Chapter 9
Omega Polynomial in Hyperdiamonds

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Abstract Hyperdiamonds are covalently bonded carbon phases, more or less related to the diamond network, having a significant amount of sp^3 carbon atoms and similar physical properties. Many of them have yet a hypothetical existence but a well-theorized description. Among these, the diamond D_5 was studied in detail, as topology, at TOPO GROUP CLUJ, Romania. The theoretical instrument used was the Omega polynomial, also developed in Cluj. It was computed in several 3D network domains and analytical formulas have been derived, not only for D_5 but also for the well-known diamond D_6 and other known networks.

9.1 Introduction

Diamond D_6 (Fig. 9.1), the beautiful classical diamond, with all-hexagonal rings of sp^3 carbon atoms crystallized in a face-centered cubic *fcc* network (space group *Fd*3*m*), has kept its leading interest among the carbon allotropes, even many "nano" varieties appeared (Decarli and Jamieson 1961; Aleksenskiĭ et al. 1997; Osawa 2007, 2008; Williams et al. 2007; Dubrovinskaia et al. 2006). Its mechanical

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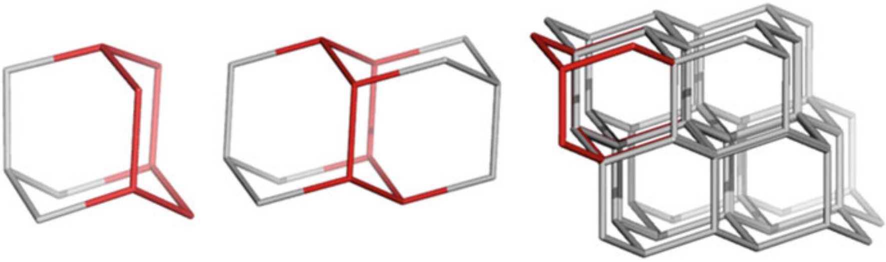

Fig. 9.1 Diamond D_6: adamantane D_6_10 (*left*), diamantane D_6_14 (*middle*), and diamond D_6_52 (a 222 net – *right*)

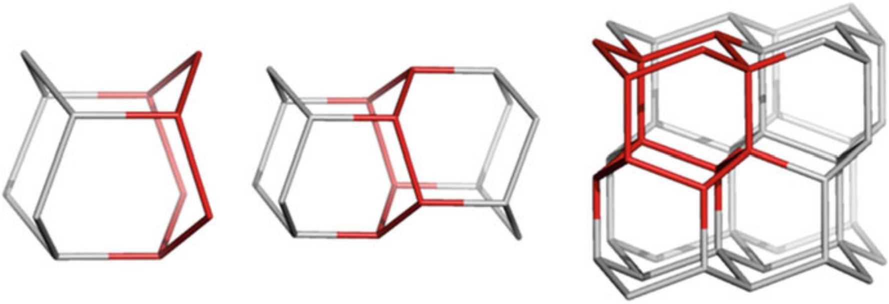

Fig. 9.2 Lonsdaleite: L_6_12 (*left*), L_6_18 (*middle*), and L_6_48 (a 222 net – *right*)

characteristics are of great importance, and composites including diamonds may overpass the resistance of steel or other metal alloys. Synthetic diamonds can be produced by a variety of methods, including high pressure-high temperature HPHT, static or detonation procedures, chemical vapor deposition CVD (Lorenz 1995), ultrasound cavitation (Khachatryan et al. 2008), or mechano-synthesis (Tarasov et al. 2011), under electronic microscopy.

A relative of the diamond D_6, called lonsdaleite L_6 (Frondel and Marvin 1967), with a hexagonal network (space group $P6_3/mmc$ – Fig. 9.2), was discovered in a meteorite in the Canyon Diablo, Arizona, in 1967. Several diamond-like networks have also been proposed (Diudea and Nagy 2007; Diudea et al. 2010a; Hyde et al. 2008).

Hyperdiamonds are covalently bonded carbon phases, more or less related to the diamond network, having a significant amount of sp^3 carbon atoms. Their physical properties are close to that of the classical diamond, sometimes with exceeding hardness and/or endurance.

Design of several hypothetical crystal networks was performed by using our software programs (Diudea 2010a) CVNET and NANO-STUDIO. Topological data were provided by NANO-STUDIO, Omega, and PI programs.

This chapter is structured as follows. After the introductory part, the main networks, diamond D_5 and lonsdaleite L_5, are presented in detail. Next, two other nets, the uninodal net, called rhr, and the hyper boron nitride, are designed. Two sections with basic definitions in Omega polynomial and in Omega-related polynomials, respectively, are developed in the following. The topology of the discussed networks will be presented in the last part. Conclusions and references will close the chapter.

9.2 Structures Construction

9.2.1 Diamond D_5 Network

Diamond $\mathbf{D_5}$, recently theorized by Diudea and collaborators (Diudea and Ilić 2011; Diudea 2010b; Diudea and Nagy 2012; Diudea et al. 2012), is a hyperdiamond, whose seed is the centrohexaquinane C_{17} (Fig. 9.3). D_5 is the *mtn* crystal 4,4,4-c trinodal network, appearing in type II clathrate hydrates; it belongs to the space group Fd-3m and has point symbol net: {5^5.6}12{5^6}5 (Dutour Sikirić et al. 2010; Delgado-Friedrichs and O'Keeffe 2006, 2010). The hyper-structures, from ada- to dia- and a larger net are illustrated in Fig. 9.4, viewed both from C_{20} (left column) and C_{28} (right column) basis, respectively (Diudea et al. 2012).

The hyperdiamond D_5_20/28 mainly consists of sp^3 carbon atoms building ada-like repeating units (C_{20} cages including C_{28} as hollows). The ratio C-sp^3/C-total trends to 1 in a large enough network. As the content of pentagons *R*[5] per total rings trends to 90 % (see Table 9.3, entry 9), this yet hypothetical carbon allotrope is called the diamond D_5.

Energetic data, calculated at various DFT levels (Diudea and Nagy 2012; Diudea et al. 2012), 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 D_5 diamond.

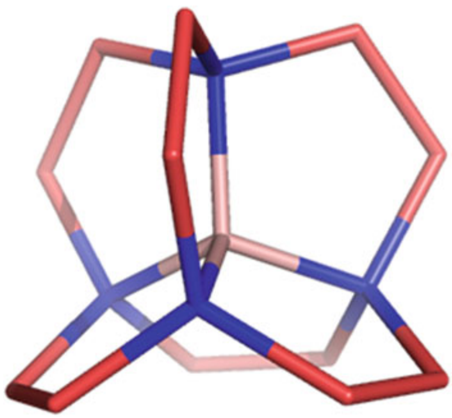

Fig. 9.3 The seed of diamond D_5: C_{17}

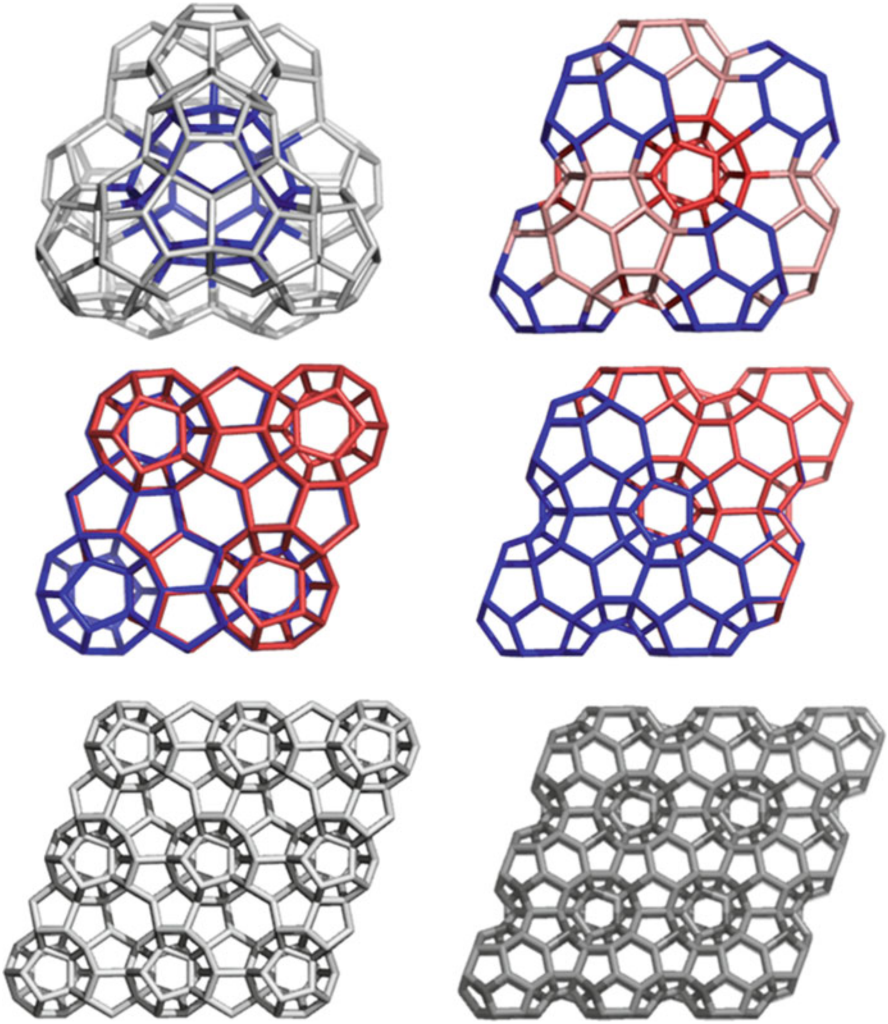

Fig. 9.4 Hyper-adamantane: ada_20_158 and ada_28_213 (*top*), diamantane: dia_20_226_222 and dia_28_292_222 (*middle*), and diamond D_5_20_860_333 and D_5_28_ 1022_333 co-net (*bottom*)

9.2.2 Lonsdaleite L_5 Network

By analogy to D_5_20/28, a lonsdaleite-like net was proposed (Diudea et al. 2012) (Fig. 9.5). The hyper-hexagons L_5_28_134 (Fig. 9.5, middle and right), whose nodes represent the C_{28} fullerene, was used as the monomer (in the chair conformation). Its corresponding co-net L_5_20 was also designed. The lonsdaleite L_5_28/20 is partially

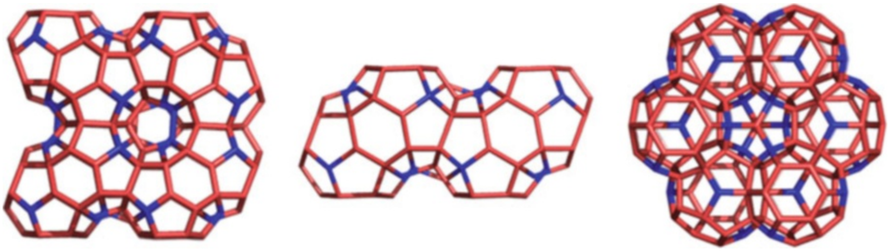

Fig. 9.5 Lonsdaleite: L_5_28_250 (*side view*, *left*), L_5_28_134 (*side view*, *middle*), and L_5_28_134 (*top view*, *right*)

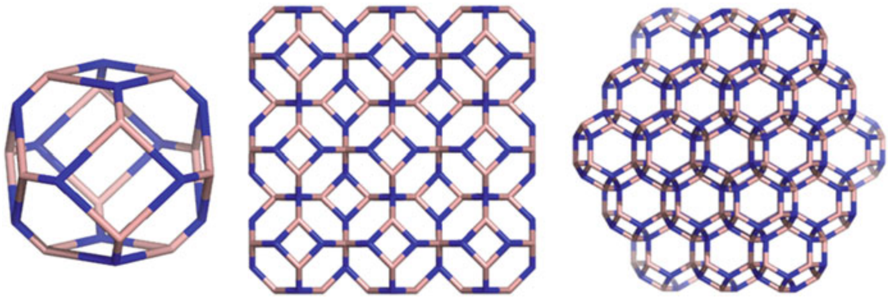

Fig. 9.6 Boron nitride $B_{12}N_{12}$: truncated octahedron (*left*), a cubic (3,3,3)_432 domain built up from truncated octahedra joined by identifying the square faces (*middle*), and a corner view (*right*)

superimposed on D_5_20/28 net. In crystallography, L_5 is known as the 7-nodal mgz-x-d net, with the point symbol: {5^5.6}12{5^6}5.

9.2.3 Hyper Boron Nitride

Boron nitride is a chemical crystallized basically as the carbon allotropes: graphite (**h-BN**), cubic-diamond D_6 (**c-BN**), and lonsdaleite L_6 (wurtzite **w-BN**). Their physicochemical properties are also similar, with small differences.

Fullerene-like cages have been synthesized and several theoretical structures have been proposed for these molecules (Soma et al. 1974; Stephan et al. 1998; Jensen and Toftlund 1993; Mei-Ling Sun et al. 1995; Fowler et al. 1999; Oku et al. 2001; Narita and Oku 2001).

Based on $B_{12}N_{12}$ unit, with the geometry of truncated octahedron, we modeled three 3D arrays: a cubic domain, Fig. 9.6; a dual of cuboctahedron domain, Fig. 9.7; and an octahedral domain, Fig. 9.8.

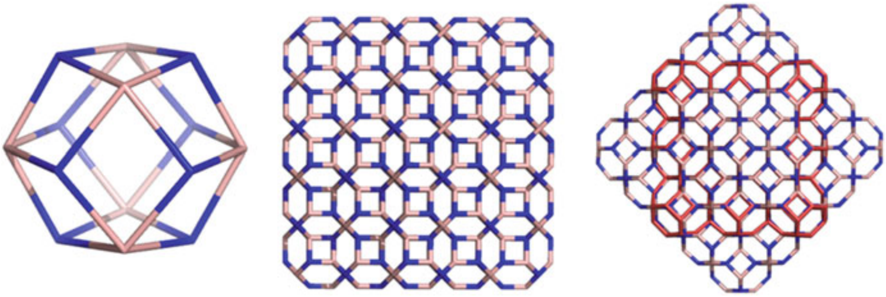

Fig. 9.7 Boron nitride $B_{12}N_{12}$: dual of cuboctahedron (*left*), a (3,3,3)_648 dual of cuboctahedron domain, constructed from truncated octahedra by identifying the square and hexagonal faces, respectively (*middle*), and its superposition with the cubic (3,3,3)_432 domain (*right*)

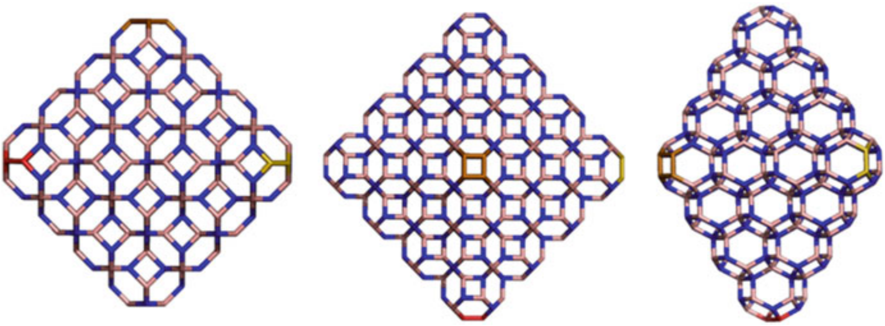

Fig. 9.8 Boron nitride $B_{12}N_{12}$: an octahedral (4,4,4)_480 domain: (1,1,0-*left*), (0,0,1-*central*), and (2,1,1-*right*) constructed from truncated octahedra by identifying the square and hexagonal faces, respectively

The topology of the above hyperdiamonds will be described by using the net parameter *k*, meaning the number of repeat units along the chosen 3D direction, and by the formalism of several counting polynomials, the largest part being devoted to Omega polynomial.

9.2.4 rhr Network

A uninodal 4-c net with a point $\{4^2.6^2.8^2\}$ was named *rhr* or sqc5544. In topological terms, its unit cell is a homeomorphic of cuboctahedron, one of the semi-regular polyhedra (Fig. 9.9). It can be obtained by making the medial operation on the cube or octahedron (Diudea 2010a). The net can be constructed by identifying the vertices of degree 2 in two repeating units, thus the resulting net will have all points of degree 4, as in the classical diamond D_6 (but the rings are both six- and eight-membered ones).

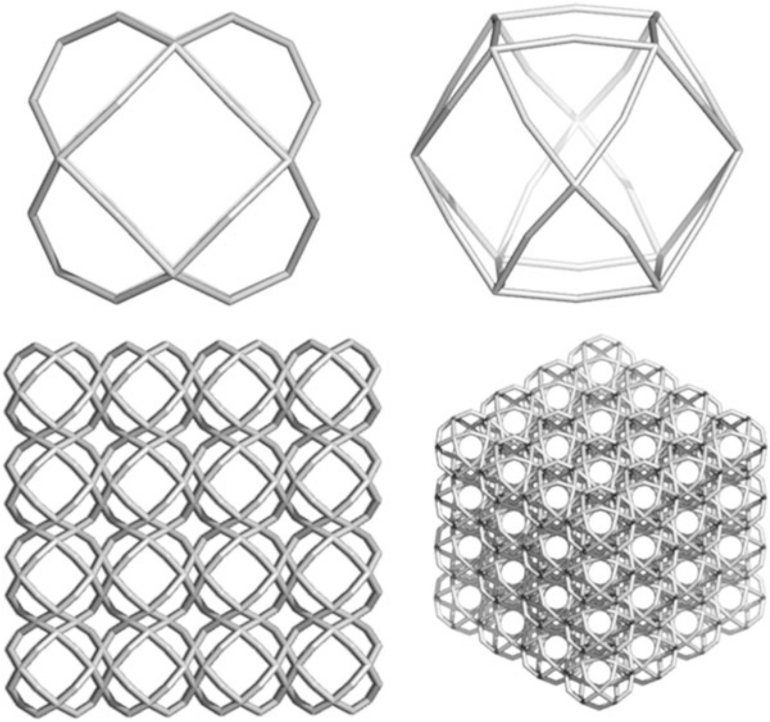

Fig. 9.9 The *rhr* unit (*top*) and network (444_1728, *bottom*: top view (*left*) and corner view (*right*))

9.3 Omega Polynomial

9.3.1 Relations co and op

Let $G = (V(G),E(G))$ be a connected graph, with the vertex set $V(G)$ and edge set $E(G)$. Two edges $e = (u,v)$ and $f = (x,y)$ of G are called *co-distant* (briefly: $e\ co\ f$) if the notation can be selected such that (Diudea 2010a; John et al. 2007; Diudea and Klavžar 2010)

$$e\ co\ f \Leftrightarrow d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y) \tag{9.1}$$

where d is the usual shortest-path distance function. Relation *co* is reflexive, that is, $e\ co\ e$ holds for any edge e of G and it is also symmetric: if $e\ co\ f$, then also $f\ co\ e$. In general, *co* is not transitive.

For an edge $e \in E(G)$, let $c(e) := \{f \in E(G);\ f\ co\ e\}$ be the set of edges co-distant to e in G. The set $c(e)$ is called an *orthogonal cut* (*oc* for short) of G, with respect to e. If G is a *co*-graph then its orthogonal cuts $C(G) = c_1,\ c_2, \ldots, c_k$ form a partition:

$$E(G) = c_1 \cup c_2 \cup \cdots \cup c_k, \quad c_i \cap c_j = \emptyset,\ \ i \neq j$$

A subgraph $H \subseteq G$ is called *isometric* if $d_H(u,v) = d_G(u,v)$, for any $(u,v) \in H$; it is *convex* if any shortest path in G between vertices of H belongs to H. The n-cube Q_n is the graph whose vertices are all binary strings of length n, two strings being adjacent if they differ in exactly one position (Harary 1969). A graph G is called a *partial cube* if there exists an integer n such that G is an isometric subgraph of Q_n.

For any edge $e = (u,v)$ of a connected graph G, let n_{uv} denote the set of vertices lying closer to u than to v: $n_{uv} = \{w \in V(G) | d(w,u) < d(w,v)\}$. By definition, it follows that $n_{uv} = \{w \in V(G) | d(w,v) = d(w,u) + 1\}$. The sets (and subgraphs) induced by these vertices, n_{uv} and n_{vu}, are called *semicubes* of G; these semicubes are *opposite* and disjoint (Diudea and Klavžar 2010; Diudea et al. 2008; Diudea 2010c).

A graph G is *bipartite* if and only if, for any edge of G, the opposite semicubes define a partition of G: $n_{uv} + n_{vu} = v = |V(G)|$.

The relation *co* is related to the $\sim$ (Djoković 1973) and Θ (Winkler 1984) relations:

$$e\ \Theta\ f \Leftrightarrow d(u,x) + d(v,y) \neq d(u,y) + d(v,x) \tag{9.2}$$

Lemma 9.1 *In any connected graph, $co = \sim$.*

In general graphs, we have $\sim \subseteq \Theta$ and in bipartite graphs $\sim = \Theta$. From this and the above lemma, it follows (Diudea and Klavžar 2010)

Proposition 9.1 *In a connected graph, $co = \sim$; if G is also bipartite, then $co = \sim = \Theta$.*

Theorem 9.1 *In a bipartite graph, the following statements are equivalent* (Diudea and Klavžar 2010):

- (i) G is a *co*-graph.
- (ii) G is a partial cube.
- (iii) All semicubes of G are convex.
- (iv) Relation Θ is transitive.

Equivalence between (i) and (ii) was observed in Klavžar (2008), equivalence between (ii) and (iii) is due to Djoković (1973), while the equivalence between (ii) and (iv) was proved by Winkler (1984).

Two 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. Then $e\ co\ f$ holds by assuming the faces are isometric. Note that relation *co* involves distances in the whole graph while *op* is defined only locally (it relates face-opposite edges). A partial cube is also a *co*-graph but the reciprocal is not always true. There are *co*-graphs which are non-bipartite (Diudea 2010d), thus being non-partial cubes.

Relation *op* partitions the edge set of *G* into *opposite* edge *strips ops*: any two subsequent edges of an *ops* are in *op*-relation, and any three subsequent edges of such a strip belong to adjacent faces.

Lemma 9.2 *If G is a co-graph, then its opposite edge strips ops* $\{s_k\}$ *superimpose over the orthogonal cuts ocs* $\{c_k\}$.

Proof Recall the *co*-relation is defined on parallel equidistant edges relation (9.1). The same is true for the *op*-relation, with the only difference (9.1) is limited to a single face. Suppose e_1*and* e_2 are two consecutive edges of *ops*; by definition, they are topologically parallel and also *co*-distant (i.e., belong to *ocs*). By induction, any newly added edge of *ops* will be parallel to the previous one and also *co*-distant. Because, in *co*-graphs, c*o*-relation is transitive, all the edges of *ops* will be *co*-distant, thus *ops* and *ocs* will coincide.

Corollary 9.1 *In a co-graph, all the edges of an ops are topologically parallel.*

Observe that the relation *co* is a particular case of the edge *equidistance eqd* relation. The equidistance of two edges $e = (uv)$ and $f = (xy)$ of a connected graph *G* includes conditions for both (i) topologically parallel edges (relation (9.1)) and (ii) topologically perpendicular edges (in the Tetrahedron and its extensions – relation (9.3)) (Diudea et al. 2008; Ashrafi et al. 2008a):

$$e\ eqd\ \ f(ii) \Leftrightarrow d(u,x) = d(u,y) = d(v,x) = d(v,y) \tag{9.3}$$

The *ops* strips can be either cycles (if they start/end in the edges e_{even} of the same even face f_{even}) or paths (if they start/end in the edges e_{odd} of the same or different odd faces f_{odd}).

Proposition 9.2 *Let G be a planar graph representing a polyhedron with the odd faces insulated from each other. The set of ops strips* $S(G) = \{s_1, s_2, \ldots, s_k\}$ *contains a number of op paths opp which is exactly half of the number of odd face edges* $e_{\text{odd}}/2$.

Proof of Proposition 9.2 was given in Diudea and Ilić (2009).

Corollary 9.2 *In a planar bipartite graph, representing a polyhedron, all ops strips are cycles.*

The *ops* is maximum possible, irrespective of the starting edge. The choice is about the maximum size of face/ring searched, and mode of face/ring counting, which will decide the length of the strip.

Definitions 9.1 *Let G be an arbitrary connected graph and* $s_1, s_2, \ldots, s_k$ *be its op strips. Then ops form a partition of* $E(G)$ *and the* Ω*-polynomial* (Diudea 2006) *of G is defined as*

$$\Omega(x) = \sum_{i=1}^{k} x^{|s_i|} \tag{9.4}$$

Let us now consider the set of edges *co*-distant to edge e in G, $c(e)$. A Θ-polynomial (Diudea et al. 2008), counting the edges equidistant to every edge e, is written as

$$\Theta(x) = \sum_{e \in E(G)} x^{|c(e)|} \tag{9.5}$$

Suppose now G is a *co*-graph, when $|c_k| = |s_k|$, then (Diudea and Klavžar 2010)

$$\Theta(x) = \sum_{e \in E(G)} x^{|c(e)|} = \sum_{i=1}^{k} \sum_{e \in S_i} x^{|c(e)|} = \sum_{e} |c(e)| x^{|c(e)|} = \sum_{i=1}^{k} |s_i| x^{|s_i|} \tag{9.6}$$

Let us simplify a little the above notations: note by $m(s)$ or simply m the number of *ops* of length $s = |s_k|$ and rewrite the Omega polynomial as (Diudea 2010a; Ashrafi et al. 2008b; Khadikar et al. 2002; Diudea et al. 2010b)

$$\Omega(x) = \sum_{s} m \cdot x^{s} \tag{9.7}$$

Next we can write Theta and other two related polynomials, as follows:

$$\Theta(x) = \sum_{s} ms \cdot x^{s} \tag{9.8}$$

$$\Pi(x) = \sum_{s} ms \cdot x^{e-s} \tag{9.9}$$

$$\mathrm{Sd}(x) = \sum_{s} m \cdot x^{e-s} \tag{9.10}$$

The polynomial $\Theta(x)$ counts equidistant edges while $\Pi(x)$ counts non-equidistant edges. The Sadhana polynomial, proposed by Ashrafi et al. (2008b) in relation with the Sadhana index $\mathrm{Sd}(G)$ proposed by Khadikar et al. (2002), counts non-opposite edges in G. Their first derivative (in $x = 1$) provides single-number topological descriptors also termed topological indices (Diudea 2010a):

$$\Omega'(1) = \sum_{s} m \cdot s = e = |E(G)| \tag{9.11}$$

$$\Theta'(1) = \sum_{s} m \cdot s^2 = \theta(G) \tag{9.12}$$

$$\Pi'(1) = \sum_{s} ms \cdot (e - s) = \Pi(G) \tag{9.13}$$

$$\mathrm{Sd}'(1) = \sum_{s} m \cdot (e - s) = e(\mathrm{Sd}(1) - 1) = \mathrm{Sd}(G) \tag{9.14}$$

Note $\mathrm{Sd}(1) = \Omega(1)$, then the first derivative given in (9.14) is the product of the number of edges $e = |E(G)|$ and the number of strips $\Omega(1)$ less one.

On Omega polynomial, the Cluj-Ilmenau index (Ashrafi et al. 2008a) $\mathrm{CI} = \mathrm{CI}(G)$ was defined as

$$\mathrm{CI}(G) = \left\{ [\Omega'(1)]^2 - [\Omega'(1) + \Omega''(1)] \right\} \tag{9.15}$$

A polynomial related to $\Pi(x)$ was defined by Ashrafi et al. (2008b) as

$$\mathrm{PI}_e(x) = \sum_{e \in E(G)} x^{n(e,u)+n(e,v)} \tag{9.16}$$

where $n(e,u)$ is the number of edges lying closer to the vertex u than to the v vertex. Its first derivative (in $x = 1$) provides the $\mathrm{PI}_e(G)$ index proposed by Khadikar (2000) and developed by Ashrafi et al. (2006).

Proposition 9.3 *In any bipartite graph*, $\Pi(G) = \mathrm{PI}_e(G)$.

Proof Ashrafi defined the equidistance of edges by considering the distance from a vertex z to the edge $e = uv$ as the minimum distance between the given point and the two endpoints of that edge (Ashrafi et al. 2006, 2008a):

$$d(z, e) = \min\{d(z, u), d(z, v)\} \tag{9.17}$$

Then, for two edges $e = (uv)$ and $f = (xy)$ of G,

$$e \; eqd \; f(iii) \Leftrightarrow d(x, e) = d(y, e) \quad \text{and} \quad d(u, f) = d(v, f) \tag{9.18}$$

In bipartite graphs, relations (9.1) and (9.3) superimpose over relations (9.17) and (9.18), then in such graphs, $\Pi(G) = \mathrm{PI}_e(G)$. In general graphs, this is, however, not true.

Proposition 9.4 *In co-graphs, the equality* $\mathrm{CI}(G) = \Pi(G)$ *holds.*

Proof By definition, one calculates

$$\mathrm{CI}(G) = \left(\sum_{i=1}^{k} |s_i| \right)^2 - \left(\sum_{i=1}^{k} |s_i| + \sum_{i=1}^{k} |s_i|(|s_i| - 1) \right)$$

$$= |E(G)|^2 - \sum_{i=1}^{k} (|s_i|)^2 = \Pi'(G, 1) = \Pi(G) \tag{9.19}$$

Relation (9.19) is valid only when assuming $|c_k| = |s_k|$, $k = 1,2,\ldots,$ thus providing the same value for the exponents of Omega and Theta polynomials; this is precisely achieved in *co*-graphs. In general graphs, however, $|s_i| \neq |c_k|$ and as a consequence, $\mathrm{CI}(G) \neq \Pi(G)$ (Diudea 2010a).

In partial cubes, which are also bipartite, the above equality can be expanded to the triple one:

$$\mathrm{CI}(G) = \Pi(G) = \mathrm{PI}_e(G) \tag{9.20}$$

a relation which is not obeyed in all *co*-graphs (e.g., in non-bipartite ones).

There is also a vertex-version of PI index, defined as (Nadjafi-Arani et al. 2009; Ilić 2010)

$$\mathrm{PI}_v(G) = \mathrm{PI}'_v(1) = \sum_{e=uv} n_{u,v} + n_{v,u} = |V|\cdot|E| - \sum_{e=uv} m_{u,v} \tag{9.21}$$

where $n_{u,v}$, $n_{v,u}$ count the non-equidistant vertices with respect to the endpoints of the edge $e = (u,v)$ while $m(u,v)$ is the number of equidistant vertices *vs* u and v. However, it is known that, in bipartite graphs, there are no equidistant vertices *vs*. any edge, so that the last term in (9.21) will miss. The value of $\mathrm{PI}_v(G)$ is thus maximal in bipartite graphs, among all graphs on the same number of vertices; this result can be used as a criterion for checking whether the graph is bipartite (Diudea 2010a).

9.3.2 Omega Polynomial of Diamond D_6 and Lonsdaleite L_6

Topology of the classical diamond D_6 and lonsdaleite L_6 is listed in Table 9.1 (Diudea et al. 2011). Along with Omega polynomial, formulas to calculate the number of atoms in a cuboid of dimensions (k,k,k) are given. Above, k is the number of repeating units along the edge of such a cubic domain. One can see that the ratio $\mathrm{C(sp^3)}/v(G)$ 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 9.2.

9.3.3 Omega Polynomial of Diamond D_5 and Lonsdaleite L_5

Topology of diamond D_5 and lonsdaleite L_5, in a cubic (k,k,k) domain, is presented in Tables 9.3, 9.4, 9.5, 9.6, 9.7, and 9.8 (Diudea et al. 2011). Formulas to calculate Omega polynomial, number of atoms, number of rings, and the limits (to infinity) for the ratio of $\mathrm{sp^3}$ C atoms over total number of atoms and also the ratio $R[5]$ over the total number of rings as well as numerical examples are given.

Table 9.1 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	$\Omega(D_6\_k_{\text{odd}}, x) = \left(\sum_{i-1}^{k} 2x^{\frac{(i+1)(i+2)}{2}}\right) + \left(\sum_{i-1}^{(k-1)/2} 2x^{\frac{(k+1)(k+2)}{2} + \frac{k\times k-1}{4} - i(i-1)}\right) + 3kx^{(k+1)^2}$
2	$\Omega(D_6\_k_{\text{even}}, x) = \left(\sum_{i-1}^{k} 2x^{\frac{(i+1)(i+2)}{2}}\right) + \left(\sum_{i-1}^{k/2} 2x^{\frac{(k+1)(k+2)}{2} + \frac{k\times k}{4} - (i-1)(i-1)}\right) - x^{\frac{(k+1)(k+2)}{2} + \frac{k\times k}{4}} + 3kx^{(k+1)^2}$
3	$\Omega'(1) = e(G) = -1 + 6k + 9k^2 + 4k^3$
4	$CI(G) = 2 - 187k/10 - k^2/4 + 305k^3/4 + 457k^4/4 + 1{,}369k^5/20 + 16k^6$
5	$v(G) = 6k + 6k^2 + 2k^3$
6	$\text{Atoms}(sp^3) = -2 + 6k + 2k^3$
7	$R[6] = 3k^2 + 4k^3$
8	$\lim_{k\to\infty}\left[\frac{\text{Atoms}(sp^3)}{v(G)} = \frac{-2 + 6k + 2k^3}{6k + 6k^2 + 2k^3}\right] = 1$
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	$\text{Atoms}(sp^3) = 2(k-1)\cdot k\cdot(k+1) = 2k(k^2-1)$
6	$R[6] = -2k + 3k^2 + 4k^3$
7	$\lim_{k\to\infty}\left[\frac{\text{Atoms}(sp^3)}{v(G)} = \frac{2k(k^2-1)}{4k + 6k^2 + 2k^3}\right] = 1$

9.3.4 Omega Polynomial of Boron Nitride Nets

Topology of boron nitride nets is treated similarly to that of D_5 and L_5 and is presented in Tables 9.9, 9.10, 9.11, 9.12, 9.13, 9.14, 9.15, 9.16, 9.17, and 9.18 (Diudea et al. 2011). Formulas to calculate Omega polynomial, number of atoms, number of rings, and the limits (to infinity) for the ratio of sp^3 C atoms over total number of atoms are given, along with numerical examples. Formulas for Omega polynomial are taken as the basis to calculate the above four related polynomials in these bipartite networks. Formulas are derived here not only for a cubic domain (in case of $c\_B_{12}N_{12}$) but also for a dual of cuboctahedron domain (case of $COD\_B_{12}N_{12}$) and for an octahedral domain (case of $Oct\_B_{12}N_{12}$).

Table 9.2 Examples, Omega polynomial in diamond D_6 and lonsdaleite L_6 nets

	Polynomial (Net)					
k	Omega(D_6); R[6]	Atoms	sp^3 atoms (%)	Bonds	CI(G)	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	5,616	44
3	$2x^3 + 2x^6 + 2x^{10} + 2x^{12} + 9x^{16}$	126	70 (55.56)	206	39,554	135
4	$2x^3 + 2x^6 + 2x^{10} + 2x^{15} + 2x^{18} + 1x^{19} + 12x^{25}$	248	150 (60.48)	423	169,680	304
5	$2x^3 + 2x^6 + 2x^{10} + 2x^{15} + 2x^{21} + 2x^{25} + 2x^{27} + 15x^{36}$	430	278 (64.65)	754	544,746	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)	1,223	1,443,182	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	1,952	40
3	$3x^{15} + x^{152}$	120	48 (40.00)	197	15,030	129
4	$4x^{24} + x^{315}$	240	120 (50.00)	411	67,392	296
5	$5x^{35} + x^{564}$	420	240 (57.14)	739	221,900	565
6	$6x^{48} + x^{917}$	672	420 (62.50)	1,205	597, 312	960

Table 9.3 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_20a); R[6]: formulas
1	$\Omega(D_5\_20a, x) = (32 - 54k + 36k^2 + 44k^3) \cdot x + (-3 + 18k - 27k^2 + 12k^3) \cdot x^2$
2	$\Omega'(1) = e(G) = -38 - 18k - 18k^2 + 68k^3$
3	$CI(G) = 1,488 + 1,350k + 1,764k^2 - 4,612k^3 - 2,124k^4 - 2,448k^5 + 4,624k^6$
4	$v(D_5\_20a) = -22 - 12k + 34k^3$
5	$\text{Atoms}(sp^3) = -10 - 36k^2 + 34k^3$
6	$R[5] = -18 - 6k - 18k^2 + 36k^3$
7	$R[6] = -1 + 6k - 9k^2 + 4k^3$
8	$R[5] + R[6] = -19 - 27k^2 + 40k^3$
9	$\lim_{k\to\infty} \frac{R[5]}{R[6]} = 9; \lim_{k\to\infty} \frac{R[5]}{R[5] + R[6]} = \frac{9}{10}$
10	$\lim_{k\to\infty} \left[\frac{\text{Atoms}(sp^3)}{v(G)} = \frac{-10 - 36k^2 + 34k^3}{-22 - 12k + 34k^3} = \frac{-(10/k^3) - (36/k) + 34}{-(22/k^3) - (12/k^2) + 34} \right] = 1$

Table 9.4 Examples, Omega polynomial in D_5_20 net

k	Omega(D_5_20a); R[6]	Atoms	sp^3 atoms (%)	Bonds	CI	R[5]	R[6]
2	$356\,x^1 + 21\,x^2$	226	118 (52.21)	398	157,964	186	7
3	$1{,}318\,x^1 + 132\,x^2$	860	584 (67.91)	1,582	2,500,878	774	44
4	$3{,}144\,x^1 + 405\,x^2$	2,106	1,590 (75.50)	3,954	15,629,352	1,974	135
5	$6{,}098\,x^1 + 912\,x^2$	4,168	3,340 (80.13)	7,922	62,748,338	4,002	304
6	$10{,}444\,x^1 + 1{,}725\,x^2$	7,250	6,038 (83.28)	13,894	193,025,892	7,074	575
7	$16{,}446\,x^1 + 2{,}916\,x^2$	11,556	9,888 (85.57)	22,278	496,281,174	11,406	972

Table 9.5 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_28a); $R[6]$; formulas
1	$\Omega(D_5\_28a, x) = (-26 - 12k - 6k^2 + 44k^3) \cdot x + (-18 + 9k^2 + 12k^3) \cdot x^2$
2	$\Omega'(1) = e(G) = -62 - 12k + 12k^2 + 68k^3$
3	$CI(G) = 3,942 + 1,500k - 1,374k^2 - 8,812k^3 - 1,488k^4 + 1,632k^5 + 4,624k^6$
4	$v(D_5\_28a) = -40 - 6k + 18k^2 + 34k^3$
5	$\text{Atoms}(sp^3) = -4 - 6k - 30k^2 + 34k^3$
6	$R[5] = -18 - 18k^2 + 36k^3$
7	$R[6] = -1 + 6k - 9k^2 + 4k^3$
8	$\lim_{k\to\infty}\left[\frac{\text{Atoms}(sp^3)}{v(G)} = \frac{-4 - 6k - 30k^2 + 34k^3}{-40 - 6k + 18k^2 + 34k^3}\right] = 1$

Table 9.6 Examples, Omega polynomial in D_5_28 co-net

k	Omega(D_5_28a); $R[6]$	Atoms	sp^3 atoms (%)	Bonds	CI	$R[5]$	$R[6]$
2	$278\,x^1 + 114\,x^2$	292	136 (46.58)	506	255,302	198	38
3	$1{,}072\,x^1 + 387\,x^2$	1,022	626 (61.25)	1,846	3,405,096	792	129
4	$2{,}646\,x^1 + 894\,x^2$	2,400	1,668 (69.50)	4,434	19,654,134	1,998	298
5	$5{,}264\,x^1 + 1{,}707\,x^2$	4,630	3,466 (74.86)	8,678	75,295,592	4,032	569
6	$9{,}190\,x^1 + 2{,}898\,x^2$	7,916	6,224 (78.63)	14,986	224,559,414	7,110	966
7	$14{,}688\,x^1 + 4{,}539\,x^2$	12,462	10,146 (81.41)	23,766	564,789,912	11,448	1,513

Table 9.7 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

	Formulas
1	$v(c\_B_{12}N_{12}) = 4k^2[6 + 3(-1 + k)]$
2	$e(G) = 12k^2(1 + 2k)$
3	$\Theta(c\_B_{12}N_{12}, x) = 6 \cdot k(4k + 2) \cdot x^{k(4k+2)} + 12\sum_{i=1}^{k-1} i(4k + 2) \cdot x^{i(4k+2)}$
4	$\Theta'(1) = 6 \cdot [k(4k + 2)]^2 + 12\sum_{i=1}^{k-1} [i(4k + 2)]^2 = 8k(2k^2 + 1)(2k + 1)^2$
5	$\Pi(c\_B_{12}N_{12}, x) = 6 \cdot k(4k+2) \cdot x^{12k^2(2k+1)-k(4k+2)} + 12\sum_{i=1}^{k-1} i(4k+2) \cdot x^{12k^2(2k+1)-i(4k+2)}$
6	$\Pi'(1) = 6 \cdot [k(4k + 2)][12k^2(2k + 1) - k(4k + 2)] + 12\sum_{i=1}^{k-1} [i(4k+2)][12k^2(2k+1) - i(4k+2)] = 8k(18k^3 - 2k^2 - 1)(2k+1)^2$
7	$Sd(c\_B_{12}N_{12}, x) = 6 \cdot x^{12k^2(2k+1)-k(4k+2)} + 12\sum_{i=1}^{k-1} x^{12k^2(2k+1)-i(4k+2)}$
8	$Sd'(1) = 6 \cdot [12k^2(2k + 1) - k(4k + 2)] + 12\sum_{i=1}^{k-1} [12k^2(2k + 1) - i(4k + 2)] = 12k^2(12k - 7)(2k + 1)$
9	$PI_v = e \cdot x^v$
10	$PI_v'(1) = e \cdot v = (12k^2)^2(2k + 1)(k + 1) = 144k^4 + 432k^5 + 288k^6$

Table 9.8 Examples, Omega polynomial in L_5_28 and L_5_20 nets

k	Polynomial (Net)						
A	Omega(L_5_28); R[6]	Atoms	sp^3 atoms (%)	Bonds	CI(G)	R[5]	R[6]
1	$232\,x + 99\,x^2$	250	110 (44.00)	430	184,272	165	33
2	$1{,}284\,x + 468\,x^2$	1,224	768 (62.75)	2,220	4,925,244	957	156
3	$3{,}684\,x + 1{,}251\,x^2$	3,330	2,382 (71.53)	6,186	38,257,908	2,809	417
4	$7{,}960\,x + 2{,}592\,x^2$	6,976	5,360 (76.83)	13,144	172,746,408	6,153	864
5	$14{,}640\,x + 4{,}635\,x^2$	12,570	10,110 (80.43)	23,910	571,654,920	11,421	1,545
6	$24{,}252\,x + 7{,}524\,x^2$	20,520	17,040 (83.04)	39,300	1,544,435,652	19,045	2,508
B	Omega(L_5_20); R[6]						
2	$356\,x + 21\,x^2$	226	118 (52.21)	398	157,964	186	7
3	$1{,}303\,x + 132\,x^2$	852	578 (67.84)	1,567	2,453,658	766	44
4	$3{,}114\,x + 405\,x^2$	2,090	1,578 (75.50)	3,924	15,393,042	1,958	135
5	$6{,}053\,x + 912\,x^2$	4,144	3,322 (80.16)	7,877	62,037,428	3,978	304
6	$10{,}384\,x + 1{,}725\,x^2$	7,218	6,014 (83.32)	13,834	191,362,272	7,042	575

Table 9.9 Omega polynomial in $c\_B_{12}N_{12}$ net, (designed by $Le(C_n)$_all) function of k = no. repeating units along the edge of a cubic (k,k,k) domain

	Omega ($c\_B_{12}N_{12}$); R[4,6]; formulas
1	$\Omega(c\_B_{12}N_{12}, x) = 6 \cdot x^{k(4k+2)} + 12 \sum_{i=1}^{k-1} x^{i(4k+2)}$
2	$\Omega'(1) = e(G) = 12k^2(1+2k)$
3	$CI(G) = -8k - 32k^2 - 48k^3 + 80k^4 + 512k^5 + 576k^6$ $= -8k(1+2k)^2(1+2k^2-18k^3)$
4	$v(c\_B_{12}N_{12}) = 4k^2[6+3(-1+k)]$
5	$\text{Atoms}(sp^3) = 12k^2(-1+k)$
6	$R[4] = 3(1-k+2k^2)$
7	$R[6] = 8k^3$
8	$m(c\_B_{12}N_{12}) = k^3$; m = no. monomer
9	$\lim_{k\to\infty}\left[\dfrac{\text{Atoms}(sp^3)}{v(G)} = \dfrac{12k^2(-1+k)}{4k^2[6+3(-1+k)]}\right] = 1$

Table 9.10 Examples, Omega polynomial in $c\_B_{12}N_{12}$ cubic (k,k,k) net

k	Omega($c\_B_{12}N_{12}$) R[4,6]	Atoms	sp^3 Atoms (%)	Bonds	CI(G)	R[4]	R[6]
1	$6x^6$	24	110 (44.00)	36	1,080	6	8
2	$12x^{10} + 6x^{20}$	144	768 (62.75)	240	54,000	42	64
3	$12x^{14} + 12x^{28} + 6x^{42}$	432	2,382 (71.53)	756	549,192	144	216
4	$12x^{18} + 12x^{36} + 12x^{54} + 6x^{72}$	960	5,360 (76.83)	1,728	2,900,448	348	512
5	$12x^{22} + 12x^{44} + 12x^{66} + 12x^{88} + 6x^{110}$	1,800	10,110 (80.43)	3,300	10,643,160	690	1,000
6	$12^{26} + 12x^{52} + 12x^{78} + 12x^{104} + 12x^{130} + 6x^{156}$	3,024	17,040 (83.04)	5,616	30,947,280	1,206	1,728

Table 9.11 Theta Θ, Pi Π, Sadhana Sd, and PI_v polynomials in $c\_B_{12}N_{12}$ cubic (*k*,*k*,*k*) net

	Formulas
1	$v(c\_B_{12}N_{12}) = 4k^2[6 + 3(-1 + k)]$
2	$e(G) = 12k^2(1 + 2k)$
3	$\Theta(c\_B_{12}N_{12}, x) = 6 \cdot k(4k + 2) \cdot x^{k(4k+2)} + 12 \sum_{i=1}^{k-1} i(4k + 2) \cdot x^{i(4k+2)}$
4	$\Theta'(1) = 6 \cdot [k(4k + 2)]^2 + 12 \sum_{i=1}^{k-1} [i(4k + 2)]^2 = 8k(2k^2 + 1)(2k + 1)^2$
5	$\Pi(c\_B_{12}N_{12}, x) = 6 \cdot k(4k+2) \cdot x^{12k^2(2k+1)-k(4k+2)} + 12 \sum_{i=1}^{k-1} i(4k+2) \cdot x^{12k^2(2k+1)-i(4k+2)}$
6	$\Pi'(1) = 6 \cdot [k(4k + 2)][12k^2(2k + 1) - k(4k + 2)] + 12\sum_{i=1}^{k-1} [i(4k+2)][12k^2(2k+1) - i(4k+2)] = 8k(18k^3 - 2k^2 - 1)(2k+1)^2$
7	$Sd(c\_B_{12}N_{12}, x) = 6 \cdot x^{12k^2(2k+1)-k(4k+2)} + 12 \sum_{i=1}^{k-1} x^{12k^2(2k+1)-i(4k+2)}$
8	$Sd'(1) = 6 \cdot [12k^2(2k + 1) - k(4k + 2)] + 12\sum_{i=1}^{k-1} [12k^2(2k + 1) - i(4k + 2)] = 12k^2(12k - 7)(2k + 1)$
9	$PI_v = e \cdot x^v$
10	$PI'_v(1) = e \cdot v = (12k^2)^2(2k + 1)(k + 1) = 144k^4 + 432k^5 + 288k^6$

Table 9.12 Examples, Theta Θ, Pi Π, Sadhana Sd, and PI_v indices in $c\_B_{12}N_{12}$ cubic (*k*,*k*,*k*) net

k	$\Theta'(1)$	$\Pi'(1)$	$Sd'(1)$	$PI'_v(1)$	$\Omega'(1)=e(G)$	$v(G)$
4	85,536	2,900,448	70,848	1,658,880	1,728	960
5	246,840	10,643,160	174,900	5,940,000	3,300	1,800
6	592,176	30,947,280	365,040	16,982,784	5,616	3,024

Table 9.13 Omega polynomial in $B_{12}N_{12}$ net function of $k =$ no. repeating units along the edge of a Du(Med(Cube)) COD (*k*_all) domain

	Omega($COD\_B_{12}N_{12}$); *R*[4,6]; formulas
1	$\Omega(COD\_B_{12}N_{12}, x) = 12 \sum_{i=0}^{k-2} x^{[2k(k+2)+4ki]} + 6x^{6k^2}$
2	$\Omega'(1) = e(G) = 12k^2(4k - 1)$
3	$CI(G) = 8k^3(2k - 1)(144k^2 - 13k + 4) = 2,304k^6 - 1,360k^5 + 168k^4 - 32k^3$
4	$v(COD\_B_{12}N_{12}) = 24k^3$
5	$Atoms(sp^3) = 24k^2(k - 1) = 24k^3 - 24k^2$
6	$R[4] = -6k^2 + 12k^3$
7	$R[6] = 4k - 12k^2 + 16k^3$
8	$\lim_{k\to\infty}\left[\frac{Atoms(sp^3)}{v(G)} = \frac{24k^2(k - 1)}{24k^3}\right] = 1$

Table 9.14 Examples, Omega polynomial in COD_$B_{12}N_{12}$ (*k*_all) net

k	Omega(COD_$B_{12}N_{12}$) *R*[4,6]	Atoms	sp^3 atoms (%)	Bonds	CI(G)	*R*[4]	*R*[6]
2	$12x^{16} + 6x^{24}$	192	96 (50.00)	336	106,368	72	88
3	$12x^{30} + 12x^{42} + 6x^{54}$	648	432 (66.67)	1,188	1,361,880	270	336
4	$12x^{48} + 12x^{64} + 12x^{80} + 6x^{96}$	1,536	1,152 (75.00)	2,880	8,085,504	672	848
5	$12x^{70} + 12x^{90} + 12x^{110} + 12x^{130} + 6x^{150}$	3,000	2,400 (80.00)	5,700	31,851,000	1,350	1,720
6	$12x^{96} + 12x^{120} + 12x^{144} + 12x^{168} + 12x^{192} + 6x^{216}$	5,184	4,320 (83.33)	9,936	97,130,880	2,376	3,048

Table 9.15 Theta, Pi, Sadhana, and PI_v polynomials in COD_$B_{12}N_{12}$ (*k*_all) net

	Formulas
1	$v(\text{COD\_B}_{12}\text{N}_{12}) = 24k^3$
2	$\Omega'(1) = e(G) = 12k^2(4k-1)$
3	$\Theta(\text{COD\_B}_{12}\text{N}_{12}, x) = 12\sum_{i=0}^{k-2}[2k(k+2)+4ki]\cdot x^{[2k(k+2)+4ki]} + 36k^2x^{6k^2}$
4	$\Theta'(1) = 12\sum_{i=0}^{k-2}[2k(k+2)+4ki]^2 + 6^3k^4 = 32k^3 - 24k^4 + 208k^5$
5	$\Pi(\text{COD\_B}_{12}\text{N}_{12}, x) = 12\sum_{i=0}^{k-2}[2k(k+2)+4ki]\cdot x^{12k^2(4k-1)-[2k(k+2)+4ki]} + 36k^2x^{12k^2(4k-1)-6k^2}$
6	$\Pi'(1) = 12\sum_{i=0}^{k-2}[2k(k+2)+4ki]\cdot[12k^2(4k-1)-[2k(k+2)+4ki]] + 36k^2[12k^2(4k-1)-6k^2] = -32k^3 + 168k^4 - 1,360k^5 + 2,304k^6$
7	$\text{Sd}(\text{COD\_B}_{12}\text{N}_{12}, x) = 12\sum_{i=0}^{k-2}x^{12k^2(4k-1)-[2k(k+2)+4ki]} + 6x^{12k^2(4k-1)-6k^2}$
8	$\text{Sd}(1) = 12\sum_{i=0}^{k-2}12k^2(4k-1)-[2k(k+2)+4ki] + 6[12k^2(4k-1)-6k^2] = 12k^2(4k-1)(12k-7) = 84k^2 - 480k^3 + 576k^4$
9	$PI_v = e\cdot x^v$
10	$PI'_v(1) = e\cdot v = 288k^5(4k-1)$

Table 9.16 Examples, Theta, Pi, Sadhana, and PI_v polynomials in COD_$B_{12}N_{12}$ (*k_all*) net

k	$\Theta'(1)$	$\Pi'(1)$	$\text{Sd}'(1)$	$PI'_v(1)$	$\Omega'(1) = e(G)$	$v(G)$
4	208,896	8,085,504	118,080	4,423,680	2,880	1,536
5	639,000	31,851,000	302,100	17,100,000	5,700	3,000
6	1,593,216	97,130,880	645,840	51,508,224	9,936	5,184

9.3.5 Omega Polynomial of rhr Network

Formulas for Omega polynomial are derived here for a cubic domain (*k*,*k*,*k*) of the *rhr* network. The results are listed in Table. 9.19.

Table 9.17 Omega polynomial in $B_{12}N_{12}$ net function of $k =$ no. repeating units along the edge of an octahedral Oct (*k*_all) domain

	Omega(Oct_$B_{12}N_{12}$); R[4,6]; formulas
1	$\Omega(\mathrm{Oct\_B_{12}N_{12}}, x, k_{\mathrm{even}}) = \sum_{i=1}^{k-1} 4x^{2i(i+2)} + \sum_{i=1}^{k/2} 8x^{1+2i-2i^2+3k(k+2)/2} + 2x^{2k(k+2)}$
2	$\Omega(\mathrm{Oct\_B_{12}N_{12}}, x, k_{\mathrm{odd}}) = \sum_{i=1}^{k-1} 4x^{2i(i+2)} + \sum_{i=1}^{(k-1)/2} 8x^{3/2-2i^2+3k(k+2)/2} + 4x^{3/2+3k(k+2)/2} + 2x^{2k(k+2)}$
3	$\Omega'(1) = e(G) = 4k(k+2)(2k+1)$
4	$\mathrm{CI}(G) = 64k^6 + 1,548k^5/5 + 480k^4 + 240k^3 + 8k^2 - 108k/5$
5	$v(\mathrm{Oct\_B_{12}N_{12}}) = 8k + 12k^2 + 4k^3$
6	$\mathrm{Atoms(sp^3)} = -8k + 4k^2 + 4k^3$
7	$R[4] = 1 - k + 4k^2 + 2k^3$
8	$R[6] = 4k/3 + 4k^2 + 8k^3/3$
9	$\lim_{k\to\infty}\left[\frac{\mathrm{Atoms(sp^3)}}{v(G)} = \frac{-8k + 4k^2 + 4k^3}{8k + 12k^2 + 4k^3}\right] = 1$

Table 9.18 Examples, Omega polynomial in Oct_$B_{12}N_{12}$ (*k*_all) net

k	Omega(Oct_$B_{12}N_{12}$) R[4,6]	Atoms	sp^3 (%)	Bonds	CI(G)	R[4]	R[6]
2	$4x^6 + 8x^{13} + 2x^{16}$	96	32 (33.33)	160	23,592	31	40
3	$4x^6 + 4x^{16} + 8x^{22} + 4x^{24} + 2x^{30}$	240	120 (50.00)	420	167,256	88	112
4	$4x^6 + 4x^{16} + 4x^{30} + 8x^{33} + 8x^{37} + 2x^{48}$	480	288 (60.00)	864	717,456	189	240
5	$4x^6 + 4x^{16} + 4x^{30} + 8x^{46} + 4x^{48} + 8x^{52} + 4x^{54} + 2x^{70}$	840	560 (66.67)	1,540	2,297,592	346	440
6	$4x^6 + 4x^{16} + 4x^{30} + 4x^{48} + 8x^{61} + 8x^{69} + 4x^{70} + 8x^{73} + 2x^{96}$	1,344	960 (71.43)	2,496	6,067,512	571	728

Table 9.19 Omega polynomial in the *rhr* net function of *k*

Omega (*x*, rhr); $R_{\max} = 6$

$\Omega(x) = 24k \sum_{i=0}^{k-1} x^{(4i+2)}$

$\mathrm{CI} = 32k^2(72k^4 - 4k^2 + 1)$

$e = |E(G)| = 48k^3$

$v = |V(G)| = 12k^2(2k+1)$

Examples

k	Omega polynomial; $R_{\max} = 6$	CI	e	v	r4	r6
1	$24x^2$	2,208	48	36	–	8
2	$48x^2 + 48x^6$	145,536	384	240	48	64
3	$72x^2 + 72x^6 + 72x^{10}$	1,669,536	1,296	756	216	216
4	$96x^2 + 96x^6 + 96x^{10} + 96x^{14}$	9,404,928	3,072	1,728	576	512
5	$120x^2 + 120x^6 + 120x^{10} + 120x^{14} + 120x^{18}$	35,920,800	6,000	3,300	1,200	1,000

9.4 Conclusions

Design of several hypothetical crystal networks was performed by using original software programs CVNET and NANO-STUDIO, developed at TOPO GROUP CLUJ. The topology of the networks was described in terms of the net parameters by several counting polynomials, calculated by our NANO-STUDIO, Omega and PI software programs.

Hyperdiamonds are structures related to the classical diamond, having a significant amount of sp^3 carbon atoms and covalent forces to join the consisting fullerenes in crystals. Design of several hypothetical crystal networks was performed by using original software programs CVNET and NANO-STUDIO, developed at TOPO GROUP CLUJ. The topology of the networks was described in terms of the net parameters and several counting polynomials, calculated by our NANO-STUDIO, Omega, and PI software programs.

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