-0.63140	2.59220	1.11410	1.24920
C2	-0.11970	-2.60740	0.27950	-3.02340	0.56970	-0.37220	2.07800	1.26940	-1.45800
C3	-1.24590	-2.30060	1.01860	-1.63850	0.06220	-2.04160	1.44600	2.16770	-0.56990
C4	2.19570	-2.05960	-0.09170	-2.22260	-1.08260	-1.55010	1.75290	2.07570	0.77670
C5	-2.29090	-2.13210	0.20180	-0.30170	0.06710	-2.39200	-0.73020	1.82620	-1.62230
C6	-1.82410	-2.05090	-1.05790	-1.32650	2.20170	-0.95180	0.06230	2.41870	-0.63510
C7	-2.36380	-0.91760	-1.56380	-2.16320	1.15290	-1.31000	1.79090	0.38390	2.09680
C8	1.81080	-1.49200	-1.32700	0.49670	1.20060	-2.15630	1.94410	-0.94110	1.77040
C9	0.46090	-1.48140	-1.77530	0.01110	2.27130	-1.42190	0.76950	-1.68420	1.70940
C10	-0.46440	-2.29850	-1.07030	-1.29190	2.59610	0.39020	0.58180	2.08180	1.46210
C11	-3.03790	-1.04470	0.50690	0.49900	-1.07930	-2.17620	0.53870	0.96860	2.29630
C12	-2.32580	-0.43480	1.56170	-0.01900	-2.13700	-1.35900	2.57140	-1.66940	-0.38970
C13	-2.14980	0.95220	1.52510	-1.39180	-2.09870	-1.06160	1.34320	-2.29780	-0.54440
C14	-3.24360	-0.31830	-0.65590	0.88570	-2.50830	-0.30740	2.88950	-0.97280	0.75060
C15	-2.98560	1.01380	-0.67280	1.78890	-0.62110	-1.99110	0.49600	-2.44340	0.54060
C16	-2.57220	1.72710	0.42520	2.66270	-1.11310	-1.09390	-0.84860	-2.43840	0.38210
C17	-0.92100	1.46290	1.86350	2.22210	-2.07820	-0.24460	-0.65450	0.22720	2.37400
C18	-1.51490	2.55450	0.10640	1.76670	0.73800	-1.89760	-0.49070	-1.18320	2.13790
C19	-0.54750	2.50430	1.07130	0.38980	-2.40160	1.02480	-1.47910	-1.83420	1.43200
C20	0.17710	0.71580	2.21740	-0.93860	-2.14950	1.23660	1.62890	-0.79550	-2.12580
C21	0.07720	-0.69730	2.24280	-1.88980	-2.28750	0.24140	2.75390	-0.79700	-1.40680
C22	-1.19090	-1.23310	1.90570	1.38440	-1.73200	1.70050	-2.30290	0.26470	-1.76130
C23	1.25120	-1.34210	1.78070	2.51740	-1.64330	0.99830	-1.12300	-0.28500	-2.24860
C24	1.30920	1.38470	1.68360	-2.93810	-1.46160	0.47320	-0.69180	-1.58040	-1.81030
C25	2.45390	0.66890	1.35070	-2.53650	-0.59350	1.43760	0.71000	-1.76450	-1.71840
C26	2.45400	-0.71220	1.49100	-1.74510	1.67220	1.33310	-3.16110	-0.31450	-0.87030
C27	0.80370	2.43580	0.86200	-2.68060	0.72260	0.98610	-2.70310	-1.48090	-0.33310
C28	3.52160	-0.28070	-0.34280	1.05680	-0.47050	2.20110	-1.53410	-2.10360	-0.77980
C29	3.16060	-1.27340	0.46490	-0.30030	-0.06190	2.34010	3.11130	0.43500	-0.96400
C30	2.41190	1.67170	-0.71560	-1.31190	-0.98890	1.97500	3.30460	0.31570	0.39920
C31	3.17300	0.96040	0.17560	-0.57510	1.29890	2.05600	-0.16130	0.75720	-2.32410
C32	-1.07670	2.17990	-1.15050	2.10140	0.38160	1.71390	1.18990	0.50580	-2.25990
C33	0.27850	2.06010	-1.41610	1.69560	1.65000	1.31100	-3.35810	0.60080	0.13590
C34	1.27560	2.40190	-0.46310	0.44140	2.13040	1.60780	-2.90220	0.02650	1.29390
C35	-1.94500	1.20470	-1.57640	2.99320	-0.37790	0.95510	-2.63840	-1.28710	1.03610
C36	2.65990	-0.39240	-1.41940	1.99020	2.09400	-0.02900	-0.48370	2.42870	0.68270
C37	2.05360	0.77560	-1.69510	2.60330	1.15380	-0.85950	-1.75460	1.92890	0.93700
C38	0.75730	0.91010	-2.08720	3.15890	-0.01750	-0.37000	-1.85730	0.80540	1.81600
C39	-0.10180	-0.21770	-2.28130	0.81640	2.77710	-0.39500	-2.03760	1.54910	-1.33600
C40	-1.49230	0.00540	-2.11360	-0.01220	2.92580	0.63440	-2.64430	1.72350	-0.11740

Coordinates of C_{40} symmetry : $C_1 - 26, C_1 - 34, C_2 - 2$.

C_{40}	$C_1 - 26$			$C_1 - 34$			$C_2 - 2$		
	x	y	z	x	y	z	x	y	z
C1	-2.96060	1.15280	0.23300	2.07430	2.09060	0.31580	3.65270	0.71860	-0.47310
C2	-2.76820	0.87260	-1.07740	1.01970	2.78380	-0.13570	2.63990	1.36310	-1.15580
C3	-2.03240	1.99330	0.69780	-0.15080	2.90080	0.49820	-1.60280	1.71360	-1.11550
C4	-1.40500	1.44640	1.81950	-0.36100	2.06580	1.60320	-0.23120	1.71250	-1.34330
C5	-0.04390	1.66210	1.99030	0.63570	1.12320	2.03770	3.59230	-0.59270	-0.82170
C6	-1.24470	2.39490	-0.38320	1.93850	1.26490	1.44760	2.45870	-0.74810	-1.60980
C7	0.07510	2.69470	-0.14820	-2.19150	2.04100	0.22410	-1.81950	-0.48960	-1.80290
C8	0.65950	2.42640	1.08560	-1.18730	2.72040	-0.38740	-0.40820	-0.60780	-1.95820
C9	1.04670	2.31940	-1.04850	-2.11420	0.44650	1.72270	0.42790	0.58340	-1.97500
C10	-0.68340	-0.50200	-2.33260	-1.66470	1.66630	1.44720	1.83640	0.46890	-1.85710
C11	-0.56240	0.93330	-2.22640	1.03180	-1.33930	1.90260	-2.45630	0.72130	-1.55560
C12	-1.62300	1.57280	-1.49170	0.15330	-0.25740	2.28260	3.29780	-1.35140	0.25340
C13	0.76710	1.38410	-2.04560	-1.23840	-0.53850	2.12740	2.18760	-2.09080	0.04800
C14	-1.07040	-0.91010	2.13570	0.74580	2.26910	-1.38790	-0.03340	-2.10380	0.93160
C15	0.29470	-0.67260	2.40600	1.68340	1.29070	-1.69130	1.29370	-1.87690	1.08250
C16	-1.96730	0.14750	1.92660	-0.62560	2.19270	-1.54280	-1.89010	-2.08280	-0.27320
C17	0.83930	0.61830	2.31900	-1.15070	1.00860	-2.03820	-0.55550	-2.31020	-0.36810
C18	2.09110	0.81940	1.65960	-0.22630	-0.03350	-2.35850	0.25370	-1.77420	-1.39600
C19	1.00010	-1.69760	1.84140	1.18550	0.03740	-2.15330	1.62720	-1.77200	-1.19630
C20	2.16750	-1.51190	1.17410	1.80570	-1.13590	-1.59070	-2.66990	-1.39400	-1.14930
C21	2.75460	-0.26860	1.04430	-2.87250	0.93960	-0.27650	2.99280	-0.46770	1.27330
C22	1.93590	1.98980	0.91460	-2.32530	0.41550	-1.48310	3.29400	0.81220	0.86020
C23	-2.92680	-1.03080	0.07600	2.64530	1.33130	-0.67740	2.25210	1.66940	0.98920
C24	-2.00350	-2.05890	0.21370	2.84230	-1.02520	-0.64850	1.04810	1.49510	1.64730
C25	-2.96710	0.00930	0.97040	3.13310	0.20820	-0.13330	0.70550	0.19110	2.14120
C26	-1.13130	-2.07410	1.30610	2.54140	-1.85970	0.37360	1.72840	-0.75620	1.80480
C27	0.17140	-2.49060	1.11770	-0.33410	-2.24570	-1.41910	0.56410	2.29610	-0.32400
C28	-1.79030	-1.13330	-1.78260	1.01470	-2.24020	-1.16130	1.89660	2.08140	-0.27350
C29	-2.81120	-0.48040	-1.19560	1.46170	-2.60370	0.11630	-1.29160	1.92740	1.11830
C30	0.79980	-2.72630	-0.11380	-0.92060	-1.18650	-2.05880	0.03210	2.16800	0.97240
C31	-0.00770	-2.37700	-1.20570	2.32400	-1.08780	1.46260	-2.20070	2.10030	0.09050
C32	-1.35280	-2.16800	-1.01830	2.72600	0.16740	1.19540	-1.04710	-1.45470	1.62580
C33	2.06290	-2.16410	-0.03180	-1.25520	-2.58140	-0.42530	-0.69130	-0.16270	2.12910
C34	2.55110	-1.28940	-0.95500	-2.16990	-0.95290	-1.57880	-1.71600	0.77740	1.79040
C35	2.24410	2.01840	-0.42300	-2.42270	-1.84550	-0.56580	-3.32100	1.35400	0.23600
C36	2.76430	0.93550	-1.04240	-2.99380	-0.00030	0.76500	-2.24210	-1.64840	0.96840
C37	3.09510	-0.17610	-0.31710	-2.75630	-1.33990	0.65290	-3.28670	-0.79730	0.81250
C38	0.43740	-1.35710	-2.09860	0.52880	-2.45680	1.14810	-2.96910	0.46730	1.23770
C39	1.72240	-0.83240	-1.97840	-0.82140	-2.54400	0.90180	-3.70840	-0.72380	-0.51710
C40	1.87040	0.53170	-2.01160	-1.71010	-1.68790	1.49290	-3.64220	0.58560	-0.84340

Coordinates of C_{40} symmetry $C_2 - 9$.

C_{40}	$C_2 - 9$		
	x	y	z
C1	-2.78290	1.04190	0.95030
C2	-2.70700	-0.29990	1.36720
C3	-1.55670	-0.71010	2.04400
C4	-1.66220	1.85860	1.11160
C5	-0.59360	1.52320	1.92340
C6	-0.61120	0.22820	2.40000
C7	1.07470	2.33640	0.38730
C8	0.75770	1.77480	1.63470
C9	-2.20670	-1.89370	-0.20780
C10	-1.06490	-2.32930	0.40710
C11	-3.15790	-1.01010	0.24880
C12	-0.73720	-1.80600	1.66640
C13	0.61950	-1.56350	1.96560
C14	-0.01860	-2.35800	-0.52050
C15	1.30370	-2.24220	-0.16790
C16	1.69240	-1.89580	1.14500
C17	0.64230	-0.25380	2.41870
C18	-0.50660	-1.65070	-1.65320
C19	-1.85130	-1.46700	-1.46720
C20	2.19410	-1.62460	-1.01120
C21	-3.48280	-0.15940	-0.78440
C22	-2.56730	-0.35870	-1.79180
C23	1.70980	-0.72320	-1.96250
C24	0.31740	-0.63860	-2.22950
C25	-3.23890	1.08410	-0.33010
C26	-2.23210	1.65290	-1.03930
C27	0.00890	2.37180	-0.53400
C28	-1.31820	2.25670	-0.19930
C29	1.83210	1.47770	-1.47130
C30	0.48860	1.66280	-1.66860
C31	-0.35370	0.66560	-2.24990
C32	-1.74770	0.75210	-2.00110
C33	2.54930	0.36510	-1.76250
C34	3.46580	0.16020	-0.75650
C35	3.22510	-1.08290	-0.29780
C36	1.58130	0.68800	2.04440
C37	2.73790	0.28120	1.36810
C38	2.81500	-1.07230	0.99720
C39	2.22220	1.92020	-0.22470
C40	3.15820	1.04010	0.25530

6.3 Coordinates of C_{60}

C_{60}	x	I_h	
		y	z
C1	2.16650	0.59060	2.58740
C2	3.03780	0.17660	1.59180
C3	1.27860	-0.30980	3.16790
C4	3.01180	-1.14340	1.16540
C5	3.10340	-1.43350	-0.19300
C6	3.15030	1.21060	0.66820
C7	3.24280	0.91490	-0.68590
C8	3.21920	-0.40230	-1.12070
C9	-0.43930	1.35270	3.12710
C10	0.43630	0.06330	3.43790
C11	-0.02960	0.06330	3.43790
C12	1.74420	1.87900	2.28300
C13	2.35190	2.26760	1.09900
C14	-0.26330	3.02680	1.63260
C15	0.33740	3.40540	0.43730
C16	1.65160	3.02780	0.17070
C17	-2.09030	-0.82250	2.59550
C18	-2.51110	0.46640	2.28540
C19	-0.84490	-1.02520	3.17380
C20	-1.68740	1.55330	2.55120
C21	-1.58430	2.58580	1.63190
C22	-3.23140	0.40610	1.10070
C23	-3.12270	1.44100	0.17460
C24	-2.29470	2.52910	0.43990
C25	-0.49080	-2.91330	1.73650
C26	-1.74300	-2.71240	1.16370
C27	-0.03930	-2.06840	2.74530
C28	-2.54860	-1.66500	1.59420
C29	-3.26020	-0.91410	0.67010
C30	-1.65430	-3.00610	-0.18970
C31	-2.35420	-2.24390	-1.11700

Details of C_{60} I_h coordinates continued on the next page.

Continuation of C_{60} I_h coordinates:

C_{60}	x	I_h y	z
C32	-3.16430	-1.19490	-0.68780
C33	2.13640	-2.05530	1.73580
C34	1.68950	-2.90090	0.72930
C35	1.27850	-1.63660	2.74350
C36	0.36780	-3.33270	0.73020
C37	-0.34400	-3.39040	-0.45940
C38	2.28890	-2.52500	-0.46400
C39	1.57900	-2.57180	-1.65800
C40	0.25600	-3.00540	-1.65310
C41	-2.18280	-0.57830	-2.59790
C42	-1.74800	-1.86940	-2.30830
C43	-0.43850	-2.24690	-2.58450
C44	-1.28150	0.31890	-3.16710
C45	-2.15260	2.05450	-1.73780
C46	-3.04850	1.15350	-1.18110
C47	-3.06560	-0.16290	-1.61070
C48	-1.26610	1.64070	-2.72710
C49	0.50390	2.93610	-1.74180
C50	-0.37880	3.35610	-0.75130
C51	-1.69430	2.91860	-0.74910
C52	0.05210	2.07300	-2.73550
C53	2.09760	0.83400	-2.60510
C54	2.55170	1.69230	-1.61070
C55	1.75890	2.74520	-1.18240
C56	0.84200	1.02060	-3.17860
C57	0.44610	-1.34950	-3.16610
C58	1.69830	-1.54850	-2.59080
C59	2.51840	-0.46230	-2.31710
C60	0.02180	-0.06450	-3.45850

6.4 Coordinates of C_{80}

Coordinates of C_{80} symmetry $C_{2v} - 3, C_{2v} - 5, D_2 - 2$.

C_{80}	$C_{2v} - 3$			$C_{2v} - 5$			$D_2 - 2$		
	x	y	z	x	y	z	x	y	z
C1	4.25960	0.00440	0.68480	-3.92270	-1.14790	0.67370	-2.10880	2.75020	-1.65590
C2	3.80430	1.09940	1.36910	-3.22680	-2.10920	1.36590	-3.26710	2.35960	-0.94080
C3	4.26110	0.00360	-0.69270	-3.92290	-1.16030	-0.69060	-3.97600	1.21550	-1.24140
C4	3.43790	2.21840	0.68880	-2.56760	-3.08130	0.68300	-1.64550	1.88220	-2.72170
C5	0.97900	0.69720	3.51020	-0.69500	-1.01420	3.62510	-2.38310	0.71460	-2.94210
C6	3.06590	0.69450	2.45890	-2.67690	-1.57090	2.49540	-3.53960	0.40090	-2.23980
C7	1.98890	1.45540	2.93100	-1.43370	-2.00900	2.99200	1.92520	2.55080	-2.29330
C8	1.62220	2.67320	2.27530	-0.72050	-3.03770	2.29830	0.57920	2.73620	-2.42720
C9	0.25120	3.10140	2.28070	0.71860	-3.04020	2.30030	-0.26880	1.82530	-3.07680
C10	2.39660	2.99230	1.12970	-1.35690	-3.54100	1.13440	2.53320	1.44010	-2.76660
C11	-0.20580	3.79990	1.13250	1.36900	-3.54690	1.14340	1.74000	0.44320	-3.29180
C12	3.44960	-2.20890	-0.69110	-3.01920	2.23130	1.35770	0.35960	0.57880	-3.49490
C13	3.45730	-2.21350	0.69460	-3.78400	1.25850	0.70130	-4.48380	-0.69750	0.07630
C14	3.81570	-1.09140	-1.37450	-3.82690	0.02650	1.37040	-4.09810	-1.50590	-0.95270
C15	3.81890	-1.09480	1.37290	-3.08960	-0.23360	2.53090	-4.48560	0.67640	-0.06320
C16	3.07410	-0.70550	2.46490	-1.12550	0.31470	3.69160	-3.63720	-0.95830	-2.13260
C17	1.99170	-1.45780	2.93530	-2.31420	0.73860	3.11790	-2.56140	-1.48640	-2.78090
C18	0.97360	-0.70910	3.50930	-2.30910	1.99310	2.52940	-3.38950	-2.55620	-0.40880
C19	0.57740	-3.91270	-0.00540	-3.78320	1.26080	-0.72760	-2.36130	-3.10480	-1.10810
C20	2.40850	-2.97530	-1.14360	-3.82600	0.02020	-1.38190	-1.94360	-2.58920	-2.30960
C21	1.84690	-3.52310	-0.00480	-2.31480	3.18730	0.65810	-0.38750	-0.62560	-3.50390
C22	1.63120	-2.67740	2.27390	-2.31320	3.19260	-0.69800	-1.76840	-0.48670	-3.30530
C23	2.41430	-2.98540	1.13250	-3.02290	2.23140	-1.38470	-0.60030	-2.78030	-2.44300
C24	-0.19880	-3.78910	1.12960	-1.17440	3.53000	1.35540	0.25200	-1.87160	-3.09360
C25	0.25930	-3.10170	2.28260	0.00150	3.91130	0.69250	-3.63320	0.92950	2.12370
C26	-0.19190	-3.77640	-1.14530	1.17710	3.53370	1.35940	-3.53040	-0.43220	2.24350
C27	0.26770	-3.08780	-2.29560	-0.00250	1.12700	3.71350	-4.09660	1.49720	0.95270
C28	1.63590	-2.66060	-2.29110	0.00430	2.39360	3.13480	-3.96740	-1.24690	1.24670
C29	1.99940	-1.44020	-2.94260	-1.17640	2.79680	2.53540	-3.25930	-2.38760	0.95930
C30	3.07570	-0.68440	-2.46190	1.18580	2.79360	2.53590	-2.37000	-0.74720	2.94320
C31	0.99050	-0.68110	-3.51680	-2.31410	1.97480	-2.55280	-1.62660	-1.91390	2.72020
C32	-1.48270	-3.72080	-0.69160	-2.30470	0.71470	-3.13370	-2.09380	-2.78210	1.65530
C33	-2.41240	-3.00370	-1.37100	-3.08160	-0.25450	-2.53500	-1.12030	-3.49860	0.90950
C34	-2.04530	-2.29080	-2.47840	-1.11640	0.28560	-3.69970	0.18020	-3.49310	1.33180
C35	-0.72240	-2.30560	-2.96400	-1.18000	2.78430	-2.54770	-1.26620	-3.60730	-0.48160
C36	-0.31940	-1.10570	-3.54140	1.17390	2.77510	-2.53610	-2.36980	3.10180	1.10850
C37	-2.42860	-3.02170	1.36020	-0.00270	2.36220	-3.14740	-1.94500	2.56340	2.29660
C38	-1.49320	-3.73360	0.68640	0.00360	1.09760	-3.72230	-3.40190	2.55600	0.42460
C39	-0.33400	-1.13540	3.53500	-0.00300	3.91660	-0.73120	-2.54400	1.44730	2.76780
C40	-0.74370	-2.33360	2.95320	-1.17770	3.54550	-1.38590	-1.75040	0.45620	3.29460
C41	-2.06820	-2.31660	2.47480	1.18160	3.53280	-1.37160	-0.59720	2.75460	2.41970

Details of C_{80} ($C_{2v} - 3, C_{2v} - 5$, and $D_2 - 2$ symmetry) coordinates continued on the next page.

Continuation of the xyz coordinates of C_{80} $C_{2v}-3$, $C_{2v}-5$ and D_2-2 :

C_{80}	$C_{2v}-3$			$C_{2v}-5$			D_2-2		
	x	y	z	x	y	z	x	y	z
C42	0.99230	0.72240	-3.51550	-0.68990	-1.04140	-3.62880	0.25560	1.84280	3.06630
C43	2.00140	1.47660	-2.93170	-1.43670	-2.02660	-2.99130	-0.36980	0.59380	3.48790
C44	3.08060	0.71840	-2.45190	-2.68170	-1.59370	-2.49020	0.60810	-2.75760	2.42670
C45	3.82660	1.11680	-1.36240	-3.24190	-2.13820	-1.36840	-0.24840	-1.84970	3.07260
C46	3.44770	2.23550	-0.69530	-2.56990	-3.10140	-0.69540	0.38720	-0.60290	3.48480
C47	0.25850	3.11530	-2.27520	0.72250	-3.04770	-2.28880	1.76600	-0.45830	3.27710
C48	1.63260	2.69390	-2.27340	-0.71750	-3.05360	-2.29380	0.15930	3.48700	-1.34040
C49	2.40750	3.01120	-1.12640	-1.35670	-3.55930	-1.13050	-1.13850	3.48380	-0.91580
C50	-0.20240	3.80420	-1.12250	1.36130	-3.54760	-1.12210	-1.27880	3.59930	0.47480
C51	0.57680	3.95500	0.00600	0.66450	-3.91980	0.01100	-0.17570	3.50070	1.32970
C52	1.84190	3.56740	0.00360	-0.65930	-3.92220	0.00540	1.12130	3.49330	0.90220
C53	-0.32040	1.14340	-3.53720	0.69280	-1.03760	-3.62590	1.26850	3.59440	-0.48830
C54	-2.05620	2.31910	-2.46120	2.67930	-1.58300	-2.47600	3.39160	2.54540	-0.42910
C55	-0.73540	2.33490	-2.94820	1.43880	-2.01830	-2.98270	2.36030	3.09670	-1.11360
C56	-2.86590	-1.16310	-2.50440	2.31220	1.97030	-2.52910	2.37990	0.74520	2.92690
C57	-2.41690	0.01280	-3.06790	2.30440	0.71290	-3.12150	1.63250	1.90850	2.70640
C58	-1.13800	0.01650	-3.58780	1.12260	0.29030	-3.69940	2.10320	2.77010	1.63820
C59	-2.86900	1.18320	-2.49810	3.08950	-0.24490	-2.51680	3.26710	2.36750	0.93780
C60	-3.40260	2.32940	-0.67970	3.93140	-1.15360	-0.67440	3.63220	-0.93250	2.10150
C61	-2.42930	3.02770	-1.35420	3.23770	-2.12670	-1.35420	3.53730	0.43060	2.22330
C62	-1.49790	3.74000	-0.67860	2.57520	-3.09300	-0.67370	3.98900	1.23280	1.22070
C63	-3.40210	2.31820	0.68740	3.92390	-1.15710	0.69180	4.09510	-1.48630	0.92130
C64	-3.68760	-1.17980	-1.36980	3.03380	2.23370	-1.36890	2.36140	-3.09570	1.09570
C65	-4.07650	-0.00130	-0.71780	3.79490	1.26160	-0.71190	1.95030	-2.57040	2.29280
C66	-3.69570	1.17990	-1.36850	3.84180	0.02540	-1.36860	2.55530	-1.46070	2.75420
C67	-3.69260	-1.18750	1.36990	3.02560	2.23830	1.36790	3.38720	-2.54650	0.39520
C68	-3.40290	-2.33570	0.67470	2.32110	3.19590	0.66790	-0.17140	-3.51620	-1.34920
C69	-3.39740	-2.32980	-0.68830	2.32340	3.19530	-0.68420	1.12780	-3.50950	-0.92940
C70	-3.69310	1.17380	1.37640	3.83050	0.02380	1.38130	1.27510	-3.60500	0.46060
C71	-4.07640	-0.00250	0.72000	3.78990	1.25840	0.71790	3.52980	-0.43670	-2.25900
C72	-1.15240	-0.00700	3.58330	1.11970	0.31330	3.69490	2.36770	-0.75760	-2.95520
C73	-2.87850	1.17180	2.51620	3.08830	-0.23830	2.53980	1.62870	-1.92800	-2.73950
C74	-2.43980	-0.01040	3.07140	2.31310	0.73670	3.12690	3.97890	-1.24810	-1.26220
C75	-2.88380	-1.18690	2.51460	2.31980	1.99170	2.54080	3.26680	-2.38910	-0.97440
C76	-1.50360	3.73800	0.69840	2.58280	-3.09580	0.70430	2.10580	-2.78950	-1.67320
C77	-2.43090	3.01310	1.36840	3.23840	-2.12310	1.38160	4.51210	0.68430	0.05420
C78	-2.06270	2.30730	2.48030	2.67840	-1.57820	2.50410	4.09950	1.49210	-0.97090
C79	-0.73830	2.31730	2.95730	1.42870	-2.00670	2.99840	3.62800	0.92660	-2.13740
C80	-0.33200	1.12020	3.53650	0.68690	-1.01480	3.62760	4.50750	-0.68300	-0.10160

Coordinates of C_{80} symmetry $D_3 - 4, D_{5d} - 1, D_{5h} - 6$.

C_{80}	$D_3 - 4$			$D_{5d} - 1$			$D_{5h} - 6$		
	x	y	z	x	y	z	x	y	z
C1	2.11670	1.67790	-2.64280	-3.72590	0.71360	2.18830	2.27000	2.09900	2.48050
C2	0.88370	2.25530	-2.84600	-2.95730	-0.20790	2.85830	1.04360	2.26610	3.11140
C3	0.64080	3.37510	-2.02840	-4.51270	0.36360	1.10560	0.52350	1.16990	3.78370
C4	-0.63550	3.72660	-1.67550	-2.96810	-1.50020	2.43550	0.15120	3.10450	2.45790
C5	-1.68160	2.98320	-2.11100	-1.78130	-2.20180	2.46680	0.45720	3.72900	1.25530
C6	2.33620	0.33430	-2.89260	-1.78170	0.34680	3.30880	1.68080	3.55020	0.59820
C7	1.31150	-0.55420	-3.28030	-0.59320	-0.35630	3.49100	2.58350	2.72300	1.27860
C8	-0.01260	0.00180	-3.47860	-0.59410	-1.73470	3.03610	-1.22210	2.85270	2.47180
C9	-0.20070	1.42520	-3.28220	1.79360	-3.23290	0.69660	-1.73720	1.74810	3.13610
C10	-1.48150	1.86130	-2.89360	0.60610	-3.18050	1.43220	-0.84270	0.91510	3.79180
C11	-0.88950	-2.20630	-2.90110	0.61100	-2.32840	2.60680	-2.83070	1.14750	2.52530
C12	-1.15310	-0.87380	-3.28220	1.80130	-1.65510	2.87660	-0.72450	3.83480	-0.78430
C13	0.38260	-2.68850	-2.64540	-3.71560	2.29640	-0.00560	-0.72570	3.87090	0.57000
C14	1.49990	-1.90820	-2.84160	-2.96120	2.64230	1.08380	-1.76490	3.32410	1.28230
C15	2.59640	-2.25150	-2.02860	-4.50950	1.16410	-0.01890	-2.84400	2.71120	0.63880
C16	-1.68170	3.94490	0.42030	-2.95700	1.85150	2.18590	-3.36820	1.61160	1.33020
C17	-2.76310	3.23320	-0.02290	-1.78150	1.67200	2.87580	2.57340	2.64730	-1.46460
C18	-0.63100	4.25100	-0.41010	-1.78080	3.23250	0.68100	1.67160	3.51140	-0.82490
C19	-2.77710	2.76940	-1.31450	-0.59640	3.19070	1.42110	0.44690	3.65570	-1.48770
C20	-3.31590	1.55920	-1.62600	-0.59330	2.34900	2.60460	-3.01360	-0.23750	2.56910
C21	-3.95890	0.77070	-0.66980	1.79720	-0.33110	3.31400	-2.10420	-1.06020	3.22190
C22	-3.96620	-0.58970	-0.94520	0.61030	0.38100	3.49240	-1.01650	-0.45900	3.83710
C23	-2.41750	-0.35090	-2.84320	0.61290	1.75980	3.03860	-1.88960	-2.29590	2.62460
C24	-2.53260	1.00030	-2.64920	1.79620	2.22560	2.46850	-3.89010	0.48390	-0.67480
C25	-3.24660	-1.13840	-2.02220	-3.73490	0.70160	-2.20660	-3.88560	0.51730	0.67940
C26	0.89640	3.81600	1.31400	-2.96870	1.84220	-2.19480	-3.66480	-0.62820	1.40470
C27	-0.13920	3.41810	2.12320	-4.52000	0.34590	-1.12740	-3.43550	-1.85560	0.77550
C28	0.66000	4.21540	0.02110	-2.95660	2.64060	-1.09660	-2.53220	-2.68320	1.45440
C29	-1.42070	3.50030	1.68890	-1.78010	3.23910	-0.71180	-1.76360	3.23830	-1.46590
C30	-2.32110	2.53330	2.03290	-1.78550	1.65390	-2.88180	-2.84740	2.66280	-0.78400
C31	-1.93900	1.45100	2.84930	-0.59730	2.33510	-2.60980	-3.38060	1.53170	-1.41240
C32	-2.68520	0.31230	2.64090	-0.59290	3.19280	-1.43840	-0.62780	-2.89740	2.64070
C33	-3.85760	1.20130	0.69510	1.79310	3.03960	1.33780	0.45490	-2.27670	3.25170
C34	-3.22600	2.39700	0.96960	0.60580	3.42250	0.71290	0.23820	-1.04730	3.85620
C35	-3.66330	0.18640	1.63360	0.61030	3.41880	-0.73920	1.67860	-2.46390	2.61900
C36	3.66990	1.58030	0.94130	1.79390	3.02280	-1.35960	-1.68260	-3.56450	-0.56290
C37	2.95730	2.73500	0.65890	-3.72100	-1.86410	-1.35560	-1.67210	-3.52540	0.79130
C38	1.99340	3.06220	1.61540	-2.95810	-1.51050	-2.43780	-0.49310	-3.65660	1.48390
C39	1.62360	2.17340	2.64160	-4.52200	-0.95900	-0.68180	0.72510	-3.82810	0.81980
C40	2.23700	0.95990	2.83780	-2.96130	-0.22060	-2.86670	1.81140	-3.21350	1.45570
C41	3.35260	0.73260	2.01320	-1.78350	0.32830	-3.31420	-3.66220	-0.70110	-1.34140
C42	3.04350	-1.59240	2.10500	-1.78100	-2.22220	-2.46280	-3.43220	-1.89870	-0.64730
C43	3.75560	-0.52490	1.66240	-0.59420	-1.75820	-3.03360	-2.54120	-2.76670	-1.28730
C44	-0.57920	1.30780	3.28970	-0.59460	-0.37940	-3.49120	2.64310	-1.45100	2.58880

As previously, details of C_{80} ($D_3 - 4, D_{5d} - 1,$ and $D_{5h} - 6$ symmetry) coordinates continued on the next page.

Continuation of the xyz coordinates of C_{80} $D_3 - 4$, $D_{5d} - 1$ and $D_{5h} - 6$:

C_{80}	$D_3 - 4$			$D_{5d} - 1$			$D_{5h} - 6$		
	x	y	z	x	y	z	x	y	z
C45	0.27740	2.35810	2.90070	1.79410	2.20860	-2.49040	2.40830	-0.21980	3.18840
C46	-2.16460	-0.94570	2.88900	0.60550	1.73470	-3.04870	1.19310	-0.04340	3.82790
C47	-0.82650	-1.16550	3.28160	0.61090	0.35260	-3.49370	2.94230	0.87380	2.51680
C48	0.01350	0.00020	3.48220	1.80180	-0.35060	-3.30780	2.84880	-2.71180	-0.60270
C49	1.44190	-0.14870	3.27970	-3.74120	-1.87220	1.36720	2.85730	-2.66720	0.75100
C50	1.91640	-1.41710	2.88850	-2.97080	-2.78320	0.68530	3.36960	-1.57630	1.41010
C51	2.65100	3.05420	-0.70190	-4.52740	-0.96050	0.69910	3.89100	-0.48260	0.71160
C52	1.48900	3.74400	-0.97220	-2.95890	-2.78330	-0.67350	3.66390	0.75180	1.33410
C53	4.18610	0.76280	-0.04710	-1.78100	-3.04230	-1.33740	-0.50760	-3.72690	-1.26440
C54	3.78430	1.00560	-1.33630	-1.78400	-3.02790	1.34690	0.72320	-3.86390	-0.60350
C55	3.01230	2.08450	-1.63520	-0.59580	-3.41650	0.72700	1.80410	-3.29580	-1.28700
C56	4.28340	-0.52400	0.39680	-0.59170	-3.42980	-0.72340	3.34530	-1.65510	-1.33570
C57	3.42010	-0.05210	-2.13000	1.79500	-1.67580	-2.87170	3.88010	-0.51810	-0.71270
C58	3.54640	-1.32570	-1.68530	0.60800	-2.35540	-2.59740	3.65310	0.67370	-1.41050
C59	4.01220	-1.59160	-0.42210	0.61270	-3.20490	-1.42130	3.44840	1.86210	-0.74370
C60	1.66860	-3.26170	1.62360	1.80110	-3.24410	-0.69560	3.45440	1.89980	0.60760
C61	2.87150	-2.69950	1.30890	3.73550	-0.71730	-2.19610	2.61960	-1.60650	-2.52030
C62	3.33090	-2.68880	0.01680	2.97590	-1.86310	-2.18160	1.15970	-0.26320	-3.80050
C63	-0.46100	-3.96990	0.95360	2.98570	-2.65870	-1.07820	2.39210	-0.39990	-3.17110
C64	0.89600	-3.93020	0.66920	4.51430	-0.37190	-1.10600	2.92780	0.74010	-2.59340
C65	-2.88900	-1.83240	2.11640	3.72050	1.85850	-1.36910	-0.64920	-3.05420	-2.47380
C66	-2.31680	-2.98080	1.67450	2.97640	1.49920	-2.45980	0.20480	-1.27410	-3.76980
C67	-1.02680	-3.26720	2.02970	2.98070	0.20970	-2.87150	0.43930	-2.47630	-3.11200
C68	-0.26810	-2.41350	2.84580	4.50000	0.94620	-0.68150	1.66890	-2.62310	-2.49540
C69	1.08620	-2.49190	2.64720	3.72410	1.86820	1.36290	-3.03420	-0.37900	-2.53950
C70	-3.36830	-2.68630	-0.41030	2.97360	2.78740	0.67100	-1.05060	-0.67640	-3.78280
C71	-3.98010	-1.55000	0.04350	2.97160	2.78100	-0.68430	-2.13540	-1.25630	-3.13470
C72	-3.76950	-1.13560	1.32830	4.50860	0.94370	0.69730	-1.91110	-2.45850	-2.48630
C73	-2.56900	-3.44490	0.40860	3.74370	-0.70940	2.20860	-1.24080	2.71300	-2.64310
C74	-1.02280	-3.79700	-1.33730	2.98080	0.22360	2.87310	-0.87180	0.70260	-3.82620
C75	-1.76140	-2.95440	-2.13050	2.97580	1.51210	2.45120	-1.77530	1.57200	-3.22550
C76	-2.92330	-2.42180	-1.68510	4.52780	-0.37000	1.12000	-2.86280	1.00180	-2.58810
C77	-1.41800	-4.01690	-0.04390	3.75290	-2.32220	0.00790	2.26140	1.96190	-2.63370
C78	2.49460	-3.16690	-0.96850	2.98050	-2.65100	1.09800	0.49520	0.95820	-3.83780
C79	1.31150	-3.83030	-0.69860	2.98050	-1.85240	2.19590	1.02620	2.10110	-3.25040
C80	0.29910	-3.66890	-1.63880	4.53670	-1.18920	0.00780	0.13030	2.97330	-2.65650

References

- [1] R. C. Haddon. C_{60} sphere or polyhedron? *J. Am. Chem. Soc.*, 119:1797–1798, 1997.
- [2] C. A. Coulson, B. O’Leary, and R. B. Mallion. *Hückel Theory for Organic Chemists*. Academic Press, London, 1978.
- [3] P. Romon. *Introduction à la géométrie différentielle discrète*. Ellipses, December 2013.
- [4] J. Guan, Z. Jin, Z. Zhu, C. Chuang, B-Y. Jin, and D. Tománek. Local curvature and stability of two-dimensional systems. *Phys. Rev. B*, 90:245403, 2014.