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Hyperdiamonds: a topological view

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ABSTRACT

Hyperdiamonds are covalently bonded fullerenes in crystalline forms, more or less related to diamond, and having a significant amount of sp3 carbon atoms. Design of several hypothetical crystal networks was performed by using our original software programs CVNET and NANO-STUDIO. The topology of the networks is described in terms of the net parameters and several counting polynomials, calculated by NANO-STUDIO, OMEGA and PI software programs.

Keywords: Hyperdiamond, crystal-like network, molecular topology, counting polynomial.

1 INTRODUCTION

Since 1985, when C_{60} was discovered, a new period, called "nano-era", has started in science and technology. This period is dominated by the carbon allotropes, which are 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 [1-3], both from theoretical reasons and applications perspective. Inorganic compounds also attracted the attention of scientists. Recent articles in crystallography promoted the idea of topological description and classification of crystal structures [4-7].

Diamond D_6 (Figure 1), the beautiful classical diamond, with all-hexagonal rings of sp^3 carbon atoms crystallized in a face-centered cubic network (space group $Fd3m$), has kept its leading interest among the carbon allotropes, even as the "nano" varieties [8-13]. Its

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mechanical characteristics are of great importance, as the composites can 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 [14], ultrasound cavitation [15], or mechano-synthesis [16], under electronic microscopy.

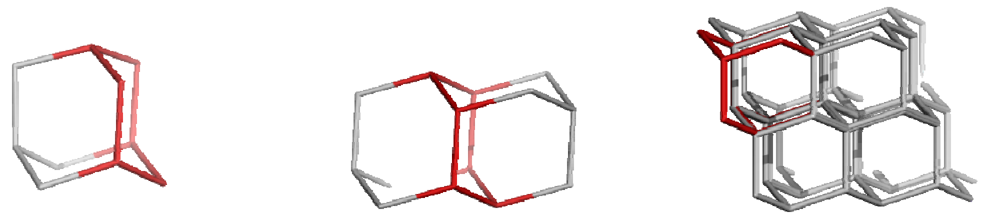


Figure 1. Diamond D_6: adamantane D_6_10_100 (left), diamantane D_6_14_211 (central) and diamond D_6_52_222 net (right)

However, the diamond D_6 is not unique: a hexagonal network (space group $P6_3/mmc$ - Figure 2), called lonsdaleite [17], was discovered in a meteorite in the Canyon Diablo, Arizona, in 1967. Several diamond-like networks have also been proposed [2,18,19].

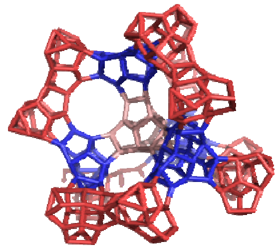
Figure 2. Losdaleite: L_6_12_111 (left), L_6_18_211 (central) and L_6_48_222 net (right)

Multi-tori MT are structures of high genera [1-3], consisting of more than one tubular ring. They are supposed to result by self-assembly of some repeating units (*i.e.*, monomers) which can be designed by opening of cages/fullerenes or by appropriate map/net operations. Multi-tori appear in processes of self-assembling of some rigid monomers [20]. Zeolites and spongy carbon [21,22] also contain multi-tori. Multi-tori can be designed starting from the Platonic solids, by using appropriate map operations [23-25].

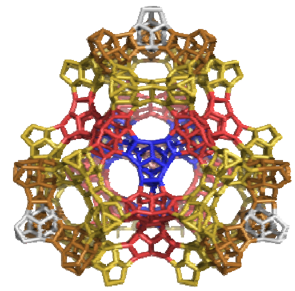
In a previous study, Diudea and Ilić [26] described some multi-tori (see Figure 3) constructed by using a unit designed by the map operation sequence $Trs(P_4(T))$. These structures consist of all pentagonal faces, observing the triangles disappear (as faces) in the building process.

Hyperdiamonds are covalently bonded fullerenes in crystalline forms, more or less related to the diamond D_6, having a significant amount of sp^3 carbon atoms.

Design of several hypothetical crystal networks was performed by using our original software programs [1] CVNET and NANO-STUDIO. Topological data were provided by NANO-STUDIO, OMEGA and PI software programs.



M$_{17}$



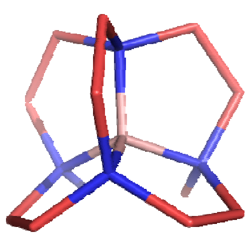
M$_{57}$

Figure 3. Multi-tori M_{17} (left) and M_{57} (right) v=972; e=1770; f_5=684

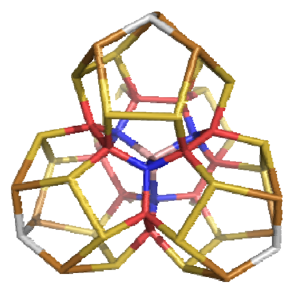
The article is structured as follows. After the introductory part, the main networks: Diamond D_5, Lonsdaleite L_5 and Hyper Boron Nitride are presented in detail. Two sections with basic definitions in Omega polynomial and in Omega related polynomials, respectively, will be next developed. In the last part, the topology of the classical diamond and the three hyperdiamond nets will be presented. Conclusions and references will close the article.

2. DIAMOND D$_5$ NETWORK

Diamond **D**$_5$, recently theorized by Diudea and collaborators [26-30], is a hyperdiamond, of which seed is the centrohexaquinane C_{17} (Figure 4, left).



C$_{17}$



C$_{57}$

Figure 4. The seed C_{17} (left) and the multi-cage C_{57}: v=57; e=94; r_5=42 (right)

C_{17} can dimerize (by a synchron cycloaddition) to $2\times C_{17}=C_{34}$ (Figure 5) and next condensing up to the multi-cage C_{57} (Figure 4, right) or to the adamantane-like ada_20_170 (Figure 5, right), or without wings, as in ada_20_158 (Figure 6, left). Compare this with adamantane (Figure 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 hyper- diamond D_5, while the last number counts the carbon atoms in the structures.

A diamantane-like unit is evidenced, as in Figure 7 (see for comparison the diamantane, Figure 1, central). Since any net has its co-net, the diamond D_5_20 net (Figure 8, left) has the co-net D_5_28 (Figure 8, right), of which corresponding units are illustrated in Figures 6 (right) and 7 (right), respectively. In fact, there is one and the same *triple* *periodic* D_5 network, built up basically from C_{20} and having as hollows the fullerene C_{28}. 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.

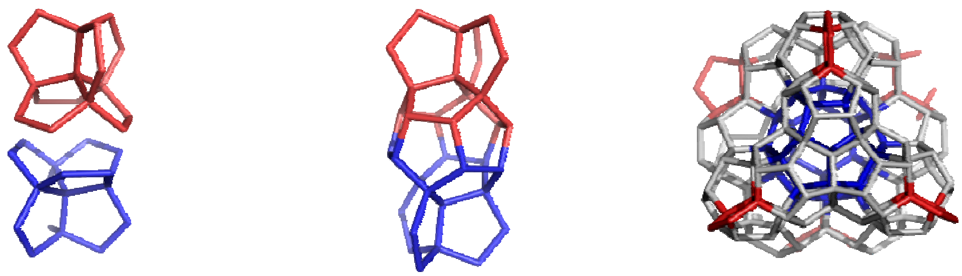


Figure 5. Way to ada_20: 2×C_{17}=C_{34} (left and central) and ada_20_170 (right).

Figure 6. Adamantane-like structures: ada_20_158 (left) and ada_28_213 (right)

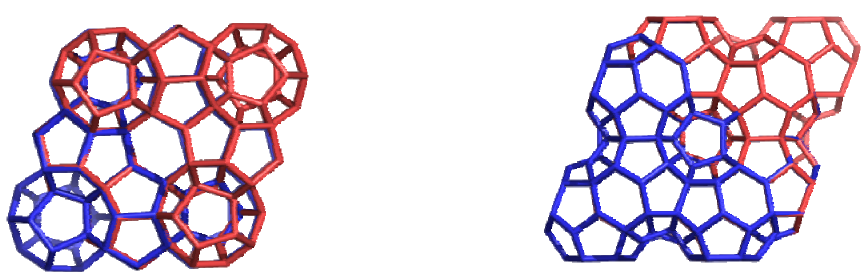


Figure 7. Diamantane-like structures: dia_20_226_222 net (left) and dia_28_292_222 co-net (right)

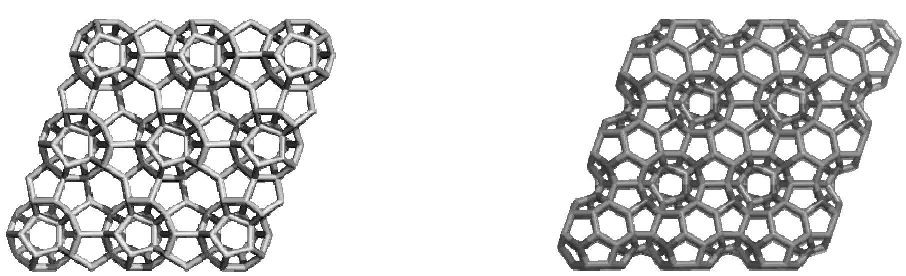


Figure 8. Diamond D_5_20_860_333 net (left) and D_5_28_ 1022_333 co-net (right)

The hyperdiamond D_5_20/28 mainly consists of sp^3 carbon atoms building ada-like repeating units (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 trend to 90% (see Table 3, entry 9) this, yet hypothetical carbon allotrope, was called the diamond D_5.

Energetic data, calculated at various DFT levels [29,30] 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. Density of the D_5 network was calculated to be around 2.8 g/cm^3.

It is noteworthy that D_5_20/28 net was identified, in the space fullerene theory [6,7,31], as the Frank-Kasper *mtn* structure, appearing in "type II clathrate hydrates"; space group Fd-3m, point symbol net: {5^5.6}12{5^6}5, 4,4,4-c trinodal net [32].

3. LONSDALEITE L_5 NETWORK

By analogy to D_5_20/28, a lonsdaleite-like net was proposed [30] (Figure 9). The hyper-hexagons L_5_28_134 (Figure 9, central and right), of which 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 superimposed on D_5_20/28 net. In crystallography, it is known as the mgz-x-d net, with the point symbol: {5^5.6}12{5^6}5; 4,4,4,4,4,4,4-c, 7-nodal net [32].

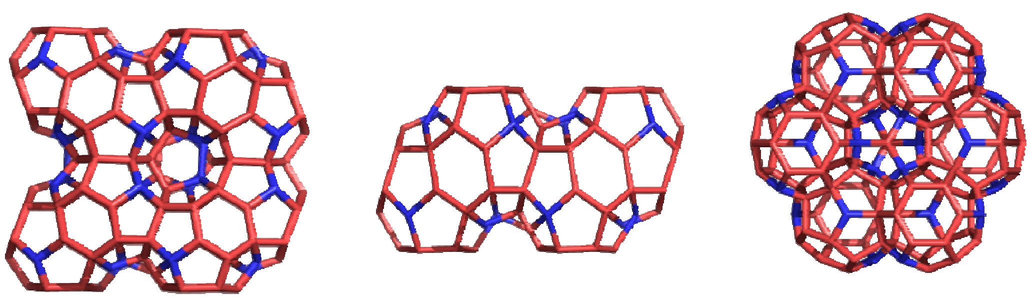


Figure 9. Losdaleite: L_5_28_250 (side view, left), L_5_28_134 (side view, central) and L_5_28_134 (top view, right).

4. 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 physico-chemical properties are also similar, with small differences.

Fullerene-like cages have been synthesized and several theoretical structures have been proposed for these molecules [33-39].

Based on $B_{12}N_{12}$ unit, designed by *Tr*(Oct) or *Le*(C) map operation, we modeled three domains of 3D arrays: a cubic domain (k,k,k), Figure 10, a dual of cubeoctahedron domain (k_all), Figure 11 and an octahedral domain (k_basis), Figure 12.

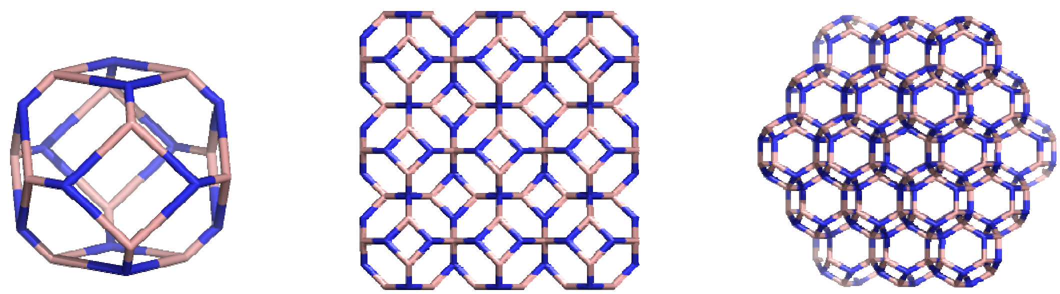


Figure 10. Boron nitride $B_{12}N_{12}$: truncated octahedron (left), a cubic (3,3,3)_432 domain built up from truncated octahedra joined by identifying the square faces (central) and its corner view (right).

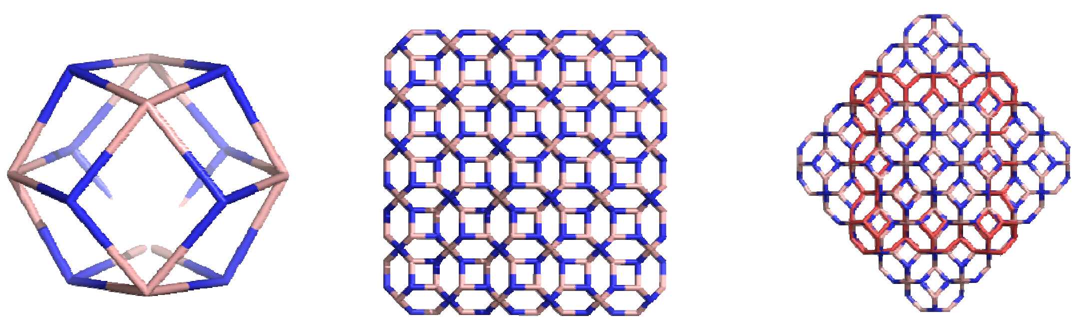


Figure 11. Boron nitride $B_{12}N_{12}$: dual of cubeoctahedron (left), a (3,3,3)_648 domain constructed from truncated octahedra joined by identifying the square and hexagonal faces, respectively, by following the dual of cubeoctahedron structure (central) and its superposition with the cubic (3,3,3)_432 domain (right).

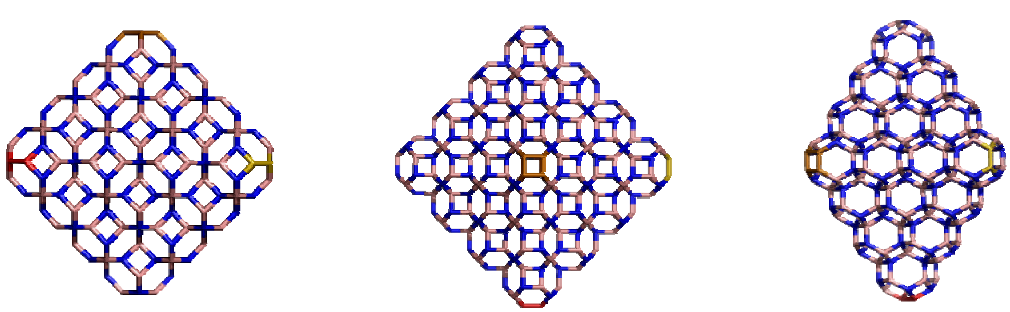


Figure 12. Boron nitride $B_{12}N_{12}$: an octahedral (4,4,4)_480 domain: (1,1,0-left), (0,0,1-central) and (2,1,1-right) constructed from truncated octahedra joined by identifying the square and hexagonal faces, respectively.

The topology of the above hyperdiamond structures 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.

5. 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 [1,40,41]

$$e\ co\ f \Leftrightarrow d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y) \quad (1)$$

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 codistant 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 $C(G) = c_1, c_2, .., c_k$ form a partition: $E(G) = c_1 \cup c_2 \cup ... \cup c_k$, $c_i \cap c_j = \varnothing, i \neq j$.

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 [42]. A graph *G* is called a *partial cube* if there exists an integer n such that G is an isometric subgraph of Qn.

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*: $n_{uv} = \{w \in V(G) \mid d(w,u) < d(w,v)\}$. By definition, it follows that $n_{uv} = \{w \in V(G) \mid d(w,v) = d(w,u) + 1\}$. The sets (and subgraphs) induced by these vertices, n_{uv} and n_{vu}, are called *semicubes* of *G*; these semicubes are *opposite* and disjoint [41,43,44].

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 ~ (Djoković [45]) and Θ (Winkler [46]) relations:

$$e\,\Theta\, f \Leftrightarrow d(u,x) + d(v,y) \neq d(u,y) + d(v,x) \quad (2)$$

LEMMA 1. In any connected graph, *co* = ~.

In general graphs, we have $\sim \subseteq \Theta$ and in bipartite graphs ~ = Θ. From this and the above lemma, it follows [41]

PROPOSITION 2. In a connected graph, *co* = ~; if *G* is also bipartite, then *co*= ~ = Θ .

THEOREM 3. In a bipartite graph, the following statements are equivalent [41]:

(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 [47], equivalence between (ii) and (iii) is due to Djoković [45], while the equivalence between (ii) and (iv) was proved by Winkler [46].

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 [48], 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 4. 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 (1). The same is true for the *op*-relation, with the only difference (1) is limited to a single face. Suppose e_1, 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, *co*-relation is transitive, all the edges of *ops* will be *co*-distant, thus *ops* and *ocs* will coincide.

COROLLARY 5. In a *co*-graph, all the edges of an *ops* are topologically parallel.

Observe 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 (1)) and (ii) topologically perpendicular edges (in the Tetrahedron and its extensions - relation (3)) [43,49]:

$$e\ eqd\ f\,(ii) \Leftrightarrow d(u,x) = d(u,y) = d(v,x) = d(v,y) \tag{3}$$

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

Proof of Proposition 6 was given in [50].

COROLLARY 7. 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.

6. OMEGA POLYNOMIAL

Let G be an arbitrary connected graph and $s_1, s_2, .., s_k$ be its *op*-strips. Then *ops* form a partition of $E(G)$ and the Ω-polynomial [51] of G is defined as

$$\Omega(x) = \sum_{i=1}^{k} x^{|s_i|} \tag{4}$$

Let now consider the set of edges *co*-distant to edge e in G, $c(e)$. A Θ-polynomial [43], counting the edges equidistant to every edge e, is written as

$$\Theta(x) = \sum_{e \in E(G)} x^{|c(e)|} \tag{5}$$

Suppose now G is a *co*-graph, when $|c_k|=|s_k|$, then [41]

$$\Theta(x) = \sum_{e \in E(G)} x^{|c(e)|} = \sum_{i=1}^{k} \sum_{e \in S_i} x^{|c(e)|} = \sum_{e} |c(e)| x^{|c(e)|} = \sum_{i=1}^{k} |s_i| x^{|s_i|} \tag{6}$$

Let's simplify a little the above notations: note by $m(s)$ or simply m the number of *ops* of length $s=|s_k|$ and re-write the Omega polynomial as [1,52,53,54]:

$$\Omega(x) = \sum_{s} m \cdot x^{s} \tag{7}$$

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

$$\Theta(x) = \sum_{s} ms \cdot x^{s} \tag{8}$$

$$\Pi(x) = \sum_{s} ms \cdot x^{e-s} \tag{9}$$

$$Sd(x) = \sum_{s} m \cdot x^{e-s} \tag{10}$$

The polynomial $\Theta(x)$ counts equidistant edges while $\Pi(x)$ non-equidistant edges. The Sadhana polynomial, proposed by Ashrafi et al. [52] in relation with the Sadhana index

$Sd(G)$ proposed by Khadikar et al. [53], counts non-opposite edges in G. Their first derivative (in x=1) provides single number topological descriptors also termed topological indices [1]:

$$\Omega'(1) = \sum_s m \cdot s = e = |E(G)| \tag{11}$$

$$\Theta'(1) = \sum_s m \cdot s^2 = \theta(G) \tag{12}$$

$$\Pi'(1) = \sum_s ms \cdot (e-s) = \Pi(G) \tag{13}$$

$$Sd'(1) = \sum_s m \cdot (e-s) = e(Sd(1)-1) = Sd(G) \tag{14}$$

Note $Sd(1) = \Omega(1)$, then the first derivative given in (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 [49] CI=$CI(G)$ was defined:

$$CI(G) = \left\{[\Omega'(1)]^2 - [\Omega'(1) + \Omega''(1)]\right\} \tag{15}$$

A polynomial related to $\Pi(x)$ was defined by Ashrafi [53] as:

$$PI_e(x) = \sum_{e \in E(G)} x^{n(e,u)+n(e,v)} \tag{16}$$

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 $PI_e(G)$ index proposed by Khadikar [55,56].

PROPOSITION 8. In any bipartite graph, $\Pi(G) = PI_e(G)$.

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 [49,56]:

$$d(z,e) = \min\{d(z,u), d(z,v)\} \tag{17}$$

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

$$e \; eqd \; f \, (iii) \Leftrightarrow d(x,e) = d(y,e) \text{ and } d(u,f) = d(v,f) \tag{18}$$

In bipartite graphs, relations (1) & (3) superimpose over relations (17)&(18), then in such graphs, $\Pi(G) = PI_e(G)$. In general graphs, this is, however, not true.

PROPOSITION 9. In *co*-graphs, the equality $CI(G) = \Pi(G)$ holds.

Proof. By definition, one calculates:

$$\begin{aligned} CI(G) &= \left(\sum_{i=1}^{k}|s_i|\right)^2 - \left(\sum_{i=1}^{k}|s_i| + \sum_{i=1}^{k}|s_i|(|s_i|-1)\right) \\ &= |E(G)|^2 - \sum_{i=1}^{k}(|s_i|)^2 = \Pi'(G,1) = \Pi(G) \end{aligned} \tag{19}$$

Relation (19) is valid only assuming $|c_k| = |s_k|$, k=1,2,.., 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, $CI(G) \neq \Pi(G)$ [1].

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

$$CI(G) = \Pi(G) = PI_e(G) \tag{20}$$

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:[57,58]

$$PI_v(G) = PI_v'(1) = \sum_{e=uv} n_{u,v} + n_{v,u} = |V|\cdot|E| - \sum_{e=uv} m_{u,v} \tag{21}$$

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 (21) will miss. The value of $PI_v(G)$ 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 [1].

7. 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 1. 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 2.

8. TOPOLOGY OF DIAMOND D_5 AND LONSDALEITE L_5 NETS

Topology of diamond D_5 and lonsdaleite L_5, in a cubic (k,k,k) domain, is presented in Tables 3 to 8: formula 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 3). Numerical examples are given.

Table 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	$\Omega(D_6\_k_{odd},x)=\left(\sum_{i-1}^{k}2x^{\frac{(i+1)(i+2)}{2}}\right)+\left(\sum_{i-1}^{(k-1)/2}2x^{\frac{(k+1)(k+2)}{2}+\frac{k\times k-1}{4}-i(i-1)}\right)+3kx^{(k+1)(k+1)}$
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	$\lim_{k\to\infty}\left[\frac{Atoms(sp^3)}{v(G)}=\frac{2k(k^2-1)}{4k+6k^2+2k^3}\right]=1$

9. TOPOLOGY OF BORON NITRDIDE NETS

Topology of boron nitride nets is treated similarly to that of D_5 and L_5 and is presented in Tables 9 to 18: 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 are given, along with numerical examples. Formulas for Omega polynomial are taken as 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 2. 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 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	$CI(G)=1488+1350k+1764k^2-4612k^3-2124k^4-2448k^5+4624k^6$
4	$v(D_5\_20a)=-22-12k+34k^3$
5	$Atoms(sp^3)=-10-36k^2+34k^3$
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	$\lim_{k\to\infty}\frac{R[5]}{R[6]}=9$; $\lim_{k\to\infty}\frac{R[5]}{R[5]+R[6]}=9/10$
10	$\lim_{k\to\infty}\left[\frac{Atoms(sp^3)}{v(G)}=\frac{-10-36k^2+34k^3}{-22-12k+34k^3}=\frac{-\frac{10}{k^3}-\frac{36}{k}+34}{-\frac{22}{k^3}-\frac{12}{k^2}+34}\right]=1$

Table 4. Examples, Omega polynomial in D_5_20 net.

k	Omega(D_5_20a); R[6]	Atoms	sp^3Atoms (%)	Bonds	CI	R[5]	R[6]
2	$356 x^1+21 x^2$	226	118 (52.21)	398	157964	186	7
3	$1318 x^1+132 x^2$	860	584 (67.91)	1582	2500878	774	44
4	$3144 x^1+405 x^2$	2106	1590 (75.50)	3954	15629352	1974	135
5	$6098 x^1+912 x^2$	4168	3340 (80.13)	7922	62748338	4002	304
6	$10444 x^1+1725 x^2$	7250	6038 (83.28)	13894	193025892	7074	575
7	$16446 x^1+2916 x^2$	11556	9888 (85.57)	22278	496281174	11406	972

Table 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	$\Omega(\mathrm{D}_5\_28a, x) = (-26-12k-6k^2+44k^3)\cdot x + (-18+9k^2+12k^3)\cdot x^2$
2	$\Omega'(1) = e(G) = -62-12k+12k^2+68k^3$
3	$CI(G) = 3942+1500k-1374k^2-8812k^3-1488k^4+1632k^5+4624k^6$
4	$v(\mathrm{D}_5\_28a) = -40-6k+18k^2+34k^3$
5	$Atoms(sp^3) = -4-6k-30k^2+34k^3$
6	$R[5] = -18-18k^2+36k^3$
7	$R[6] = -1+6k-9k^2+4k^3$
8	$\lim_{k\to\infty}\left[\frac{Atoms(sp^3)}{v(G)} = \frac{-4-6k-30k^2+34k^3}{-40-6k+18k^2+34k^3}\right] = 1$

Table 6. Examples, Omega polynomial in D_5_28 co-net.

k	Omega(D_5_28a); R[6]	Atoms	sp^3Atoms (%)	Bonds	CI	R[5]	R[6]
2	$278 x^1+114 x^2$	292	136 (46.58)	506	255302	198	38
3	$1072 x^1+387 x^2$	1022	626 (61.25)	1846	3405096	792	129
4	$2646 x^1+894 x^2$	2400	1668 (69.50)	4434	19654134	1998	298
5	$5264 x^1+1707 x^2$	4630	3466 (74.86)	8678	75295592	4032	569
6	$9190 x^1+2898 x^2$	7916	6224 (78.63)	14986	224559414	7110	966
7	$14688 x^1+4539 x^2$	12462	10146 (81.41)	23766	564789912	11448	1513

Table 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.

	Network
A	Omega (L_5_28); R[6]
1	$\Omega(\mathrm{L}_5\_28, x) = 2k(-1+73k+44k^2)\cdot x + 3k(4+21k+8k^2)\cdot x^2$
2	$\Omega'(1) = e(G) = 2k(11+136k+68k^2)$
3	$CI(G) =$ 2k(-23 $+43k+5892k^2+39984k^3+36992k^4+9248k^5)$
4	$v(\mathrm{L}_5\_28) = 2k(12+79k+34k^2)$
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	$\lim_{k\to\infty}\left[\frac{Atoms(sp^3)}{v(G)} = \frac{2-6k-36k^2+34k^3}{-6-20k+34k^3}\right] = 1$

10. CONCLUSIONS

Hyperdiamonds are structures having a significant amount of sp^3 carbon atoms and covalent forces to join the consisting fullerenes in crystalline forms, related to the classical diamond. 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 is described in terms of the net parameters and several counting polynomials, calculated by our NANO-STUDIO, OMEGA and PI software programs.

Table 8. 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	$232x + 99x^2$	250	110 (44.00)	430	184272	165	33
2	$1284x + 468x^2$	1224	768 (62.75)	2220	4925244	957	156
3	$3684x + 1251x^2$	3330	2382 (71.53)	6186	38257908	2809	417
4	$7960x + 2592x^2$	6976	5360 (76.83)	13144	172746408	6153	864
5	$14640x + 4635x^2$	12570	10110 (80.43)	23910	571654920	11421	1545
6	$24252x + 7524x^2$	20520	17040 (83.04)	39300	1544435652	19045	2508
B	Omega(L_5_20); R[6]						
2	$356x + 21x^2$	226	118 (52.21)	398	157964	186	7
3	$1303x + 132x^2$	852	578 (67.84)	1567	2453658	766	44
4	$3114x + 405x^2$	2090	1578 (75.50)	3924	15393042	1958	135
5	$6053x + 912x^2$	4144	3322 (80.16)	7877	62037428	3978	304
6	$10384x + 1725x^2$	7218	6014 (83.32)	13834	191362272	7042	575

Table 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	$Atoms(sp^3) = 12k^2(-1+k)$
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	$\lim_{k\to\infty}\left[\frac{Atoms(sp^3)}{v(G)} = \frac{12k^2(-1+k)}{4k^2[6+3(-1+k)]}\right] = 1$

Table 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^3Atoms (%)	Bonds	CI(G)	R[4]	R[6]
1	$6x^{6}$	24	110 (44.00)	36	1080	6	8
2	$12x^{10}+6x^{20}$	144	768 (62.75)	240	54000	42	64
3	$12x^{14}+12x^{28}+6x^{42}$	432	2382 (71.53)	756	549192	144	216
4	$12x^{18}+12x^{36}+12x^{54}+6x^{72}$	960	5360 (76.83)	1728	2900448	348	512
5	$12x^{22}+12x^{44}+12x^{66}+12x^{88}+6x^{110}$	1800	10110 (80.43)	3300	10643160	690	1000
6	$12^{26}+12x^{52}+12x^{78}+12x^{104}+12x^{130}+6x^{156}$	3024	17040 (83.04)	5616	30947280	1206	1728

Table 11. Theta Θ, Pi Π, Sadhana Sd and PI_v polynomials in c_$B_{12}N_{12}$ cubic (*k*,*k*,*k*) net.

	Formulas
1	$v(\mathrm{c\_B_{12}N_{12}}) = 4k^2[6+3(-1+k)]$
2	$e(G) = 12k^2(1+2k)$
3	$\Theta(\mathrm{c\_B_{12}N_{12}}, x) = 6\cdot k(4k+2)\cdot x^{k(4k+2)} + 12\sum_{i=1}^{k-1} i(4k+2)\cdot x^{i(4k+2)}$
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	$\Pi(\mathrm{c\_B_{12}N_{12}}, x) = 6\cdot k(4k+2)\cdot x^{12k^2(2k+1)-k(4k+2)} + 12\sum_{i=1}^{k-1} i(4k+2)\cdot x^{12k^2(2k+1)-i(4k+2)}$
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	$Sd(\mathrm{c\_B_{12}N_{12}}, x) = 6\cdot x^{12k^2(2k+1)-k(4k+2)} + 12\sum_{i=1}^{k-1} x^{12k^2(2k+1)-i(4k+2)}$
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 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	85536	2900448	70848	1658880	1728	960
5	246840	10643160	174900	5940000	3300	1800
6	592176	30947280	365040	16982784	5616	3024

Table 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	$\Omega(\mathrm{COD\_B_{12}N_{12}},x)=12\sum_{i=0}^{k-2}x^{[2k(k+2)+4ki]}+6x^{6k^2}$
2	$\Omega'(1)=e(G)=12k^2(4k-1)$
3	$CI(G)=\ 8k^3(2k-1)(144k^2-13k+4)=2304k^6-1360k^5+168k^4-32k^3$
4	$v(\mathrm{COD\_B_{12}N_{12}})=24k^3$
5	$Atoms(sp3)=24k^2(k-1)=24k^3-24k^2$
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 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^3Atoms (%)	Bonds	CI(G)	R[4]	R[6]
2	$12x^{16}+6x^{24}$	192	96 (50.00)	336	106368	72	88
3	$12x^{30}+12x^{42}+6x^{54}$	648	432 (66.67)	1188	1361880	270	336
4	$12x^{48}+12x^{64}+12x^{80}+6x^{96}$	1536	1152 (75.00)	2880	8085504	672	848
5	$12x^{70}+12x^{90}+12x^{110}+12x^{130}+6x^{150}$	3000	2400 (80.00)	5700	31851000	1350	1720
6	$12x^{96}+12x^{120}+12x^{144}+12x^{168}+12x^{192}+6x^{216}$	5184	4320 (83.33)	9936	97130880	2376	3048

Table 15. Theta, Pi, Sadhana and PI_v polynomials in COD_$B_{12}N_{12}$ (k_all) net.

	Formulas
1	$v(\mathrm{COD\_B_{12}N_{12}})=24k^3$
2	$\Omega'(1)=e(G)=12k^2(4k-1)$
3	$\Theta(\mathrm{COD\_B_{12}N_{12}},x)=12\sum_{i=0}^{k-2}[2k(k+2)+4ki]\cdot x^{[2k(k+2)+4ki]}+36k^2x^{6k^2}$
4	$\Theta'(1)=12\sum_{i=0}^{k-2}[2k(k+2)+4ki]^2+6^3k^4\ =32k^3-24k^4+208k^5$
5	$\Pi(\mathrm{COD\_B_{12}N_{12}},x)=12\sum_{i=0}^{k-2}[2k(k+2)+4ki]\cdot x^{12k^2(4k-1)-[2k(k+2)+4ki]}+36k^2x^{12k^2(4k-1)-6k^2}$
6	$\Pi'(1)=12\sum_{i=0}^{k-2}[2k(k+2)+4ki]\cdot[12k^2(4k-1)-[2k(k+2)+4ki]]+36k^2[12k^2(4k-1)-6k^2]$ $=-32k^3+168k^4-1360k^5+2304k^6$
7	$Sd(\mathrm{COD\_B_{12}N_{12}},x)=12\sum_{i=0}^{k-2}x^{12k^2(4k-1)-[2k(k+2)+4ki]}+6x^{12k^2(4k-1)-6k^2}$
8	$Sd(1)=12\sum_{i=0}^{k-2}12k^2(4k-1)-[2k(k+2)+4ki]+6[12k^2(4k-1)-6k^2]$ $=12k^2(4k-1)(12k-7)=84k^2-480k^3+576k^4$
9	$PI_v=e\cdot x^v$
10	$PI_v{}'(1)=e\cdot v=288k^5(4k-1)$

Table 16. Examples, Theta, Pi, Sadhana and PI_v polynomials in $COD\_B_{12}N_{12}$ (*k_all*) net.

k	$\Theta'(1)$	$\Pi'(1)$	Sd\`(1)	PI_v\`(1)	$\Omega'(1) = e(G)$	$v(G)$
4	208896	8085504	118080	4423680	2880	1536
5	639000	31851000	302100	17100000	5700	3000
6	1593216	97130880	645840	51508224	9936	5184

Table 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	$\Omega(Oct\_B_{12}N_{12}, x, k_{even}) = \sum_{i=1}^{k-1} 4x^{2i(i+2)} + \sum_{i=1}^{k/2} 8x^{1+2i-2i^2+3k(k+2)/2} + 2x^{2k(k+2)}$
2	$\Omega(Oct\_B_{12}N_{12}, x, k_{odd}) = \sum_{i=1}^{k-1} 4x^{2i(i+2)} + \sum_{i=1}^{(k-1)/2} 8x^{3/2-2i^2+3k(k+2)/2} + 4x^{3/2+3k(k+2)/2} + 2x^{2k(k+2)}$
3	$\Omega'(1) = e(G) = 4k(k+2)(2k+1)$
4	$CI(G) = 64k^6 + 1548k^5/5 + 480k^4 + 240k^3 + 8k^2 - 108k/5$
5	$v(Oct\_B_{12}N_{12}) = 8k + 12k^2 + 4k^3$
6	$Atoms(sp^3) = -8k + 4k^2 + 4k^3$
7	$R[4] = 1 - k + 4k^2 + 2k^3$
8	$R[6] = 4k/3 + 4k^2 + 8k^3/3$
9	$\lim_{k\to\infty}\left[\frac{Atoms(sp^3)}{v(G)} = \frac{-8k+4k^2+4k^3}{8k+12k^2+4k^3}\right] = 1$

Table 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^3Atoms (%)	Bonds	CI(G)	R[4]	R[6]
2	$4x^6+8x^{13}+2x^{16}$	96	32(33.33)	160	23592	31	40
3	$4x^6+4x^{16}+8x^{22}+4x^{24}+2x^{30}$	240	120(50.00)	420	167256	88	112
4	$4x^6+4x^{16}+4x^{30}+8x^{33}+8x^{37}+2x^{48}$	480	288(60.00)	864	717456	189	240
5	$4x^6+4x^{16}+4x^{30}+8x^{46}+4x^{48}+8x^{52}+4x^{54}+2x^{70}$	840	560(66.67)	1540	2297592	346	440
6	$4x^6+4x^{16}+4x^{30}+4x^{48}+8x^{61}+8x^{69}+4x^{70}+8x^{73}+2x^{96}$	1344	960(71.43)	2496	6067512	571	728

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