Chapter 11
Diamond D_5, a Novel Class of Carbon Allotropes

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Abstract Design of hypothetical crystal networks, consisting of most pentagon rings and generically called diamond D_5, is presented. It is shown that the seed and repeat-units, as hydrogenated species, show good stability, compared with that of C_{60} fullerene, as calculated at DFT levels of theory. The topology of the network is described in terms of the net parameters and Omega polynomial.

11.1 Introduction

The nano-era, a period starting since 1985 with the discovery of C_{60}, is dominated by the carbon allotropes, studied for applications in nano-technology. Among the carbon structures, fullerenes (zero-dimensional), nanotubes (one dimensional), graphene (two dimensional), diamond and spongy nanostructures (three dimensional) were the most studied (Diudea 2005; Diudea and Nagy 2007). Inorganic compounds also attracted the attention of scientists. Recent articles in crystallography promoted the idea of topological description and classification of crystal structures (Blatov et al. 2004, 2009; Delgado-Friedrichs and O'Keeffe 2005).

Diamond D_6 (Fig. 11.1), the classical, beautiful and useful diamond has kept its leading interest among the carbon allotropes, even as the newer "nano" varieties. Along with electronic properties, the mechanical characteristics appear of great

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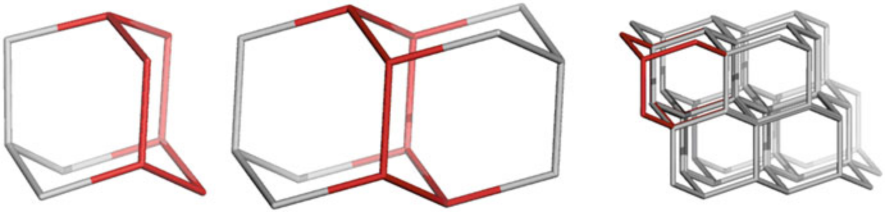

Fig. 11.1 Diamond, a triple periodic network: Ada(mantane) D_6_10_111 (*left*), Dia(mantane) D_6_14_211 (*central*) and Diamond D_6_52_222 net (*right*)

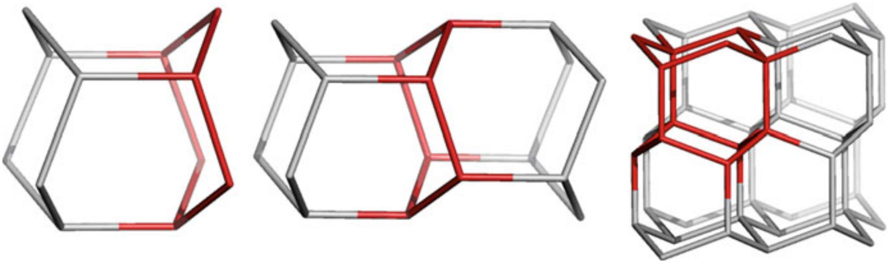

Fig. 11.2 Losdaleite, a double periodic network: L_6_12_111 (*left*), L_6_18_211 (*central*) and L_6_48_222 net (*right*)

importance, as the composites can overpass the resistance of steel or other metal alloys. A lot of efforts were done in the production and purification of "synthetic" diamonds, from detonation products (Decarli and Jamieson 1961; Aleksenskiĭ et al. 1997; Osawa 2007, 2008) and other synthetic ways (Khachatryan et al. 2008; Mochalin and Gogotsi 2009).

However, the diamond D_6 is not unique: out of the classical structure, showing all-hexagonal rings of sp^3 carbon atoms in a cubic network (space group $Fd3m$), there is Lonsdaleite (Frondel and Marvin 1967; He et al. 2002) a rare stone of pure carbon discovered at Meteor Crater, Arizona, in 1967 and also several hypothetical diamond-like networks (Sunada 2008; Diudea et al. 2010). The Lonsdaleite hexagonal network (space group $P6_3/mmc$) is illustrated in Fig. 11.2.

Dendrimers are hyper-branched nano-structures, made by a large number of (one or more types) substructures called monomers, synthetically joined within a rigorously tailored architecture (Tomalia et al. 1990; Newkome et al. 2001; Diudea and Katona 1999). They can be functionalized at terminal branches, thus finding a broad pallet of applications in chemistry, medicine, etc.

Multi-tori MT are structures of high genera (Diudea 2010a), consisting of more than one tubular ring. They are supposed to result by self-assembly of some repeat units (i.e., monomers) which can be designed by opening of cages/fullerenes or by appropriate map/net operations. Multi-tori, rather than dendrimers, appear in processes of self-assembling of some rigid monomers. Zeloites and spongy carbon, recently synthesized (Barborini et al. 2002; Benedek et al. 2003) also contain multi-tori.

Structures of high genera, like multi-tori, can be designed starting from the Platonic solids, by using appropriate map operations (Diudea 2010a). Such structures have before been modeled by Lenosky et al. (1992) and Terrones and Mackay (1997) etc.

11.2 Dendrimer Design and Stability

A tetrapodal monomer M_1(Fig. 11.3, *left*), designed by $Trs(P_4(\mathrm{T}))$ sequence of map operations (Diudea and Ilić 2011) and consisting of all pentagonal faces, can self-arrange to a dendrimer M_5, at the first generation stage (Fig. 11.3, *right*).

The "growing process" is imagined occurring by identification of the trigonal faces of two opposite M_1 units; at the second generation, six pentagonal hypercycles are closed, as in molecule M_{17}, Fig. 11.4 (Diudea and Ilić 2011).

The process is drown as a "dendrimer growth", and is limited here at the fifth generation (Fig. 11.4), when a tetrahedral array results: $4S\_MT = M_{57}$.

Multi-tori herein considered can be viewed either as infinite (*i.e.*, open) structures or as closed cages; then, it is not trivial to count the number of simple tori (*i.e.*, the genus g) in such complex structures.

The Euler's formula [Euler (1758)]: $v - e + f = 2(1 - g)$, where v, e and f are the number of vertices/atoms, edges/bonds, and faces, respectively, is applicable only in case of single shell structures. In multi shell structures (Diudea and Nagy 2008), have modified the Euler formula as: $v - e + r - p(s - 1) = 2(1 - g)$, where r stands for the number of hard rings (*i.e.*, those rings which are nor the sum of some smaller rings), p is the number of smallest polyhedra filling the space of the considered structure while s is the number of shells. In case of an infinite structure, the external trigonal faces are not added to the total count of faces/rings. The calculated g-values are given in Fig. 11.4.

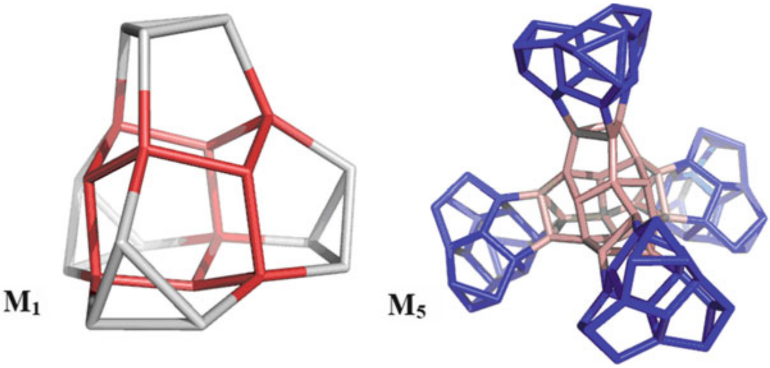

Fig. 11.3 Tetrapodal unit designed by $Trs(P_4(\mathrm{T}))$ and the corresponding dendrimer, at first generation stage

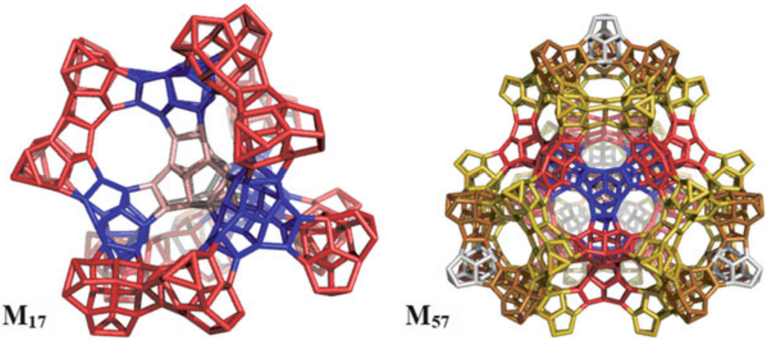

Fig. 11.4 Dendrimer at second (*left*) and fifth (*right*) generation stage; $M_{57} = 4S\_MT$; $v = 972$; $e = 1770$; $f_5 = 684$; $g = 58$ (infinite structure); adding $f_3 = 40$, then $g = 38$ (finite structure)

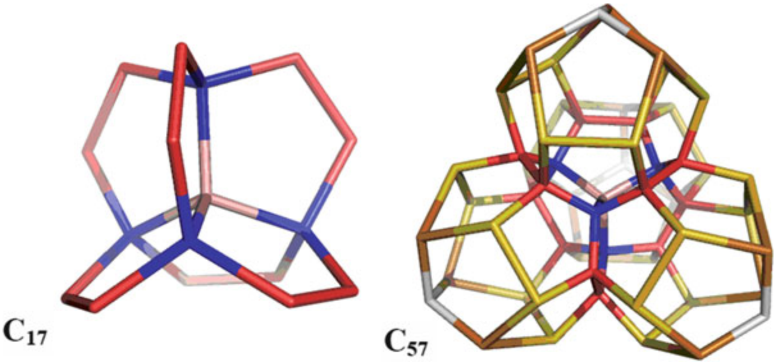

Fig. 11.5 Reduced graphs at 2nd (*left*) and 5th (*right*) generation stage; C_{57}: $v = 57$; $e = 94$; $r_5 = 42$; $g = 0.5$; $R(C_{57}, x) = 42x^5 + 82x^9 + 144x^{10}$

The number of tetrapodal monomers, added at each generation, up to the fifth one, realized as M_{57}, is: 1; 4; 12, 24, 12, 4. The connections in M_{57} are complex and to elucidate the large structures up to the fifth generation, the design of the corresponding reduced graphs (Fig. 11.5) was needed (Diudea 2010b, 2011).

The structure C_{17} (Fig. 11.5, *left*) we call the "seed" of all the hereafter structures. The structure C_{57} (Fig. 11.5, *right*) corresponds to the above M_{57} and is equivalent to 4 "condensed" dodecahedra, sharing a common point. By considering this common point as an internal shell *s*, the modified (Diudea and Nagy 2008) Euler formula will give (for $v = 57$; $e = 94$; $r = 42$; $p = 4$ and $s = 2$) a (non-integer) genus $g = 0.5$. The ring polynomial R(x) is also given, at the *bottom* of Fig. 11.5.

11.3 Diamond D_5 Networks

11.3.1 Spongy D_5

A monomer C_{81}, derived from C_{57} and consisting of four closed C_{20} units and four open units, and its mirror image (Fig. 11.6) was used by (Diudea and Nagy 2011a) to build the alternant network of spongy diamond SD_5 (Fig. 11.7). The nodes of diamond SD_5 network consist of C_{57} units and the network is triple periodic.

The number of atoms v, bonds e, and C_{57} monomers m, and the content in sp^3 carbon, given as a function of k – the number of monomers along the edge of a cubic (k,k,k) domain. At limit, in an infinitely large net, the content of sp^3 carbon approaches 77% (see Appendix 2, Table 11. 4). The density of the net varies around an average of $d = 1.6$ g/cm^3, in agreement with the "spongy" structure of D_5 net (Fig. 11.7).

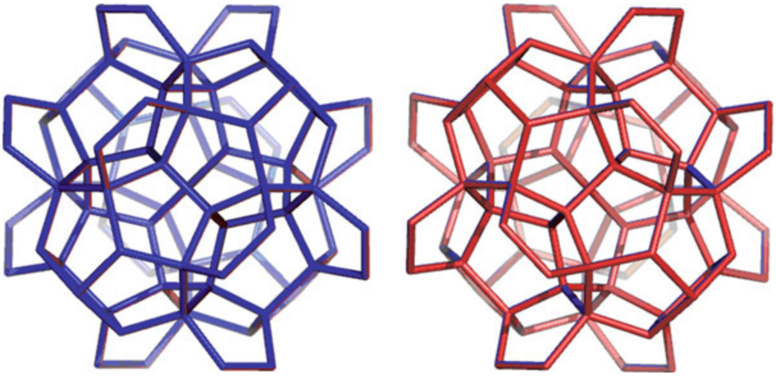

Fig. 11.6 Monomer C_{81} unit (*left-up*), and its mirror image-pair (*right-up*); the monomers as in the triple periodic network of diamond SD_5

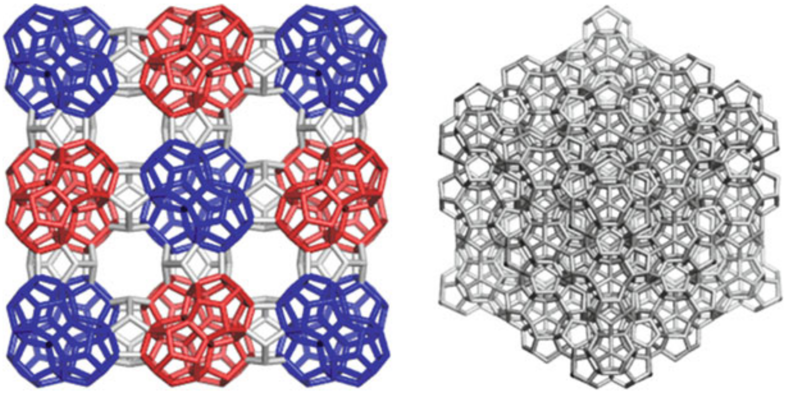

Fig. 11.7 SD_5 (C_{57}) triple periodic network: top view (*left*) and corner view (*right*)

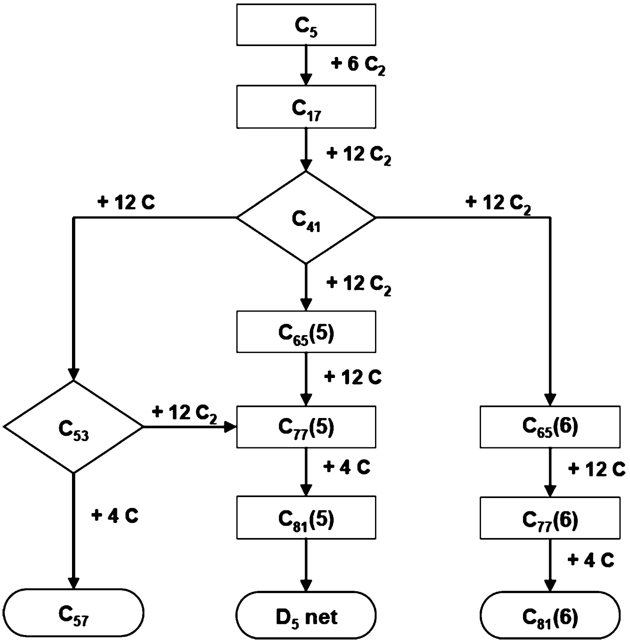

Fig. 11.8 Pathway to D_5

A possible pathway to D_5 was proposed by Diudea and Nagy (2011a) (Fig. 11.8): The main intermediate structures in this scheme are: C_{17} (the "seed" of D_5), C_{41}, C_{53} and $C_{81}(5)$ (see Fig. 11.8). The stability of these structures was evaluated as hydrogenated species. The C_{81} monomer has a C_{57} core and contains 12 flaps which represent half of the junctions between the SD_5 nodes.

To avoid the non-wished side products $C_{65}(6)$ to $C_{81}(6)$ (containing six-membered rings), the suggested way is through C_{53}. In a next step, one can reach either C_{57} as a final structure (which can, however, lead to some dense species of D_5) or go to $C_{81}(5)$, the monomer of SD_5 network.

Of course, the scientist will choose the most convenient route in an attempt to synthesize these structures.

11.3.2 Dense D_5

There is a chance to reach D_5 just from C_{17}, a centrohexaquinane (Paquette and Vazeux 1981; Kuck 2006) which can dimerize (Diudea and Nagy 2011b; Eaton 1979) to $2 \times C_{17} = C_{34}$ and this last condensing to $4 \times C_{17} = C_{51}$ (Fig. 11.9, *top row*).

A linear $4 \times C_{17} = C_{57}$ is also energetically possible (see Table 11.1). The angular tetramer $4 \times C_{17} = C_{51}$ will compose the six edges of a tetrahedron to form the corresponding Adamantane-like Ada_20_170, bearing six pentagonal

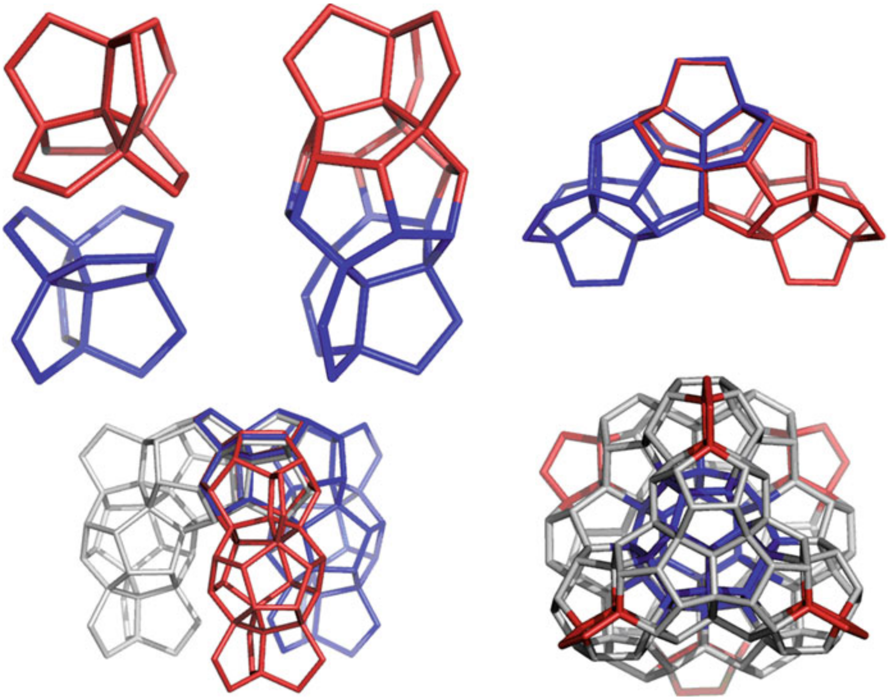

Fig. 11.9 Way to Ada_20: 2 × C_{17} = C_{34} (*top-left and central*), 4 × C_{17} = C_{51} (*top-right*), 3(4 × C_{17}) = C_{119} (*bottom-left*) and Ada_20_170 (*bottom-right*)

Table 11.1 Single point calculation results (HOMO-LUMO gap in eV and total energy E_{tot} in a.u.) at the B3LYP/6-31 G(d,p) levels of theory; C_{60} is taken as reference structure

		B3LYP		
Struct	Sym	E_{tot}	Gap	E_{tot}/N
$C_{17}H_{12}$	T_d	−650.66	6.04	−38.27
$C_{34}H_{12}$	C_{2h}	−1302.36	3.23	−38.31
$C_{51}H_{14}$-ang	C_{2v}	−1951.13	3.34	−38.26
$C_{57}H_{18}$-lin	D_{3h}	−2182.07	2.97	−38.28
$C_{158}H_{12}$	T_d	−6025.94	3.24	−38.139
$C_{170}H_{12}$	T_d	−6483.08	3.17	−38.136
$C_{20}H_{20}$	I_h	−774.21	8.00	−38.71
C_{20}	D_2	−761.44	1.94	−38.07
C_{60}	I_h	−2286.17	2.76	−38.10

wings (in red – Fig. 11.9, *right*, *bottom*), or without wings, as in Ada_20_158 (Fig. 11.10, *left*). Compare this with Adamantane (Fig. 11.1, *left*) in the structure of classical diamond D_6. In the above symbols, "20" refers to C_{20}, which is the main unit of the dense diamond D_5 (Figs. 11.10–11.12) while the last number counts the carbon atoms in the structures.

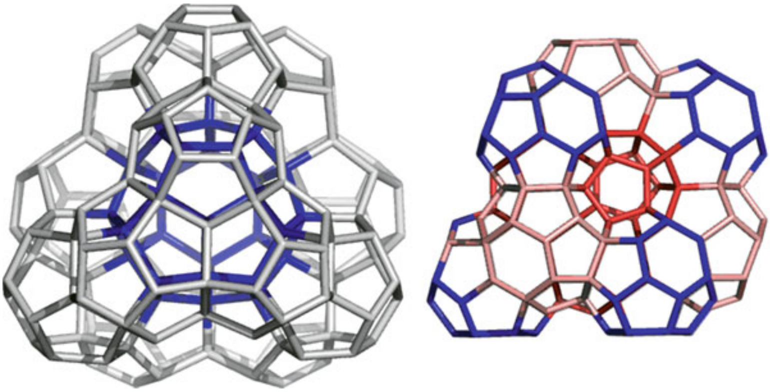

Fig. 11.10 Adamantane-like structures: Ada_20_170 (*left*) and Ada_28_213 (*right*)

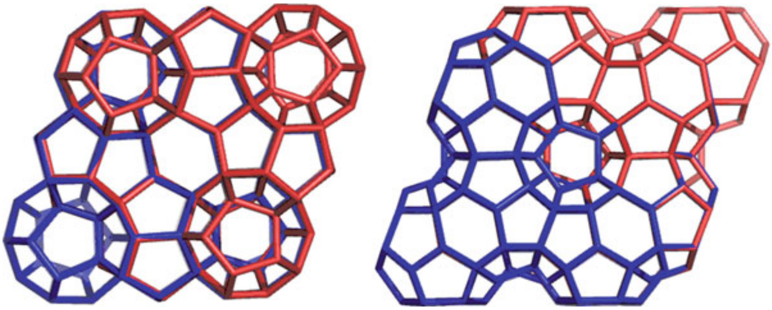

Fig. 11.11 Diamantane-like structures: Dia_20_226 net (*left*) and Dia_28_292 co-net (*right*)

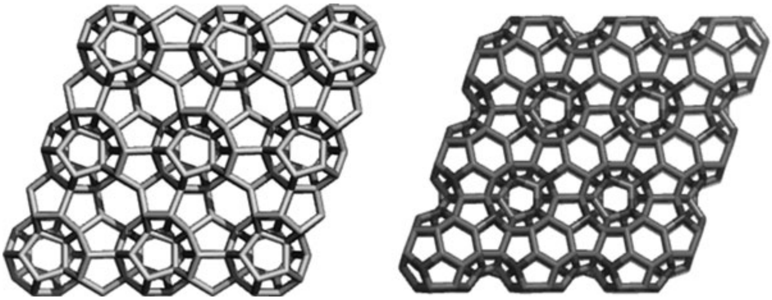

Fig. 11.12 Diamond D_5_20_860_333 net (*left*) and D_5_28_ 1022_333 co-net (*right*)

A diamantane-like unit is evidenced, as in Fig. 11.11 (see for comparison the diamantane, Fig. 11.1, *central*). Since any net has its co-net, the diamond D_5_20 net has the co-net D_5_28 (Fig. 11.12, *right*), of which corresponding units are illustrated in Figs 11.10 (*right*)–11.11 (*right*), respectively. In fact is one and the same *triple periodic* D_5 network, built up basically from C_{20} and having as hollows the fullerene C_{28} (Diudea and Nagy 2011b). The co-net D_5_28 cannot be reached from C_{28} alone since the hollows of such a net consist of C_{57} units (a C_{20}-based structure, see above) or higher tetrahedral arrays of C_{20} thus needing extra C atoms per Ada-like unit. The C_{28}-based hyperdiamond reported by Bylander and Kleinman (1993) consists of only C_{28} fullerenes joined by the tetrahedrally disposed neightbors by *only one covalent bond*.

Our D_5_20/28 hyperdiamond mainly consists of sp^3-bonded carbon atoms building Ada-like repeating units (including C_{28} as hollows), the cohesive bonds of these units being the same sp^3 covalent (and the same distributed) bonds as within the repeating units. This is in high contrast to the (Bylander and Kleinman 1993) hyperdiamond. The ratio C-sp^3/C-total trends to 1 in a large enough network. The topology of the D_5 networks is detailed in the last section.

Since the smallest C_{20} fullerene is the highest reactive one, it is expected to spontaneously stabilize in an sp^3-crystalline form, e.g., bcc-C_{20} (Chen et al. 2004; Ivanovskii 2008) or D_5_20/28 (Diudea and Nagy 2011b). A similar behavior is expected from the C_{20}-derivative $2 \times C_{17} = C_{34}$ (Fig. 11.9) to provide the Ada-like repeating units of the proposed D_5-diamond.

As the content of pentagons R[5] per total rings trend to 90% (see Table 11.5, entry 9) we called this, yet hypothetical carbon allotrope, the diamond D_5. Since the large hollows in the above spongy diamond are not counted, and the small rings are all pentagons, we also called it (S)D_5.

The presence of pentagons in diamond-like fullerides and particularly the ratio R[5]/R[6] seems to be important for the superconducting properties of such solid phases (Breda et al. 2000). In D_5 this ratio trends to 9 (see Table 11.5).

Energetic data, calculated at the DFT level in Table 11.1 – (Diudea and Nagy 2011a, b) show a good stability of the start and intermediate structures. Limited cubic domains of the D_5 networks have also been evaluated for stability, data proving a pertinent stability of the (yet) hypothetical D_5 diamond.

The calculated data show these structures as energetic minima, as supported by the simulated IR vibrations. All-together, these data reveal the proposed structures as pertinent candidates to the status of real molecules.

Density of the D_5 networks was calculated with the approximate (maximal) volume of a cubic domain. The values range from 1.5 (SD_5) to 2.8 (D_5).

11.4 Lonsdaleite L_5_28 Network

By analogy to D_5_20/28, a lonsdaleite-like net was built up (Fig. 11.13).

As a monomer, the hyper-hexagons L_5_28_134 (Fig. 11.13, *left* and *central*), in the chair conformation, of which nodes represent the C_{28} fullerene, was used. Its corresponding co-net L_5_20 was also designed. The lonsdaleite L_5_28/20 is a double periodic network, partially superimposed to the D_5_20/28 net (Diudea and Nagy 2011b).

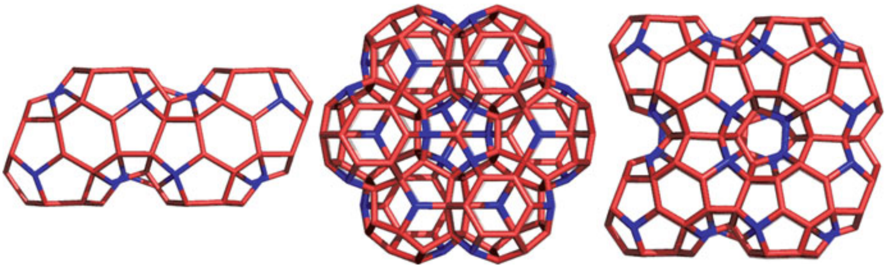

Fig. 11.13 Losdaleite, a double periodic network: L_5_28_134 (*left*), L_5_28_134 (*top view, central*) and L_5_28_250 (*side view, right*)

11.5 Omega Polynomial

In a connected graph $G(V,E)$, with the vertex set $V(G)$ and edge set $E(G)$, two edges $e = uv$ and $f = xy$ of G are called *codistant e co f* if they obey the relation [John et al (2007)]:

$$d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y) \tag{11.1}$$

which is reflexive, that is, *e co e* holds for any edge *e* of *G*, and symmetric, if *e co f* then *f co e*. In general, relation *co* is not transitive; if "*co*" is also transitive, thus it is an equivalence relation, then *G* is called a *co-graph* and the set of edges $C \times (e) := \{f \in E(G);\ f\ co\ e\}$ is called an *orthogonal cut oc* of *G*, *E*(*G*) being the union of disjoint orthogonal cuts: $E(G) = C_1 \cup C_2 \cup \ldots \cup C_k,\ \ C_i \cap C_j = \emptyset,\ i \neq j$. Klavžar has shown (Klavžar 2008) that relation *co* is a theta Djoković-Winkler relation (1973–1984).

We say that edges *e* and *f* of a plane graph *G* are in relation *opposite, e op f,* if they are opposite edges of an inner face of *G*. Note that the relation *co* is defined in the whole graph while *op* is defined only in faces. Using the relation *op* we can partition the edge set of *G* into *opposite* edge *strips, ops*. An *ops* is a quasi-orthogonal cut *qoc*, since *ops* is not transitive.

Let *G* be a connected graph and $S_1, S_2, \ldots, S_k$ be the *ops* strips of *G*. Then the *ops* strips form a partition of *E(G)*. The length of *ops* is taken as maximum. It depends on the size of the maximum fold face/ring F_{max}/R_{max} considered, so that any result on Omega polynomial will have this specification.

Denote by *m*(*G*,*s*) the number of *ops* of length *s* and define the Omega polynomial as (Diudea 2006; Diudea et al. 2008; Diudea and Katona 2009):

$$\Omega(G,x) = \sum\nolimits_s m(G,s) \cdot x^s \tag{11.2}$$

Its first derivative (in $x = 1$) equals the number of edges in the graph:

$$\Omega'(G,1) = \sum\nolimits_s m(G,s) \cdot s = e = |E(G)| \tag{11.3}$$

On Omega polynomial, the Cluj-Ilmenau [John et al (2007)] index, $CI = CI(G)$, was defined:

$$CI(G) = \{[\Omega'(G,1)]^2 - [\Omega'(G,1) + \Omega''(G,1)]\} \tag{11.4}$$

This counting polynomial found utility in predicting stability of small fullerenes (Diudea 2010a) and in description of various polyhedral nanostructures.

11.5.1 Topology of Diamond D_6 and Lonsdaleite L_6 Nets

Topology of the classical diamond D_6 and Lonsdaleite L_6 are listed in Table 11.2. Along with Omega polynomial, formulas to calculate the number of atoms in a cuboid of dimensions (k,k,k) are given. In the above, k is the number of repeating units along the edge of such a cubic domain. One can see that the ratio $C(sp^3)/v(G)$ approaches the unity; this means that in a large enough net almost all atoms are tetra-connected, a basic condition for a structure to be diamondoid. Examples of calculus are given in Table 11.3.

11.5.2 Topology of Spongy Diamond SD_5

In describing the topology of the spongy diamond SD_5, we considered only the pentagons, the larger hollows being omitted. Thus, only the basic data of the net are presented in Table 11.4; the ratio $C(sp^3)/v(G)$ is here far from unity, because of many carbon atoms are exposed to exterior.

11.5.3 Topology of Dense Diamond D_5 and Lonsdaleite L_5

Topology of the dense diamond D_5 and lonsdaleite L_5 is presented in Tables 11.5–11.10: formulas to calculate Omega polynomial, number of atoms, number of rings and the limits (at infinity) for the ratio of sp^3 C atoms over total number of atoms and also the ratio R[5] over the total number of rings (Table 11.5). Numerical examples are given.

Table 11.2 Omega polynomial in Diamond D_6 and Lonsdaleite L_6 nets, function of the number of repeating units along the edge of a cubic (k,k,k) domain

	Network
A	Omega(D_6); R[6]
1	$\Omega(D_{6}\_k_{odd},x) = \left(\sum_{i-1}^{k} 2x^{\frac{(i+1)(i+2)}{2}}\right) + \left(\sum_{i-1}^{(k-1)/2} 2x^{\frac{(k+1)(k+2)}{2}+\frac{k\times k-1}{4}-i(i-1)}\right) + 3kx^{(k+1)(k+1)}$
2	$\Omega(D_{6}\_k_{even},x) = \left(\sum_{i-1}^{k} 2x^{\frac{(i+1)(i+2)}{2}}\right) + \left(\sum_{i-1}^{k/2} 2x^{\frac{(k+1)(k+2)}{2}+\frac{k\times k}{4}-(i-1)(i-1)}\right) - x^{\frac{(k+1)(k+2)}{2}+\frac{k\times k}{4}} + 3kx^{(k+1)(k+1)}$
3	$\Omega'(1) = e(G) = -1 + 6k + 9k^2 + 4k^3$
4	$CI(G) = 2 - 187k/10 - k^2/4 + 305k^3/4 + 457k^4/4 + 1369k^5/20 + 16k^6$
5	$v(G) = 6k + 6k^2 + 2k^3$
6	$Atoms(sp^3) = -2 + 6k + 2k^3$
7	$R[6] = 3k^2 + 4k^3$
8	$\lim_{k\to\infty}\left[\frac{Atoms(sp^3)}{v(G)} = \frac{-2+6k+2k^3}{6k+6k^2+2k^3}\right] = 1$
B	Omega(L_6); R[6]
1	$\Omega(L_6,x) = k\cdot x^{k(k+2)} + x^{(k+1)(3k^2+4k-1)}$
2	$\Omega'(1) = e(G) = -1 + 3k + 9k^2 + 4k^3$
3	$CI(G) = k^2(k+2)(7k^3 + 15k^2 + 4k - 2)$
4	$v(G) = 2k(k+1)(k+2) = 4k + 6k^2 + 2k^3$
5	$Atoms(sp3) = 2(k-1)\cdot k\cdot(k+1) = 2k(k^2-1)$
6	$R[6] = -2k + 3k^2 + 4k^3$
7	$\lim_{k\to\infty}\left[\frac{Atoms(sp^3)}{v(G)} = \frac{2k(k^2-1)}{4k+6k^2+2k^3}\right] = 1$

Table 11.3 Examples, omega polynomial in diamond D_6 and lonsdaleite L_6 nets

k	Polynomial (Net)	Atoms	sp^3Atoms (%)	Bonds	CI(G)	R[6]
	Omega(D_6); R[6]					
1	$2x^3 + 3x^4$ (Diamantane)	14	–	18	258	7
2	$2x^3 + 2x^6 + 1x^7 + 6x^9$	52	26 (50.00)	79	5616	44
3	$2x^3 + 2x^6 + 2x^{10} + 2x^{12} + 9x^{16}$	126	70 (55.56)	206	39554	135
4	$2x^3 + 2x^6 + 2x^{10} + 2x^{15} + 2x^{18} + 1x^{19} + 12x^{25}$	248	150 (60.48)	423	169680	304
5	$2x^3 + 2x^6 + 2x^{10} + 2x^{15} + 2x^{21} + 2x^{25} + 2x^{27} + 15x^{36}$	430	278 (64.65)	754	544746	575
6	$2x^3 + 2x^6 + 2x^{10} + 2x^{15} + 2x^{21} + 2x^{28} + 2x^{33} + 2x^{36} + 1x^{37} + 18x^{49}$	684	466 (68.13)	1223	1443182	972
	Omega(L_6); R[6]					
1	$1x^3 + x^{12}$	12	–	15	72	5
2	$2x^8 + x^{57}$	48	12 (25.00)	73	1952	40
3	$3x^{15} + x^{152}$	120	48 (40.00)	197	15030	129
4	$4x^{24} + x^{315}$	240	120 (50.00)	411	67392	296
5	$5x^{35} + x^{564}$	420	240 (57.14)	739	221900	565
6	$6x^{48} + x^{917}$	672	420 (62.50)	1205	597312	960

Table 11.4 Topology of the spongy SD_5_20

	Formulas
	C_{57}-*based net*
1	$v(SD_5\_57) = k^2(69k - 12)$
2	$e(SD_5\_57) = 2k^2(65k - 18)$
3	$m(SD_5\_57) = k^3$; $m =$ monomer; $k = 1,2,\ldots$
4	$Atoms(sp^3) = k^2(53k - 36)$
	$R[5] = 6k^2(11k - 4)$
5	$\lim_{k\to\infty} \frac{Atoms(sp^3)}{v(G)} = 53/69 \simeq 0.768116$
	C_{81}-*based net*
6	$v(SD_5\_81) = 3k^2[27 + 23(k - 1)] = 69k^3 + 12k^2$
7	$e(SD_5\_81) = 130k^3$
8	$m(SD_5) = k^3$; $m =$ monomer
9	$Atoms(sp^3) = 53k^3 - 12k^2$
10	$\lim_{k\to\infty} \frac{Atoms(sp^3)}{v(G)} = 53/69 \simeq 0.768116$

Table 11.5 Omega polynomial in Diamond D_5_20 net function of $k =$ no. ada_20 units along the edge of a cubic (k,k,k) domain

	Omega(D_5_20[a]); R[6]; Formulas
1	$\Omega(D_5\_20b, x) = (4 - 54k + 36k^2 + 44k^3) \cdot x + (-3 + 18k - 27k^2 + 12k^3) \cdot x^2$
2	$\Omega'(1) = e(G) = -2 - 18k - 18k^2 + 68k^3$
3	$CI(G) = 12 + 54k + 468k^2 + 284k^3 - 2124k^4 - 2448k^5 + 4624k^6$
4	$v(D_5\_20b) = -2 - 12k + 34k^3 = v(Dia\_20a) + 20$
5	$Atoms(sp^3) = 2 - 36k^2 + 34k^3$
6	$R[5] = -6k - 18k^2 + 36k^3$
7	$R[6] = -1 + 6k - 9k^2 + 4k^3$
8	$\lim_{k\to\infty}\left[\frac{Atoms(sp^3)}{v(G)} = \frac{2 - 36k^2 + 34k^3}{-2 - 12k + 34k^3}\right] = 1$
9	$\lim_{k\to\infty}\frac{R[5]}{R(total\ no.)} = 9/10$; $\lim_{k\to\infty}\frac{R[5]}{R[6]} = 9$

[a]counting refers to lattices with complete tetrahedral ending

Table 11.6 Examples, omega polynomial in D_5_20 net

k	Omega(D_5_20[a]); R[6]	Atoms	sp^3Atoms (%)	Bonds	CI	R[5]	R[6]
2	$392\ x^1 + 21\ x^2$	246	130 (52.85)	434	187880	204	7
3	$1354\ x^1 + 132\ x^2$	880	596 (67.73)	1618	2616042	792	44
4	$3180\ x^1 + 405\ x^2$	2126	1602 (75.35)	3990	15915300	1992	135
5	$6134\ x^1 + 912\ x^2$	4188	3352 (80.04)	7958	63319982	4020	304
6	$10480\ x^1 + 1725\ x^2$	7270	6050 (83.22)	13930	194027520	7092	575
7	$16482\ x^1 + 2916\ x^2$	11576	9900 (85.52)	22314	497886450	11424	972

[a]counting refers to lattices with complete tetrahedral ending

Table 11.7 Omega polynomial in D_5_28 co-net function of k = no. ada_20 units along the edge of a cubic (k,k,k) domain

	Omega ($D_5\_28^a$); R[6]
1	$\Omega(D_5\_28b, x) = (10 - 12k - 6k^2 + 44k^3) \cdot x + (9k^2 + 12k^3) \cdot x^2$
2	$\Omega'(1) = e(G) = 10 - 12k + 12k^2 + 68k^3$
3	$CI(G) = 12 + 54k + 468k^2 + 284k^3 - 2124k^4 - 2448k^5 + 4624k^6$
4	$v(D_5\_28b) = 4 - 6k + 18k^2 + 34k^3$
5	$Atoms(sp^3) = 8 - 6k - 30k^2 + 34k^3$
6	$R[5] = 6 - 18k^2 + 36k^3$
7	$R[6] = 5 + 6k - 9k^2 + 4k^3$
8	$\lim_{k\to\infty}\left[\frac{Atoms(sp^3)}{v(G)} = \frac{8 - 6k - 30k^2 + 34k^3}{4 - 6k + 18k^2 + 34k^3}\right] = 1$ The limit when k tends to infinity of sp^3 atoms to all atoms is 1. This means that for large k, almost all atoms are sp^3.

[a] counting refers to lattices with complete tetrahedral ending

Table 11.8 Examples, omega polynomial in D_5_28 co-net

k	Omega($D_5\_28^a$); R[6]	Atoms	sp^3Atoms (%)	Bonds	CI	R[5]	R[6]
2	$314 x^1 + 132 x^2$	336	148 (44.05)	578	333242	222	44
3	$1108 x^1 + 405 x^2$	1066	638 (59.85)	1918	3675996	816	135
4	$2682 x^1 + 912 x^2$	2444	1680 (68.74)	4506	20297706	2022	304
5	$5300 x^1 + 1725 x^2$	4674	3478 (74.41)	8750	76550300	4056	575
6	$9226 x^1 + 2916 x^2$	7960	6236 (78.34)	15058	226722474	7134	972
7	$14724 x^1 + 4557 x^2$	12506	10158 (81.23)	23838	568217292	11472	1519

[a] counting refers to lattices with complete tetrahedral ending

Table 11.9 Omega polynomial in Lonsdaleite-like L_5_28 and L_5_20 nets function of k = no. repeating units along the edge of a cubic (k,k,k) domain

	Network
A	Omega (L_5_28); R[6]
1	$\Omega(L_5\_28, x) = 2k(-1 + 73k + 44k^2) \cdot x + 3k(4 + 21k + 8k^2) \cdot x^2$
2	$\Omega'(1) = e(G) = 2k(11 + 136k + 68k^2)$
3	$CI(G) = 2\text{k}(-23 + 43k + 5892k^2 + 39984k^3 + 36992k^4 + 9248k^5)$
4	$v(L_5\_28) = 2k(12 + 79k + 34k^2)$
5	$Atoms(sp^3) = 2k(-14 + 35k + 34k^2)$
6	$R[5] = 1 - 6k + 98k^2 + 72k^3$
7	$R[6] = k(4 + 21k + 8k^2)$
8	$\lim_{k\to\infty}\left[\frac{Atoms(sp^3)}{v(G)} = \frac{2k(-14 + 35k + 34k^2)}{2k(12 + 79k + 34k^2)}\right] = 1$
B	Omega (L_5_20); R[6]
1	$\Omega(L_5\_20, x) = (-2 - 69k + 36k^2 + 44k^3) \cdot x + 3(k-1)^2(4k-1) \cdot x^2$
2	$\Omega'(1) = e(G) = -8 - 33k - 18k^2 + 68k^3$
3	$CI(G) = 78 + 525k + 1449k^2 + 8k^3 - 4164k^4 - 2448k^5 + 4624k^6$
4	$v(L_5\_28) = -6 - 20k + 34k^3$
5	$Atoms(sp^3) = 2 - 6k - 36k^2 + 34k^3$
6	$R[5] = -2 - 14k - 18k^2 + 36k^3$
7	$R[6] = (k-1)^2(4k-1)$
8	$\lim_{k\to\infty}\left[\frac{Atoms(sp^3)}{v(G)} = \frac{2 - 6k - 36k^2 + 34k^3}{-6 - 20k + 34k^3}\right] = 1$

Table 11.10 Examples, omega polynomial in L_5_28 and L_5_20 nets

k	Polynomial (Net)	Atoms	sp^3Atoms (%)	Bonds	CI(G)	R[5]	R[6]
A	Omega(L_5_28); R[6]						
1	$232 x + 99 x^2$	250	110 (44.00)	430	184272	165	33
2	$1284 x + 468 x^2$	1224	768 (62.75)	2220	4925244	957	156
3	$3684 x + 1251 x^2$	3330	2382 (71.53)	6186	38257908	2809	417
4	$7960 x + 2592 x^2$	6976	5360 (76.83)	13144	172746408	6153	864
5	$14640 x + 4635 x^2$	12570	10110 (80.43)	23910	571654920	11421	1545
6	$24252 x + 7524 x^2$	20520	17040 (83.04)	39300	1544435652	19045	2508
B	Omega(L_5_28); R[6]						
2	$356 x + 21 x^2$	226	118 (52.21)	398	157964	186	7
3	$1303 x + 132 x^2$	852	578 (67.84)	1567	2453658	766	44
4	$3114 x + 405 x^2$	2090	1578 (75.50)	3924	15393042	1958	135
5	$6053 x + 912 x^2$	4144	3322 (80.16)	7877	62037428	3978	304
6	$10384 x + 1725 x^2$	7218	6014 (83.32)	13834	191362272	7042	575

11.6 Conclusions

A novel class of (hypothetical) carbon allotropes, consisting mostly of pentagon rings (going up to 90% in the total number of pentagon/hexagon rings), was here presented. The seed of these allotropes, C_{17} and the adamantane-like repeating-units, as hydrogenated species, show a good stability, comparable with that of C_{60} fullerene, as calculated at DFT levels of theory. The main representatives of these allotropes are the diamond D_5 and lonsdaleite L_5, in fact hyper-structures corresponding to the classical diamond D_6 and lonsdaleite L_6. The topology of the networks was described in terms of the net parameter *k* and Omega polynomial.

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