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Omega Polynomial in Puzzle Zeolites

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Abstract

The topology of puzzle-like zeolites is described in terms of Omega counting polynomial. Close formulas for calculating the polynomial and the Cluj-Ilmenau index derived from this polynomial are given.

1. Introduction

There are inorganic compounds of various classes including oxides, sulfides, selenides, borates, silicates, etc. of many metals possessing ordered structures at the nano-scale. In the last years, oxides and other above-mentioned inorganic substances found applications in the design of nanostructured functional materials as films, nanorods, porous systems, nanoclusters, nanocrystallites or nanofibers.[1-10]

Zeolites are natural or synthetic aluminosilicates with an open three-dimensional crystal structure. Zeolites are members of the family of microporous solids known as "molecular sieves." The term molecular sieve refers to the property of these materials to

This paper is dedicated to Professor Milan Randić, Drake University, Iowa, USA, for his bright contribution to the development of Chemical Graph Theory.

selectively sort molecules based primarily on a size exclusion process. This is due to a regular structure of pores, of molecular dimensions, forming channels. The maximum size of the molecular or ionic species that can enter the pores of a zeolite is controlled by the dimensions of the channels.[11-15]

The rigorous and often aesthetically appealing architecture of crystal lattices, attracted the interest of scientists in a broad area, from crystallographers, to chemists and mathematicians.[16-24] The studies on classification have been followed by studies on the usefulness, in chemical reactions or in physical devices, and more recently by applied mathematical studies, in an effort to give a new, more appropriate characterization of the world of crystals. Thus, recent articles in crystallography promoted the idea of topological description and classification of crystal structures.[16-21] They present data on real, but also hypothetical lattices designed by computer.

The present study is devoted to the study of a puzzle-like lattice of a hypothetical zeolite, by using a topological description in terms of the Omega counting polynomial.

2. Omega polynomial

Let $G(V,E)$ be a connected graph, with the vertex set $V(G)$ and edge set $E(G)$. Two edges $e = uv$ and $f = xy$ of G are called *codistant e co f* if they obey the following relation:[23,25]

$$d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y) \qquad (1)$$

Relation *co* is reflexive, that is, *e co e* holds for any edge e of G; it is also symmetric, if *e co f* then *f co e*. In general, relation *co* is not transitive, an example showing this fact is the complete bipartite graph $K_{2,n}$. If "*co*" is also transitive, thus an equivalence relation, then G is called a *co-graph* and the set of edges $C(e) := \{f \in E(G);\ f\ co\ e\}$ is called an *orthogonal cut oc* of G, $E(G)$ being the union of disjoint orthogonal cuts: $E(G) = C_1 \cup C_2 \cup ... \cup C_k$, $C_i \cap C_j = \varnothing$, $i \neq j$. Klavžar[26] has shown that relation *co* is a theta Djoković-Winkler relation.[27,28]

Let $e = uv$ and $f = xy$ be two edges of G which are *opposite* or topologically parallel and denote this relation by *e op f*. A set of opposite edges, within the same face/ring, eventually forming a strip of adjacent faces/rings, is called an *opposite* edge

strip ops, which is a quasi-ortogonal cut *qoc* (*i.e.*, the transitivity relation is not necessarily obeyed). Note that *co* relation is defined in the whole graph while *op* is defined only in a face/ring.

The *ops* relation has the properties: (i) any two subsequent edges of such a strip are in *op* relation; (ii) any three subsequent edges belong to adjacent (edge sharing) faces/ rings; (iii) the inner dual of an *ops* is a path or a cycle, thus neither revisiting nor branching is allowed.

An *ops* starts/ends in either one even face/ring or in two odd faces/rings; in the first case, the *ops* is a cycle while in the second one it is a path. In case of open structures, the open (or infinite) faces are equivalent to the odd faces. There are cases in which the two odd faces/rings superimpose and *ops* is a *pseudo* cycle, because the *op* relation in the first/last odd face/ring is not obeyed.[23]

The length of *ops* is maximal irrespective of the starting edge. The choice is about the maximum size of face/ring, and the mode of face/ring counting, which will decide the length of the strip. In case of ring mode counting, the procedure will search for the detour of the inner duals of *ops*.

Let $m(G,s)$ be the number of *ops* strips of length s. The Omega polynomial is defined as[29]

$$\Omega(G,x)=\sum_s m(G,s)\cdot x^s \tag{2}$$

The first derivative (in x=1) equals the number of edges in the graph

$$\Omega'(G,1)=\sum_s m(G,s)\cdot s=e=\left|E(G)\right| \tag{3}$$

A topological index, called Cluj-Ilmenau,[30] $CI=CI(G)$, was defined on Omega polynomial

$$CI(G)=\left\{[\Omega'(G,1)]^2-[\Omega'(G,1)+\Omega''(G,1)]\right\} \tag{4}$$

An example is given in Figure 1, which illustrates just the pattern of studied lattice.

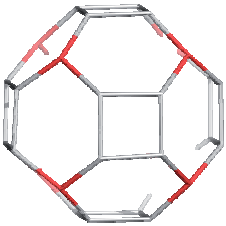

Figure 1. Q(C); v=32; $\Omega(G,X)=4X^6+3X^8$; $\Omega'(G,1)=48=e(G)$; $CI(G)=1968$

Data were calculated by an original program called Nano Studio,[31] developed at the TOPO Group Cluj.

3. Lattice building

The lattice was built up starting from the unit in Figure 1 (designed by applying the quadrupling/chamfering map operation[32-37] on the cube C), by identifying the hexagonal faces of six units, in a circular manner. Different views of circular/toroidal units, in various stacking can be seen in Figures 2 and 3.

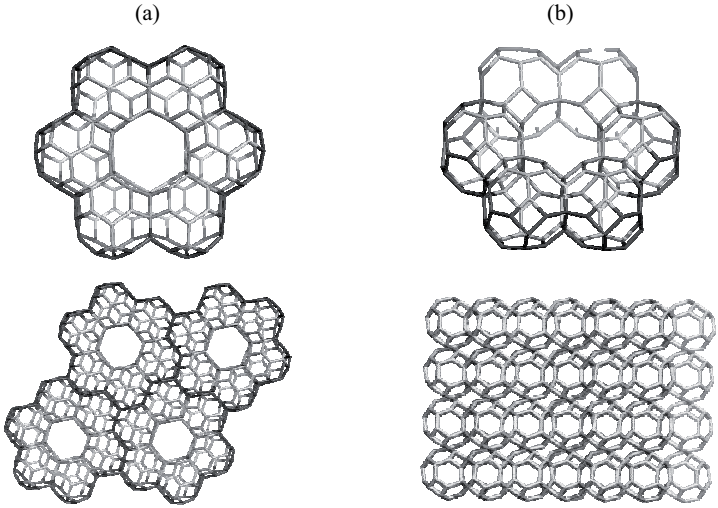

Figure 2. Circular units in the sheet-like stacking: top view (column a) and side view (column b).

It is easily seen that the puzzle-like stacking (either in sheet- of coronene-like manner) leaves channels/hollows parallel to the Z-coordinate, a required property of zeolites (see above).

4. Main results

In calculating Omega polynomial, the maximum considered ring R_{max} was six. Thus, squares and hexagons are counted in the *ops* appearing in these puzzle-like structures, as shown in Table 1. In coronene lattice CorL, there is no *ops* of length 18 (consisting by only hexagons) or 26 (mixed squares and hexagons); the number of *Q*(C) units is easily seen in Figures 2 and 3.

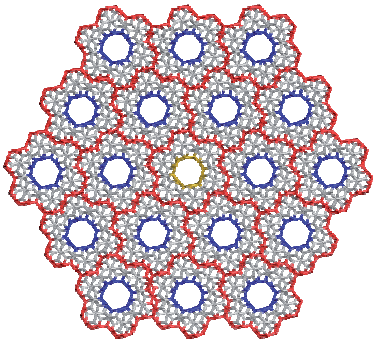

Figure 3. Toroidal units in the coronene-like stacking; u=19

Table 1. *ops* length in the lattice structures

Q(C) Units	1	2	3	4	5	6	Increment
Hexagons	6	10	14	18	22	26	+4
Squares & Hexagons	8	14	20	26	32	38	+6

In the opposite, the sheet-like stacking shows these *ops* provided by four *Q*(C) units.

Keeping in mind the data in Table 1 it is easily to derive the number of *ops* (i.e., the coefficients) of a given length (*i.e.*, the exponents). The lattice parameters (number of units u_{156} and vertices v) as well as the polynomial and *CI* index are given in the

following tables, for coronene-like CorL structures, sheet-like parallelogram domains and linear ones.

To calculate the number of vertices of coronene-like structures, a composition rule of the form: Core(k) & Contour(k+1) was used. In case of evaluating the maximum exponent of the polynomial, the simple planar coronene-like structure CorS was built up. The maximum length *ops* in the CorL structure is just the number of vertices in CorS. Next, for counting the number of vertices in CorL, the same composition rule was used; it follows the rule of construction by joining, by a simple formal bonding, the points of lower valence in the core and contour. Alternatively, the rule superimposes over the construction by identification of the core, at level k, with the contour in the next level k+1,to give the whole structure at k+1 level, the common points (namely 72(2k+1)) being taken only once (see Table 2).

Table 3 contains data for the sheet-like structures. Tables 2 and 3 also contain information about the (structural) source of the formulas for maximum exponents, finally included in the formula of Omega polynomial. Table 4 lists examples for the above formulas.

Table 2. Omega polynomial in puzzle-like lattice: coronenes.

Counting	Info source	Formula
e max	CoreS(k) + ContourS(k+1)	$e_{\max}(\mathrm{CorL}) = v(\mathrm{CorS})$
Polynomial		
CorL	$\Omega(\mathrm{CorL}, X) = 6(2k+1)X^6 + 6(2k+1)X^8 + 6X^{10} + 6(2k+1)X^{14} + 6(2k)X^{20}$	
	$+6(2k)X^{22} + 9k(k-1)X^{26} + 6(2k)X^{32} + 9k(k-1)X^{38} + X^{6(4+10k+7k^2)}$	
	$\Omega'(G,1) = 618k^2 + 708k + 252$; $\Omega''(G,1) = 1764k^4 + 5040k^3 + 24078k^2 + 9540k + 2700$;	
	$CI(\mathrm{CorL}) = 380160k^4 + 870048k^3 + 788040k^2 + 346584k + 60552$	
v		
ContourS		$v(\mathrm{ContourS}) = 120k;\ k = 0,1,2,..$
CorS	$24 + \sum_{i=1}^{k}\{120i - 9[4(i-1)+2]\}$	$v(\mathrm{CorS}) = 6(4 + 10k + 7k^2)$
ContourL		$v(\mathrm{ContourL}) = 2 \cdot 71 \cdot u(\mathrm{contourL}) = 852k$
CoreL	$84 + \sum_{i=2}^{k} 12\{6[9 + 10(i-2)] - i + k\}$	$v(\mathrm{CoreL}) = 156 - 426k + 354k^2$
CorL	CoreL(k) & ContourL(k+1)	$v(\mathrm{CorL}(k+1)) = 156 + 426k + 354k^2$
	CorL(k) & ContourL(k+1)	$v(\mathrm{CorL}(k+1)) = \mathrm{CorL}(k) + \mathrm{ContourL}(k+1) - 72(2k+1)$
u_{156}		
ContourL		$u(\mathrm{contourL}) = 6k$
CorL	$1 + \sum_{i=1}^{k} 6i$	$u(\mathrm{CorL}) = 1 + 3k + 3k^2$

Table 3. Omega polynomial in puzzle-like lattice: parallelograms and linear structures.

Counting	Info source	Formula
e max	$24+2\sum_{i=1}^{k}(14i+13)$	$24+40k+14k^2$
Polynomial		
Parallel-ogram structure	$\Omega(Parallel,X)=(6+8k)X^6+(6+8k)X^8+6X^{10}+(6+8k)X^{14}+2X^{18}+8kX^{20}$ $+(12+8(k-2))X^{22}+(4-6k+3k^2)X^{26}+(12+8(k-2))X^{32}+(2-6k+3k^2)X^{38}+X^{24+40k+14k^2}$	
	$\Omega'(G,1)=206k^2+472k+252$; $\Omega''(G,1)=196k^4+1120k^3+8426k^2+6360k+2908$ $CI(Parallel)=42240k^4+193344k^3+317976k^2+231056k+60344$	
Linear structure	$\Omega(Linear,X)=[6+4(k-1)]X^6+[6+4(k-1)]X^8+[6+2(k-1)]X^{10}+[6+4(k-1)]X^{14}$ $+(k-1)X^{18}+2(k-1)X^{20}+(k-1)X^{26}+X^{(20k+4)}$	
	$\Omega'(G,1)=236k+16$; $\Omega''(G,1)=400k^2+3108k-808$ $CI(Linear)=55296k^2+4208k+1048$	
v		
v(Parallel)	$156+\sum_{i=1}^{k-1}(236i+166)$	$v(\text{Parallel})=-10+48k+118k^2$
v(Linear)		$v(\text{Linear})=156+142k$

Table 4. Omega polynomial in puzzle-like lattice: examples.

k	Omega; CorL	CI	v
0	$6X^6+6X^8+6X^{10}+6X^{14}+1X^{24}$	60552	156
1	$18X^6+18X^8+6X^{10}+18X^{14}+12X^{20}+12X^{22}+12X^{32}+1X^{126}$	2445384	936
2	$30X^6+30X^8+6X^{10}+30X^{14}+24X^{20}+24X^{22}+18X^{26}+24X^{32}+18X^{38}+1X^{312}$	16948824	2424
	Omega; Parallel		
0	$6X^6+6X^8+6X^{10}+6X^{14}+1X^{24}$	60552	156
1	$14X^6+14X^8+6X^{10}+14X^{14}+3X^{18}+8X^{20}+2X^{22}+3X^{26}+2X^{32}+1X^{78}$	844856	558
2	$22X^6+22X^8+6X^{10}+22X^{14}+2X^{18}+16X^{20}+12X^{22}+4X^{26}+12X^{32}+2X^{38}+1X^{160}$	4016952	1196
	Omega; Linear		
0	$6X^6+6X^8+6X^{10}+6X^{14}+1X^{24}$	60552	156
1	$10X^6+10X^8+8X^{10}+10X^{14}+1X^{18}+2X^{20}+1X^{26}+1X^{44}$	230648	298
2	$14X^6+14X^8+10X^{10}+14X^{14}+2X^{18}+4X^{20}+2X^{26}+1X^{64}$	511336	440

The number of atoms in the lattice is function of the number of layers *s* and the toroidal units *u* (namely u_{156}) in the plane (*i.e*., the number of hollows):

$$v_s = sv_1 - (s-1)\cdot 6u \quad (5)$$

Omega polynomial coefficients of a given planar arrangement are simply multiplied by *s* in the multi-layer lattice to give the polynomial for the whole structure (Table 5).

Table 5. Multi-layer puzzle lattice: examples.

s	Omega; *u*=7(Cor)	*CI*	*v*
1	$18X^6+18X^8+6X^{10}+18X^{14}+12X^{20}+12X^{22}+12X^{32}+X^{126}$	2445384	936
2	$36X^6+36X^8+12X^{10}+36X^{14}+24X^{20}+24X^{22}+24X^{32}+2X^{126}$	9870936	1830
3	$54X^6+54X^8+18X^{10}+54X^{14}+36X^{20}+36X^{22}+36X^{32}+3X^{126}$	22276656	2724

5. Conclusions

The topology of puzzle-like lattices can be described by using the Omega counting polynomial. Close formulas for calculating the polynomial and the Cluj-Ilmenau index derived from this polynomial, as well as for the lattice parameters were given. It was proven that Omega polynomial is a useful tool for topological description of crystal-like lattices.

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