J Math Chem (2009) 45:316–329
DOI 10.1007/s10910-008-9408-1

ORIGINAL PAPER

Omega polynomial and its use in nanostructure description

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Abstract A new counting polynomial, called “Omega” $\Omega(G, x)$, was recently proposed by Diudea. It is defined on the ground of *quasi-orthogonal cut “qoc”* edge strips. Three topological descriptors: (1) *CI* (Cluj-Ilmenau), eventually equal to the well-known *PI* index, in planar, bipartite graphs; (2) I_Ω-defined on all the normalized derivatives of the above polynomial and (3) the coefficient of the first power term, called n_p are exemplified and used in nanostructures (e.g., fullerenes, nanotubes and tori) description. Good ability of these descriptors in predicting the heat of formation and strain energy in small fullerenes or the resonance energy in planar benzenoids was found. Omega polynomial is useful in describing the topology of tubular nanostructures.

Keywords Omega polynomial · Topological indices · Nanostructures · Fullerene stability

1 Introduction

Counting polynomials are related to finite sequences of numbers representing some graph-theoretical categories/properties, such as the distance degree sequence or the sequence of selections of k-independent edges. A counting polynomial can be written as:

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$$P(G,x)=\sum_k p(G,k)\cdot x^k \tag{1}$$

where $p(G,k)$ is the frequency of occurrence of the selections (i.e., property partitions) of G, of extent/length k, and x is simply a parameter to hold k.

Counting polynomials were introduced, in the Mathematical Chemistry literature, by Hosoya [1,2], with his *Z-counting* (of the independent edge sets) and the *distance degree* (initially called Wiener and later Hosoya) [3–6] polynomials. Their roots and coefficients are used for the characterization of topological nature of hydrocarbons.

Hosoya also proposed the sextet polynomial [7–10] for counting the resonant rings in a benzenoid molecule. The sextet polynomial is important in connection with the Clar aromatic sextets[11,12], expected to stabilize the aromatic molecules.

Related to the above polynomials are: the *independence* polynomial [13–17] (counting selections of k-independent vertices of G), the *king*, *color*, *star* and *clique* polynomials [18–27]. More about polynomials the reader can find in ref [28].

In case of some distance-related properties, the polynomial coefficients are calculable from the layer/shell matrices [29–31], built up according to the vertex distance partitions of a graph. The info (square) matrices can be obtained within some weighting schemes, so that the derived polynomials could take account of the chemical nature of the atoms/vertices of a chemical graph. Such counting polynomials have been presented elsewhere [32].

The present paper is organized as follows. The second section introduces the Omega polynomial, along with two derived topological indices. In the third part of this work, a parallel between the Omega and PI polynomials is made. Analytical relations for calculating $\Omega(G,x)$ polynomial and related numerical descriptors, in tubular nanostructures, are given in the forth part. Their ability in predicting the stability of small fullerenes and the resonance energy of planar benzenoids is presented in the fifth part. Conclusions and references will close this article.

2 Omega polynomial

Let $G(V,E)$ be a connected bipartite graph with the vertex set $V=V(G)$ and edge set $E=E(G)$, without loops.

Two edges $e=(1,2)$ and $e'=(1',2')$ of G are called *codistant* (briefly: $e\ co\ e'$) if for $k=0,1,2,\ldots$ there exist the relations: $d(1,1')=d(2,2')=k$ and $d(1,2')=d(2,1')=k+1$ or vice versa. For some edges of a connected graph G there are the following relations satisfied [33,34]:

$$e\ co\ e \tag{2}$$

$$e\ co\ e' \Leftrightarrow e'co\ e \tag{3}$$

$$e\ co\ e' \& e' co\ e'' \Rightarrow e\ co\ e'' \tag{4}$$

though the relation (4) is not always valid. An example is given in Fig. 1.

Let $C(e) := \{e' \in E(G); e'\ co\ e\}$ denote the set of all edges of G which are codistant to the edge e. If all the elements of $C(e)$ satisfy the relations (2–4) then $C(e)$ is called

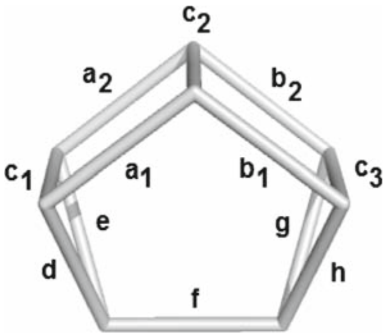


Fig. 1 Counting the *qoc* strips: f and c_2 are codistant but *do not belong to one and the same face*, thus they cannot be counted in a same strip. The polynomial and the derived indices for these graphs are: $\Omega(g, x) = 5x + 2x^2 + x^3$; $CI = 122$; $I_\Omega = 1.41495$

an *orthogonal cut "oc"* of the graph G. The graph G is called *co-graph* if and only if the edge set $E(G)$ is the union of disjoint orthogonal cuts: $C_1 \cup C_2 \cup \ldots \cup C_k = E$ and $C_i \cap C_j = \emptyset$ for $i \neq j, i, j = 1, 2, \ldots, k$.

If any two consecutive edges of a cut edge sequence are codistant (obeying the relations (2) and (3)) and belong to one and the same face of the covering, such a sequence is called a *quasi-orthogonal cut "qoc"* strip. This means that the transitivity relation (4) is not necessarily obeyed.

A *qoc* strip starts and ends either out of G (at an edge with endpoints of degree lower than 3, if G is an open lattice) or in the same starting polygon (if G is a closed lattice). Any *oc* strip is a *qoc* strip but the reverse is not always true.

The *Omega* $\Omega(G, x)$ polynomial for counting *qoc* strips in G is defined as [35,36]:

$$\Omega(G, x) = \sum\nolimits_c m(G, c) \cdot x^c \tag{5}$$

with $m(G, c)$ being the number of strips of length c. The summation runs up to the maximum length of *qoc* strips in G.

Two single number descriptors are derived from $\Omega(G, x)$ as:

$$CI(G) = (\Omega')^2 - (\Omega' + \Omega'')\Big|_{x=1} \tag{6}$$

$$I_\Omega(G) = (1/\Omega'(G, x)) \cdot \sum\nolimits_d (\Omega^d(G, x))^{1/d}\Big|_{x=1} \tag{7}$$

In case I_Ω, summation runs over all possible derivatives d in the corresponding polynomial. When one or more edges do not belong to an already counted strip, such edges are added as "strips of length 1".

This counting polynomial is useful in topological description of benzenoid structures as well as in counting some single number descriptors, i.e., topological indices. The *qoc* strips could give account for the helicity of polyhex nanotubes and tori. The Omega 1.1 software program includes the *qoc* strips procedure [37].

3 Omega polynomial in tubular nano-structures

A (6, 3) tessellation is a polyhex covering, embeddable either in orientable (plane, tube and torus) or non-orientable (Klein bottle) surfaces [38].

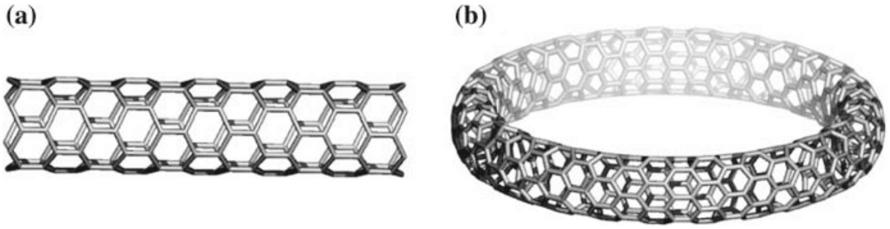
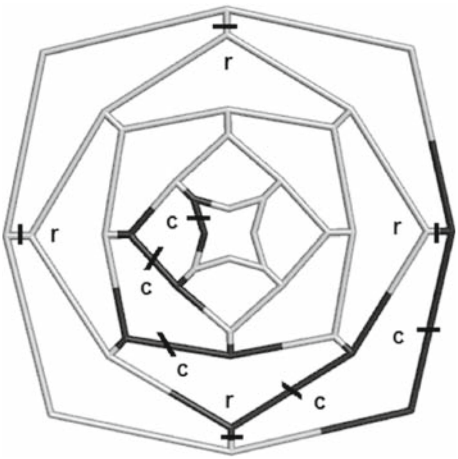


Fig. 2 The (6, 3) "zig-zag" covering. (**a**) Tu(6, 3)H[12,12]; (**b**) T(6, 3)H[12,50]; $v = 600$

Fig. 3 Tube TU(6, 3)H[8,5]; $p = 4$; $q = 5$; $\Omega(G, x) = 4 \cdot x^4 + 8 \cdot x^5$; $CI = 2872$; $I_\Omega = 1.578425$; Torus T(6, 3)V[4,8]; $p = 4$; $q = 4$; $\Omega(G, x) = 4 \cdot x^4 + 4 \cdot x^8$; $CI = 1984$; $I_\Omega = 2.274070$. The points of degree 2 lying on the central circle of a tube have to be pairwise identified to the opposite ones on the external circle to give the corresponding torus



Embedding in cylinder, as open structure, leads to tubular structures corresponding to carbon nanotubes; according to the cross-section feature, "zig-zag" (Fig. 2a) and "armchair" (Fig. 4a, see below) nanotubes can be distinguished. The toroidal polyhexes (Figs. 2b and 4b) are hypothesized to result by gluing together the two open ends of the tubes (Figs. 3 and 5). In a Schlegel-like representation [39], the points (of degree two) lying on the central circle have to be identified with the opposite ones on the external circle to give the corresponding torus.

Two types of cuts of such polyhexes appear in the Schlegel-like representation, one radial (denoted R) and another one circular (denoted C), as given in the corresponding polynomial [36]:

$$\Omega(G, x) = R(G, x) + C(G, x) \tag{8}$$

3.1 The "zig-zag" embedding

Optimized structures of a nanotube (a) and a torus (b) having a "zig-zag" embedding of the (6, 3) covering are illustrated in Fig. 2. Their topological properties and nomenclature, according to Diudea's cutting procedure, have been presented elsewhere [40,41].

Figure 3 details the cutting mode in the "zig-zag" embedding.

(a) *Case of zig-zag tubes* TU(6, 3)H[2p,q] (Fig. 3, $p = 4$; $q = 5$).

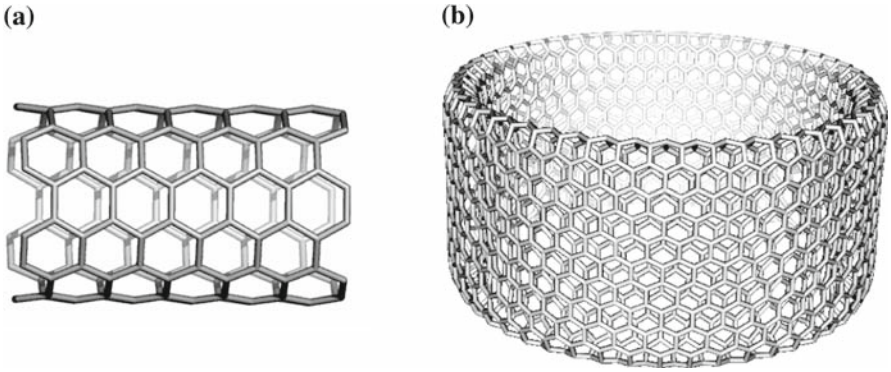


Fig. 4 The $(6,3)$ "armchair" covering. (**a**) Tu(6,3)V[12,12]; (**b**) T$(6,3)$V$[20,100]$; $v = 2000$

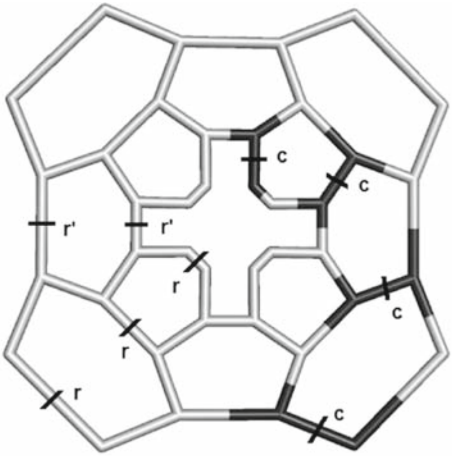


Fig. 5 Tube TU$(6,3)$V[8,5]; $p = 4; q = 5$; $\Omega(G,x) = 4\cdot x^2 + 4\cdot x^3 + 8\cdot x^4$; $CI = 2524$; $I_\Omega = 1.4045$; Torus T$(6,3)$H$[4,8]$; $p = 4$; $q = 4$; $\Omega(G,x) = 8\cdot x^2 + 4\cdot x^8$; $CI = 2016$; $I_\Omega = 2.2472$. The points of degree 2 lying on the central circle of a tube have to be pairwise identified to the opposite ones on the external circle to give the corresponding torus

The circular and radial terms are as follows:

$$C(G,x) = (q-1)\cdot x^p \tag{9}$$

$$R(G,x) = 2p\cdot x^q \tag{10}$$

and the corresponding index:

$$\begin{aligned} CI(\mathrm{TU}(6,3)\mathrm{H}[2p,q]) &= p^2(3q-1)^2 - (q-1)p^2 - 2pq^2 \\ &= 9p^2q^2 - 7p^2q + 2p^2 - 2pq^2 \end{aligned} \tag{11}$$

(b) *Case of tori*, T$(6,3)$V$[q,2p]$.

These tori correspond to "zig-zag" tubes, in a Schlegel-like projection (Fig. 3, $p = 4$; $q = 4$). The circular term C is the same for all the cases:

$$C(G,x) = q\cdot x^p \tag{12}$$

and the radial term R varies as follows:

$$R(G,x) = k \cdot x^{2pq/k} \tag{13}$$

with k being as above.

The index CI is calculable as:

$$\begin{aligned} CI(\mathrm{T}(6,3)\mathrm{V}[q,2p]) &= 9p^2q^2 - k(2pq/k)^2 - p^2q \\ &= (9kp^2q^2 - 4p^2q^2 - kp^2q)/k \end{aligned} \tag{14}$$

3.2 “Armchair” embedding

Optimized structures showing the “armchair” embedding of the (6, 3) covering are illustrated in Fig. 4.

Figure 5 details the cutting mode in the “armchair” embedding.

(a) *Case of “armchair” tubes*, TU(6, 3)V[$2p, q$], or TU(6, 3)V[c, n] in general, in Diudea’s nomenclature [40–42], with $p = c/2$ and $q = n$, as given in Fig. 5.

For all polyhex armchair tubes the circular term C is the same:

$$C(G,x) = 2p \cdot x^{q-1} \tag{15}$$

The radial term R varies function of the tube structure:

$q = even$:

$$R(G,x) = 2p \cdot x^{q/2} \tag{16}$$

The corresponding CI index is:

$$\begin{aligned} CI(\mathrm{TU}(6,3)\mathrm{V}[2p,q_e]) &= p^2(3q-2)^2 - 2p(q-1)^2 - pq^2/2 \\ &= 9p^2q^2 - 12p^2q + 4p^2 - (5/2)pq^2 + 4pq - 2p \end{aligned} \tag{17}$$

$q = odd$:

$$R(G,x) = p \cdot x^{(q+1)/2} + p \cdot x^{(q-1)/2} \tag{18}$$

$$\begin{aligned} CI(\mathrm{TU}(6,3)\mathrm{V}[2p,q_o]) &= p^2(3q-2)^2 - 2p(q-1)^2 - (p/2)(q^2+1) \\ &= 9p^2q^2 - 12p^2q \\ &\quad + 4p^2 - (5/2)pq^2 + 4pq - (5/2)p \end{aligned} \tag{19}$$

(b) *Case of tori*, T(6, 3)H[$q, 2p$]. An “armchair” nanotube TU(6, 3)V[$2p, q + 1$] (Fig. 5, $p = 4$; $q = 4$), transforms in a torus T(6, 3)H[$q, 2p$] as above mentioned, with q (q = even, always by this construction) winding around the tube while p around the central hollow of the torus.

The radial term in such tori is the same for all the cases:

$$R(G, x) = 2p \cdot x^{q/2} \tag{20}$$

and the circular term Cvary as:

$$C(G, x) = k \cdot x^{2pq/k} \tag{21}$$

with k being the greatest common divisor of q and $2p$.

The index is calculated as:

$$\begin{aligned} CI(\mathrm{T}(6,3)\mathrm{H}[q, 2p]) &= 9p^2q^2 - k(2pq/k)^2 - 2p(q/2)^2 \\ &= (18kp^2q^2 - 8p^2q^2 - kpq^2)/(2k) \end{aligned} \tag{22}$$

4 Correlating ability

Among the single number descriptors provided by the Omega polynomial, one is of particular importance: n_p, the number of *pentagon fusions*, appearing as the *coefficient of the first power term*, which accounts for more than 90% of the variance in heat of formation HF of small fullerenes, e.g., C_{40} and C_{50}.

Pentagon fusion is a major destabilizing factor in the classical fullerenes. To account for this, Albertazzi et al. [43] have proposed the number n_p, of pentagon-adjacency: $n_p \leq 30$ for any fullerene and varies from 20 to 10 within the C_{40} set. The maximum value occurs for the hemidodecahedral capped isomer 40:1, and the minimum for the two isomers 40:38 and 40:39.

Semiempirical calculations have been performed on a Pentium IV PC by using the PM3 Hamiltonian, in standard parametrization supplied by HyperChem software (optimization by Polak-Ribiere conjugate-gradient method, at RMS gradient <0.01 kcal/(Å mol)).

The ordering of fullerene graphs, in Table A2, is that resulting from their *spiral codes* [44]. The structures of C_{40} isomers are tabulated in Appendix (Table A1) along with their topological and energetical parameters (Table A2) while the plots are given in Figs. 6 and 7.

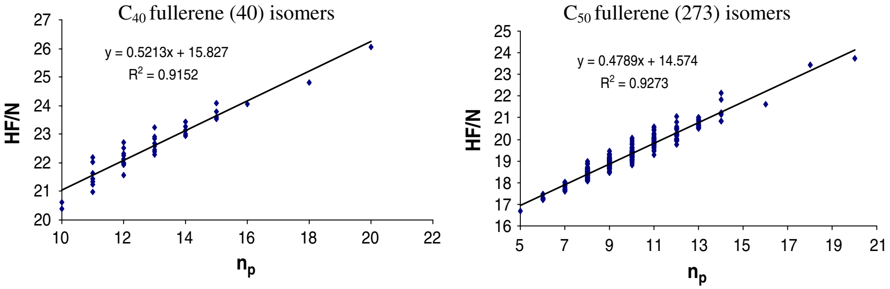


Fig. 6 The plot heat of formation HF (kcal/mol) vs n_p in C_{40} and C_{50} fullerene isomers

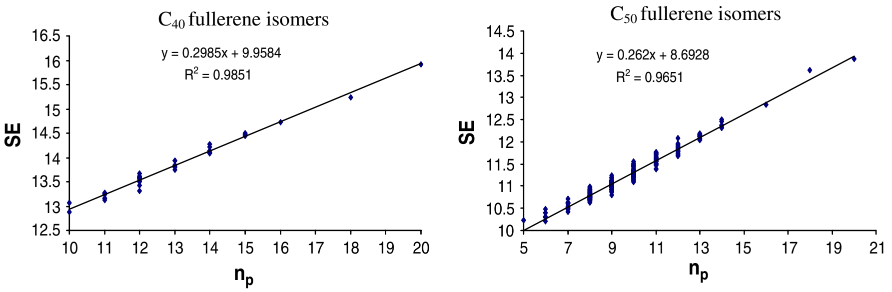


Fig. 7 The plot POAV1 strain energy SE (kcal/mol) vs n_p in C_{40} and C_{50} fullerene isomers

The other two indices CI and I_Ω, derived from the Omega polynomial, contribute rather poor to the global correlation.

Even better is correlated the strain energy SE, calculated according to POAV1 procedure [45–47]. The less strained isomer is 38-D_2.

Resuming to the n_p descriptor, it can be derived from the relations:

$$n_p = 180 - pv \tag{23}$$

$$pv_k = (1/2)\sum_{pi} [\mathbf{LV}(Du(\mathrm{M}))]_{i,k} \tag{24}$$

with summation running over all entries, in the layer matrix of valences LV, corresponding to pentavalent vertices in the *dual* of molecular graph. The pv_k parameter is the sum of faces size at the kth shell around each pentagon, in the original graph. In case $k = 1$, (the subscript k omitted), it varies between 150 (in C_{20}) and 180 (in IPR fullerenes), and from 160 to 170 within the set of C_{40} isomers (see Table A2). In IPR fullerenes, $n_p = 0$, as expected. The number 180 is calculated as: $(12 \times 5 \times 6)/2$ and represents the maximum value of v_p.

A set of 12 pyrenes (see Appendix, Table A3) has been selected among several planar benzenoids, published by Randić [48], and submitted to correlating test with their resonance energy RE with single number descriptors derived from the Omega polynomial (Table A4). The model obtained is:

$$RE = -3.209 + 3.858 I_\Omega + 0.00076 CI \tag{25}$$

$$n = 12;\ R^2 = 0.9669;\ F = 131.609$$

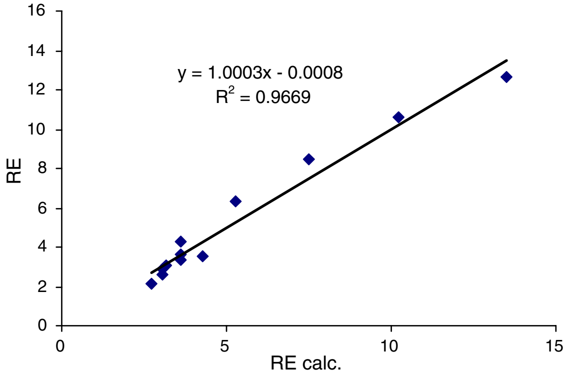
and the plot is presented in Fig. 8.

The result of Eq. 25 is appreciated as good, since no size effect within this series congeners has been hypothesized; however, no direct comparison with similar results could be made, due to the lack of papers in the field.

5 Conclusions

The newly proposed Omega counting polynomial, recently defined by Diudea on the ground of *quasi-orthogonal cut "qoc"* edge strips, proved to be a useful description of

Fig. 8 Predicting the resonance energy RE by indices derived from Omega polynomial



polyhedral coverings appearing in nanostructures. The three topological descriptors: CI, I_{Ω} and n_p have found utility in predicting the stability of small fullerenes, as well as the resonance energy of planar benzenoids. Omega polynomial is also useful in describing the topology of tubular nanostructures.

Acknowledgements the authors gratefully acknowledge the financial support by Romanian CEEX 41/2006.

Appendix

Table A1 Structure of the C_{40} isomers

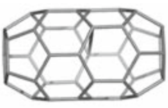
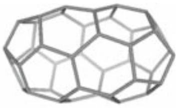
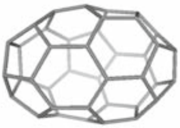
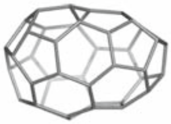
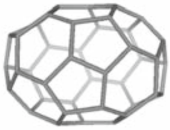
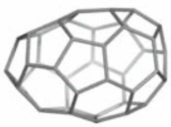
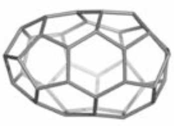
 C_{40}:1	 C_{40}:2	 C_{40}:3
 C_{40}:4	 C_{40}:5	 C_{40}:6
 C_{40}:7	 C_{40}:8	 C_{40}:9
 C_{40}:10	 C_{40}:11	 C_{40}:12

Table A1 continued

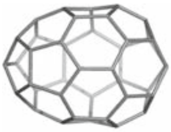
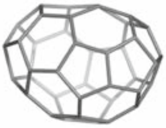
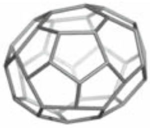
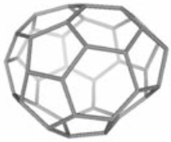
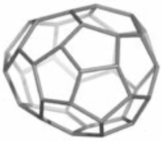
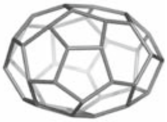
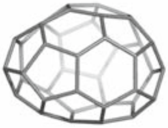
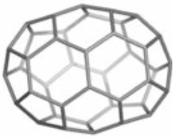
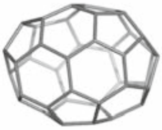
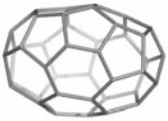
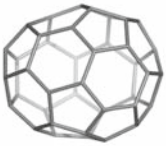
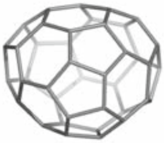
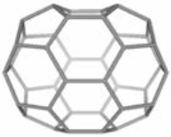
 C_{40}:13	 C_{40}:14	 C_{40}:15
 C_{40}:16	 C_{40}:17	 C_{40}:18
 C_{40}:19	 C_{40}:20	 C_{40}:21
 C_{40}:22	 C_{40}:23	 C_{40}:24
 C_{40}:25	 C_{40}:26	 C_{40}:27
 C_{40}:28	 C_{40}:29	 C_{40}:30
 C_{40}:31	 C_{40}:32	 C_{40}:33

Table A1 continued

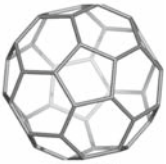
C_{40}:34

C_{40}:35

C_{40}:36

C_{40}:37

C_{40}:38



C_{40}:39

C_{40}:40

Table A2 Topological and energetical parameters of C_{40} isomers

$C_{40:i}$	n_p	pv	PM3 HF/atom (kcal/mol)	SE/atom (kcal/mol)
1-D_{5d}	20	160	26.053	15.908
2-C_2	16	164	24.057	14.724
3-D_2	18	162	24.809	15.243
4-C_1	15	165	23.542	14.474
5-C_s	14	166	23.008	14.264
6-C_1	14	166	22.960	14.111
7-C_s	15	165	23.811	14.443
8-C_{2v}	15	165	23.589	14.492
9-C_2	13	167	22.847	13.838
10-C_1	13	167	22.588	13.810
11-C_2	15	165	24.081	14.464
12-C_1	13	167	22.304	13.794
13-C_s	13	167	22.692	13.809
14-C_s	12	168	21.982	13.577
15-C_2	12	168	22.520	13.677
16-C_2	13	167	22.469	13.839
17-C_1	13	167	22.395	13.742
18-C_2	14	166	23.151	14.143
19-C_2	13	167	22.903	13.934
20-C_{3v}	12	168	22.721	13.552
21-C_2	12	168	22.325	13.603
22-C_1	12	168	21.991	13.527
23-C_2	13	167	23.235	13.935
24-C_s	11	169	21.638	13.281
25-C_2	12	168	22.134	13.578
26-C_1	11	169	21.444	13.249
27-C_2	12	168	21.967	13.431
28-C_s	12	168	21.927	13.597
29-C_2	11	169	21.328	13.227

Table A2 continued

$C_{40:i}$	n_p	pv	PM3 HF/atom (kcal/mol)	SE/atom (kcal/mol)
30-C_3	12	168	22.272	13.610
31-C_s	11	169	20.972	13.166
32-D_2	14	166	23.425	14.082
33-D_{2h}	14	166	24.922	14.212
34-C_1	12	168	22.113	13.494
35-C_2	11	169	22.192	13.262
36-C_2	11	169	22.042	13.166
37-C_{2v}	11	169	21.231	13.123
38-D_2	10	170	20.408	12.887
39-D_{5d}	10	170	20.629	13.066
40-T_d	12	168	21.569	13.312

Table A3 Pyrenic structures and their Omega polynomial

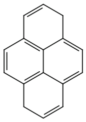
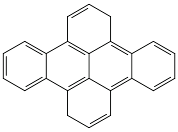
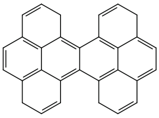
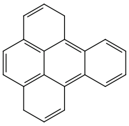
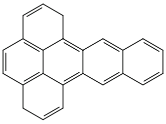
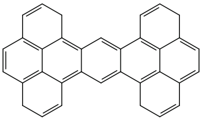
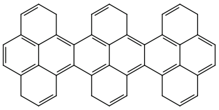
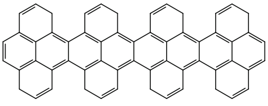
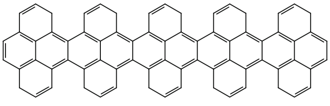
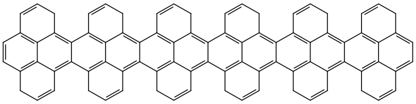
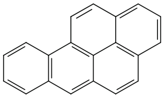
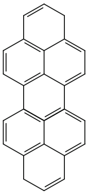
		
1 2X^2+5*X^3	**2** 6*X^2+4*X^3+1*X^5	**3** 4*X^2+8*X^3+1*X^5
		
4 4*X^2+4*X^3+1*X^4	**5** 6*X^2+4*X^3+1*X^5	**6** 6*X^2+8*X^3+1*X^6
		
7 6*X^2+12*X^3+1*X^7	**8** 8*X^2+16*X^3+1*X^9	**9** 10*X^2+20*X^3+1*X^11
		
10 12*X^2+24*X^3+1*X^13		**11** 4*X^2+4*X^3+1*X^4
		
12 3*X^2+6*X^3+2*X^4		

Table A4 Topologica indices and resonance energy for pyrenic structures in Table A3

Structure	I	CI	RE	RE Calc.*
1	1.470	308	2.133	2.697
2	1.613	756	3.669	3.585
3	1.524	1256	4.243	3.621
4	1.520	508	2.906	3.039
5	1.613	756	3.319	3.585
6	1.621	1632	3.527	4.278
7	1.645	2844	6.351	5.287
8	1.785	5072	8.459	7.509
9	1.932	7940	10.571	10.246
10	2.084	11448	12.675	13.482
11	1.520	508	2.585	3.039
12	1.473	926	3.116	3.174

* Calculated cf. Eq. 32

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