Omega and Related Polynomials in Crystal-like Structures

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Abstract

Counting polynomials are those polynomials having at exponent the extent of a property partition and as coefficients the number of the corresponding partition. In the present paper four related counting polynomials are discussed: Omega Ω, Pi Π, Theta Θ and Sadhana Sd. Analytical close formulas for the calculation of these polynomials in some hypothetical crystal-like lattices are derived.

1. Introduction

A graph can be described by a connection table, a sequence of numbers, a matrix, a polynomial or by a single number (often called a topological index). A counting polynomial can be written as:

\[ P(G,x) = \sum_k m(G,k) \cdot X^k \]

with the exponents showing the extent of partitions \( p(G) \), \( \cup p(G) = P(G) \) of a graph property \( P(G) \) while the coefficients \( m(G,k) \) are related to the number of partitions of extent \( k \).

Counting polynomials have been introduced, in the Mathematical Chemistry literature, by Hosoya: \(^1\) \(^2\) \( Z(G,X) \) counts independent edge sets while \( H(G,X) \) (initially...
called Wiener and later Hosoya\(^3,4\) counts the distances in the graph. Hosoya also proposed the sextet polynomial\(^5-8\) for counting the resonant rings in a benzenoid molecule. More about polynomials the reader can find in ref\(^9\).

Some distance-related properties can be expressed in polynomial form, with coefficients calculable from the layer and shell matrices.\(^{10-13}\) These matrices are built up according to the vertex distance partitions of a graph, as provided by the TOPOCLUJ software package.\(^{14}\) The most important, in this respect, is the evaluation of the coefficients of Hosoya \(H(G,X)\) polynomial from the layer of counting LC matrix.

### 2. Definitions

Let \(G(V,E)\) be a connected bipartite 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 codistant: \(e \; co \; f\) if

\[
d(v, x) = d(v, y) + 1 = d(u, x) + 1 = d(u, y)
\]

If \(co\) is an equivalence relation:\(^{15,16}\)

\[
e \; co \; e \\
e \; co \; f \iff f \; co \; e \\
e \; co \; f \; & \; f \; co \; h \implies e \; co \; h
\]

Then, \(C(e) := \{ f \in E(G) ; f \; co \; e \}\) is the set of edges in \(G\), codistant to the edge \(e \in E(G)\) and \(G\) is called a co-graph. Consequently, \(C(e)\) is called an orthogonal cut set \(ocs\) of \(G\) and \(E(G)\) is the union of disjoint orthogonal cuts: \(C_1 \cup C_2 \cup \ldots \cup C_k\) and \(C_i \cap C_j = \emptyset\) for \(i \neq j\) and \(i,j=1,2,\ldots,k\).

Observe \(co\) is a \(\theta\) relation, (Djoković-Winkler relation)\(^{17,18}\), and \(G\) is a co-graph if and only if it is a partial cube, a result due to Klavžar.\(^{19}\) In a plane bipartite graph, an edge \(e\) is in relation \(\theta\) with any opposite edge \(f\) if the faces of the plane graph are isometric (which is the case of the most chemical graphs). Then an orthogonal cut \(oc\) with respect to a given edge is the smallest subset of edges closed under this operation and \(C(e)\) is precisely a \(\theta\)-class of \(G\).

Concluding, a graph \(G\) is a co-graph if and only if it is a partial cube. A partial cube is always a bipartite graph, but the reciprocal is not true (see Figure 1 and Table 1).

A set of opposite edges \(S(e) := \{ f \in E(G) ; f \; op \; e \}\) within the same face/ring eventually forming a strip of adjacent faces/rings of a covering/tiling, is called an “opposite edge strip” \(ops\). Under \(ops\) relation, \(E(G)\) is the union of disjoint \(ops\): \(S_1 \cup S_2 \cup \ldots \cup S_k\) and \(S_i \cap S_j = \emptyset\)
for $i \neq j$ and $i, j = 1, 2, \ldots, k$. The relation $ops$ is not necessarily transitive. Observe $ops$ is an ocs only in partial cubes.

\[
\text{Figure 1. Bipartite, non-partial (a) and partial (b) Cubes}
\]

**Table 1.** Polynomials of cubic structures in Figure 1.

<table>
<thead>
<tr>
<th>Cubic Cage (Figure 1a)</th>
<th>Cubic Net (Figure 1b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
<td>Polynomial</td>
</tr>
<tr>
<td>$\Omega(G, x)$</td>
<td>$6X^8$</td>
</tr>
<tr>
<td>$Sd(G, x)$</td>
<td>$6X^{40}$</td>
</tr>
<tr>
<td>$\Theta(G, x)$</td>
<td>$24X^8 + 24X^{10}$</td>
</tr>
<tr>
<td>$\Pi(G, x)$</td>
<td>$24X^{38} + 24X^{40}$</td>
</tr>
</tbody>
</table>

Omega polynomial\(^2\) is defined on $ops$ as:

$$\Omega(G, X) = \sum_s m(G, s) \cdot X^s$$

where $m(G, s)$ is the number of opposite edge strips of length $s$.

If $ops$ is an ocs, as in partial cubes, we can write the following counting polynomials:

$$\Omega(G, X) = \sum_k m \cdot X^k$$

$$Sd(G, X) = \sum_k m \cdot X^{e-k}$$

$$\Theta(G, X) = \sum_k m \cdot k \cdot X^k$$

$$\Pi(G, X) = \sum_k m \cdot k \cdot X^{e-k}$$

$\Omega(G, X)$ and $\Theta(G, X)$ count equidistant edges in $G$ while $Sd(G, X)$ and $\Pi(G, X)$, count non-equidistant edges. The first two polynomials are counted once for a strip while the last two are counted for each edge, so that the coefficients are multiplied with $k$.

In a counting polynomial, the first derivative (in $X=1$) defines the type of property which is counted. For the above polynomials they are:

$$\Omega'(G, 1) = \sum_k m \cdot k = e = |E(G)|$$

\(^2\) Omega polynomial is defined on $ops$ as:

$$\Omega(G, X) = \sum_s m(G, s) \cdot X^s$$

where $m(G, s)$ is the number of opposite edge strips of length $s$. If $ops$ is an ocs, as in partial cubes, we can write the following counting polynomials:

$$\Omega(G, X) = \sum_k m \cdot X^k$$

$$Sd(G, X) = \sum_k m \cdot X^{e-k}$$

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$$\Pi(G, X) = \sum_k m \cdot k \cdot X^{e-k}$$

$\Omega(G, X)$ and $\Theta(G, X)$ count equidistant edges in $G$ while $Sd(G, X)$ and $\Pi(G, X)$, count non-equidistant edges. The first two polynomials are counted once for a strip while the last two are counted for each edge, so that the coefficients are multiplied with $k$.

In a counting polynomial, the first derivative (in $X=1$) defines the type of property which is counted. For the above polynomials they are:

$$\Omega'(G, 1) = \sum_k m \cdot k = e = |E(G)|$$
\[ Sd'(G,1) = \sum_k m \cdot (e - k) = Sd(G) \] (12)
\[ \Theta'(G,1) = \sum_k m \cdot k^2 = \theta(G) \] (13)
\[ \Pi'(G,1) = \sum_k m \cdot k \cdot (e - k) = \Pi(G) \] (14)

An index, called Cluj-Ilmenau \( CI(G) \), is defined on \( \Omega(G,X) \):
\[ CI(G) = \left\{ \left[ \Omega'(G,1) \right]^2 - \left[ \Omega'(G,1) + \Omega''(G,1) \right] \right\} \] (15)

3. Properties of counting polynomials

In general, \( k \) is different for the two pairs \( \{ \Omega(G,X) ; Sd(G,X) \} \) and \( \{ \Theta(G,X) ; \Pi(G,X) \} \).

**Proposition:** In partial cubes \( k \) takes the same value in the all above polynomials, meaning the opposite edge sets superimpose to the equidistant edge ones and ops is an ocs.

**Consequence:** In partial cubes \( CI(G) = \Pi(G) \). Applying definition (15), \( CI \) is calculated as:
\[ CI(G) = \left( \sum_c m \cdot c \right)^2 - \left[ \sum_c m \cdot c + \sum_c m \cdot c \cdot (c-1) \right] = e^2 - \sum_c m \cdot c^2 = \Pi(G) \] (16)

This is the case of cubic lattice (Figure 1b), of planar bipartite graphs, like those of acene or phenacene benzenoids, and also of some bipartite 3D structures, as that in Figure 2. However, in the bipartite cage in Figure 1a, ops is not an ocs, the two opposite red edges at the top and bottom, respectively, being not equidistant (see also Table 1).

One can reformulate (14) function of (11) and (13) to write:
\[ \Pi(G) = e^2 - \sum_c m \cdot c^2 = \left\{ \left[ \Omega'(G,1) \right]^2 - \Theta'(G,1) \right\} \] (17)

![Figure 2](image)

**Figure 2.** Bipartite, partial cubes: (a) five fold and (b) two fold symmetry, of the cage designed by sequence \( Du(Med(D)) \): \( v=32; \ e=60; \ f_3=30; \ \Omega(G,x) = 6X^{10}; \ \Pi(G,X) = 60X^{50}; \ CI(G) = \Pi(G) = 3000 \)
The first part of relation (17) and the last part of (16) as well, is just the formula proposed by John et al.\(^{15}\) to calculate the Khadikar’s \(PI=PI(G)\) topological index\(^{22}\) (which counts the non-equidistant edges in \(G\)). Note that our \(\Pi(G,X)\) equals \(PI(G)\) only in partial cubes, in part because the edge equidistance relation includes, besides parallel edges condition (\(op\) relation, (2)), a condition for perpendicular edges (tetrahedron condition):

\[
d(u, x) = d(u, y) = d(v, x) = d(v, y)
\]  

(18)

It is noteworthy that Ashrafi et al.\(^{23}\) was first who proposed a polynomial \(PI(G,X)\), of which first derivative (in \(X=1\)) eventually gives the Khadikar’s \(PI\) index. Differences in version of \(PI\) index calculation appeared also because of the \(min\)-condition put in evaluating the edge equidistance.\(^{24}\)

An interesting degeneracy of \(CI(G)\) and \(\Pi(G)\) may appear: the coefficients in the pair \(\{\Theta(G, X) ; \Pi(G, X)\}\) correspond to the product \(m \cdot k\) (as in \(\Omega(G, X)\), see relation (10)) but the exponents are such that \(\Pi(G) = CI(G)\). Examples are given for two bipartite tori, in Table 2.

**Table 2.** Polynomials of two bipartite tori showing degenerate \(CI(G)\) and \(\Pi(G)\) values

<table>
<thead>
<tr>
<th>Polynomial Index</th>
<th>Polynomial</th>
<th>Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\Omega = 12X^4 + 4X^{24})</td>
<td>(CI(G) = 18240)</td>
<td>(CI(G) = 52960)</td>
</tr>
<tr>
<td>(Sd = 4X^{120} + 12X^{140})</td>
<td>(Sd(G) = 2160)</td>
<td>(Sd(G) = 18240)</td>
</tr>
<tr>
<td>(\Theta = 48X^8 + 96X^{22})</td>
<td>(\Theta(G) = 2496)</td>
<td>(\Theta(G) = 52960)</td>
</tr>
<tr>
<td>(\Pi = 96X^{122} + 48X^{136})</td>
<td>(\Pi(G) = 2160)</td>
<td>(\Pi(G) = 2496)</td>
</tr>
</tbody>
</table>

It is easily seen that, for a single \(ops\), called Hamiltonian strip, by analogy to the path visiting once all the vertices of the graph, one calculates the polynomial:

\[
\Omega(G, X) = 1 \times X^8
\]  
and the index \(CI(G) = s^2 - (s + s(s - 1)) = s^2 - s^2 = 0\).

In tree graphs, the Omega polynomial is either not defined or it simply counts the non-opposite edges, being included in the term of exponent \(s=1\), thus: \(\Omega(G, X) = m \times X^1\); \(\Omega'(G, 1) = m \times 1 = e(G)\); \(CI(G) = m(m - 1) = e(e - 1) = \Pi(G)\), \(m\) being the number of edges in that tree graph. Also, \(PI(G) = (v - 1)(v - 2)\), a result known from Khadikar\(^{13}\) and \(e = v - 1\), the tree graphs being partial cubes. In such graphs, Omega and Theta polynomials show the same expression (compare (9) and (10)).

**4. Counting polynomials in crystal-like lattices**

Omega polynomial was thought to describe the covering of polyhedral nano-structures or the tiling of crystal-like lattices. In this section we present four infinite, periodic,
networks designed by using some operations on maps/nets.\textsuperscript{25-29} The first three nets are obtained by map operations applied on the Cube C, while the last one on the Icosahedron I.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Figure3.png}
\caption{Triple periodic lattice designed by $Le(C)$ and identifying $f_4$ faces.}
\end{figure}

By applying the leapfrog $Le$ and Chamfering $Q$ on the Cube, results in the repeat units illustrated in Figures 3a to 5a. Next, by iteratively identifying, faces of size (4,4) or (4,6) it results in various networks, even the starting object is one and the same (see the cases of $Q$-transformed objects).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Figure4.png}
\caption{By applying the leapfrog $Le$ and Chamfering $Q$ on the Cube, results in the repeat units illustrated in Figures 3a to 5a.}
\end{figure}
Figure 4. Triple periodic lattice designed by Q(C) and identifying $f_i$ faces.

Observe, the networks in Figures 3 to 5 are defined by eight units, to express their periodicity: the first two structures $Le_4(C(2,2,2))$ and $Q_4(C(2,2,2))$ are triple-periodic while the third, $Q_4,6(C(2,2,2))$ is only double-periodic. The analytical formulas were developed for either incomplete $(a,b,c)$, $a \geq b \geq c$ or complete $(a,a,a)$ cube lattice (see below).

$G=Le_4(C(a,b,c)); \ a \geq b \geq c$:

$$
\Omega(G, X) = 4 \sum_{i=1}^{c-1} X^{4ai+2i} + 2(b - c + 1)X^{(4a+2)c} + 4 \sum_{i=1}^{b-1} X^{4bi+2i} + 2(a - c + 1)X^{(4b+2)c} + 4 \sum_{i=1}^{h-1} X^{4ci+2i} + 2(a - b + 1)X^{(4c+2)b}
$$

$G=Le_4(C(a,a,a))$:

$$
\Omega(G, X) = 12 \sum_{i=1}^{a-1} X^{2i(2a+1)} + 6X^{2a(2a+1)}
$$

$\Omega(G, 1) = 12a^2(2a+1)$

$G=Q_4(C(a,b,c)); \ a \geq b \geq c$:

$$
\Omega(G, X) = 4abcX^6 + aX^{4bc+2b+2c} + bX^{4ac+2a+2c} + cX^{4ab+2a+2b}
$$

$G=Q_4(C(a,a,a))$:

$$
\Omega(G, X) = 4a^3X^6 + 3aX^{4a(a+1)}
$$

$\Omega(G, 1) = 12a^2(3a+1)$
\( Q_{4,6}(C(1,1,1)); v=32 \)
\( \Omega(C,X) = 4X^6 + 3X^8; Cl=1968 \)

\( Q_{4,6}(C(4,4,4)); v=1280 \)

\( Q_{4,6}(C(2,2,2)); v=192; (a) \)

\( Q_{4,6}(C(2,2,2)); v=192; (b,c) \)

Figure 5. Double periodic lattice designed by \( Q(C(a,b,c)) \) and identifying \( f_4 \) & \( f_6 \) faces.

\( G=Q_{4,6}(C(a,b,c)); a \geq b \geq c : \)

\[
\Omega(G,X) = 4 \sum_{i=1}^{b-1} X^{2((3c+1)i)} + 2(a-b+1)X^{2((3c+1)b)} +
4 \sum_{i=1}^{c-1} X^{2((2a+1)i)} + 2(b-c+1)X^{2((2a+1)c)} +
4 \sum_{i=1}^{c-1} X^{2((2b+1)i)} + 2(a-c+1)X^{2((2b+1)c)} + cX^{4ab+2a+2b}
\]

\( G=Q_{4,6}(C(a,a,a)):\)

\[
\Omega(G,X) = 4 \sum_{i=1}^{a-1} X^{2((3a+1)i)} + 8 \sum_{i=1}^{a-1} X^{2((2a+1)i)} + 2X^{2a(3a+1)} + 4X^{2a(2a+1)} + aX^{4a(a+1)}
\]

\[\Omega'(G,1) = 16a^2(2a+1)\]

Examples are given for each discussed lattice, both for polynomials and indices, in the tables below.
Table 3. Examples for $Le_4(C(a,b,c))$ lattice

<table>
<thead>
<tr>
<th>$Le_4(C(a,b,c))$_atoms</th>
<th>Omega polynomial</th>
<th>$CI$ _Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>111_24</td>
<td>$6X^0$</td>
<td>1080</td>
</tr>
<tr>
<td>222_144</td>
<td>$12X^{10}+6X^{20}$</td>
<td>54000</td>
</tr>
<tr>
<td>422_272</td>
<td>$4X^{10}+4X^{14}+4X^{18}+6X^{20}+6X^{28}+2X^{36}+2X^{44}$</td>
<td>363408</td>
</tr>
<tr>
<td>442_512</td>
<td>$4X^{14}+8X^{18}+4X^{28}+12X^{36}+4X^{42}+2X^{56}+2X^{80}$</td>
<td>1353664</td>
</tr>
<tr>
<td>444_960</td>
<td>$12X^{18}+12X^{36}+12X^{44}+6X^{72}$</td>
<td>2900448</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sadhana polynomial</th>
<th>$Sd$ _Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>111_24</td>
<td>$6X^{10}$</td>
</tr>
<tr>
<td>222_144</td>
<td>$6X^{220}+12X^{230}$</td>
</tr>
<tr>
<td>422_272</td>
<td>$2X^{572}+2X^{580}+6X^{588}+6X^{596}+4X^{598}+4X^{602}+4X^{606}$</td>
</tr>
<tr>
<td>442_512</td>
<td>$2X^{1104}+2X^{1128}+4X^{1142}+12X^{1148}+4X^{1156}+8X^{1166}+4X^{1170}$</td>
</tr>
<tr>
<td>444_960</td>
<td>$6X^{1656}+12X^{1674}+12X^{1692}+12X^{1710}$</td>
</tr>
</tbody>
</table>

Table 4. Examples for $Q_4(C(a,b,c))$ lattice

<table>
<thead>
<tr>
<th>$Q_4(C(a,b,c))$_atoms</th>
<th>Omega polynomial</th>
<th>$CI$ _Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>111_32</td>
<td>$4X^4+3X^6$</td>
<td>1968</td>
</tr>
<tr>
<td>222_208</td>
<td>$32X^2+6X^{24}$</td>
<td>108288</td>
</tr>
<tr>
<td>331_240</td>
<td>$36X^6+6X^{29}+1X^{48}$</td>
<td>141456</td>
</tr>
<tr>
<td>332_444</td>
<td>$72X^8+6X^{14}+2X^{48}$</td>
<td>521688</td>
</tr>
<tr>
<td>333_648</td>
<td>$108X^6+9X^{48}$</td>
<td>1141776</td>
</tr>
<tr>
<td>444_1472</td>
<td>$256X^8+12X^{48}$</td>
<td>6140000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sadhana polynomial</th>
<th>$Sd$ _Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>111_32</td>
<td>$3X^{40}+4X^{42}$</td>
</tr>
<tr>
<td>222_208</td>
<td>$6X^{312}+32X^{330}$</td>
</tr>
<tr>
<td>331_240</td>
<td>$X^{336}+6X^{364}+36X^{378}$</td>
</tr>
<tr>
<td>332_444</td>
<td>$2X^{584}+6X^{598}+72X^{726}$</td>
</tr>
<tr>
<td>333_648</td>
<td>$9X^{1032}+108X^{1074}$</td>
</tr>
<tr>
<td>444_1472</td>
<td>$12X^{2416}+256X^{2490}$</td>
</tr>
</tbody>
</table>

The last lattice (Figure 6) is constructed by identifying parts of the $Med(Med(IP))$, designed by applying twice the Medial $Med$ operation on the centered Icosahedron IP, so that the structure be periodic on the X-coordinate.

Table 5. Examples for $Q_4,6(C(a,b,c))$ lattice

<table>
<thead>
<tr>
<th>$Q_4,6(C(a,b,c))$_atoms</th>
<th>Omega polynomial</th>
<th>$CI$ _Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>222_192</td>
<td>$8X^{10}+4X^{14}+4X^{30}+2X^{34}+2X^{28}$</td>
<td>96496</td>
</tr>
<tr>
<td>422_360</td>
<td>$4X^{10}+4X^{14}+4X^{18}+6X^{20}+6X^{28}+2X^{36}+2X^{44}$</td>
<td>363408</td>
</tr>
<tr>
<td>442_672</td>
<td>$4X^{14}+8X^{18}+4X^{28}+12X^{36}+4X^{42}+2X^{56}+2X^{80}$</td>
<td>1353664</td>
</tr>
<tr>
<td>444_1280</td>
<td>$8X^{18}+4X^{26}+8X^{36}+4X^{32}+8X^{54}+4X^{72}+4X^{78}+4X^{40}+2X^{104}$</td>
<td>5166304</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sadhana polynomial</th>
<th>$Sd$ _Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>222_192</td>
<td>$2X^{292}+2X^{296}+4X^{300}+4X^{306}+8X^{310}$</td>
</tr>
<tr>
<td>422_360</td>
<td>$2X^{572}+2X^{580}+6X^{588}+6X^{596}+4X^{598}+4X^{602}+4X^{606}$</td>
</tr>
<tr>
<td>442_672</td>
<td>$2X^{1104}+2X^{1128}+4X^{1142}+12X^{1148}+4X^{1156}+8X^{1166}+4X^{1170}$</td>
</tr>
<tr>
<td>444_1280</td>
<td>$2X^{2200}+4X^{2224}+4X^{2226}+4X^{2232}+8X^{2250}+4X^{2252}+8X^{2268}+4X^{2278}+8X^{2280}$</td>
</tr>
</tbody>
</table>
Formulas for Omega polynomial are given as a function of the number of polytopes \( n \) consisting the periodic structure. The reader is invited to consult, in this respect, a recent paper of our group.\(^{30}\) Table 6 provides examples of polynomial and index calculations.

\[
\Omega(G, X, R < 6) = \left[ 120 + 90(n - 1) \right] X^2 + 10(n + 2)X^3 + 5(n - 1)X^4 + \left[ 12 + 11(n - 1) \right] X^5
\]

\[
\Omega(G, 1) = 105 + 285n; \quad \Omega'(G, 1) = 140 + 520n
\]

\[
CI(G) = 10780 + 59045n + 81225n^2
\]

\[
\Omega(G, X, R \geq 6) = 1X^{390n - 105(n - 1)}; \quad CI = 0; \quad \text{Hamiltonian ops}
\]

Note the difference in Omega polynomial function of the maximum ring size, in case of \( Med(Med(IP)) \) lattice: when ring \( R \geq 6 \), a unique strip is obtained, called here \( Hamiltonian \ ops \), because it visited once all the edges in the graph. Of course, in such a case, \( CI = 0 \).

### Table 6. Examples for \( Med(Med(IP)) \) lattice

<table>
<thead>
<tr>
<th>( n )</th>
<th>Omega polynomial</th>
<th>( CI )</th>
<th>Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( 120X^5 + 30X^4 + 12X^3 )</td>
<td></td>
<td>151050</td>
</tr>
<tr>
<td>2</td>
<td>( 210X^5 + 40X^4 + 5X^3 + 23X^2 )</td>
<td></td>
<td>453770</td>
</tr>
<tr>
<td>4</td>
<td>( 390X^5 + 60X^4 + 15X^3 + 45X^2 )</td>
<td></td>
<td>1546560</td>
</tr>
<tr>
<td>5</td>
<td>( 480X^5 + 70X^4 + 20X^3 + 56X^2 )</td>
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<tr>
<td>7</td>
<td>( 660X^5 + 90X^4 + 30X^3 + 78X^2 )</td>
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<table>
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<tr>
<th>( n )</th>
<th>Sadhana polynomial</th>
<th>( Sd )</th>
<th>Index</th>
</tr>
</thead>
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Figure 6. \( Med(Med(IP)) \); \( n \) (number of polytopes) = 4
Sadhana polynomial is immediately derived, keeping in mind its definition (relation 8) and that the first derivative of Omega polynomial in $X=1$ is just the number of edges in $G$. The other two polynomials $\Theta(G,X)$ and $\Pi(G,X)$ show, in general, more terms than the pair $\Omega(G,X)$ and $Sd(G,X)$ while the interpretation of relation polynomial-graph structure is rather laborious.

Calculation of polynomials and corresponding indices were performed on our original software Omega counter$^{31}$ and Nano_Studio.$^{32}$

5. Conclusions

Omega and three related counting polynomials were investigated in view of establishing mutual inter-relations. All these polynomials count sets of edges related to edge-cut procedures used for calculating some topological indices, such as Szeged and PI indices.

It was shown that the indices $CI(G)$ and $\Pi(G)$ show identical values in graphs embeddable in the hypercube. Examples of graphs showing $CI(G) = \Pi(G)$ and $CI(G) \neq \Pi(G)$, respectively, were presented.

Extension from faces to rings (namely strong rings, which are not the sum of other smaller rings) enabled calculation of $\Omega(G,X)$ in 3D networks. Analytical close formulas for Omega polynomial in some crystal-like lattices were derived.

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References