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CI INDEX IN TUBULAR NANOSTRUCTURES

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Abstract. A new topological index is proposed, on the ground of ***quasi-orthogonal cut "qoc"*** edge strips in a bipartite lattice. Within a *qoc* not all cut edges are necessarily orthogonal, meaning not all are pairwise ***codistant***. A topological index *CI* (Cluj-Ilmenau), eventually equal to the well-known *PI* index, in planar bipartite graphs, is defined and exemplified. Closed analytical formulas for *CI* in polyhex tubes and tori are given.

INTRODUCTION

Let G be a molecular graph, the vertex and edge sets of which being represented by $V(G)$ and $E(G)$ respectively.

The *PI* index was defined by Khadikar as:[1-3]

$$PI = PI(G) = \sum_{e \in E} [n_1(e) + n_2(e)] \tag{1}$$

where n_1 and n_2 denote the edges closer to the endpoint 1 and to the point 2, respectively of any edge e = (1,2) of G. Two edges e = (1,2) and e' = (1',2') of G are called *codistant* (briefly: $e\ co\ e'$) if for k = 0,1,2,… there exist the relations: d(1,1') = d(2,2') = k and d(1,2') = d(2,1') = k+1 or vice versa. For some edges of a bipartite connected graph G the following relations are satisfied:[4]

$$e\ co\ e \tag{2}$$

$$e\ co\ e' \Leftrightarrow e'\ co\ e \tag{3}$$

$$e\ co\ e'\ \&\ e'\ co\ e'' \Rightarrow e\ co\ e'' \tag{4}$$

though the relation (4) is not always valid. A simple counterexample is given in Figure 1.

Let $C(e) := \{e' \in E(G);\ e'\ co\ e\}$ denote the set of all edges of G which are codistant to the edge e. If all the elements of $C(e)$ satisfy the relations (2-4) then $C(e)$ is called an *orthogonal cut "oc"* of the graph *G*. The graph *G* is called *co-graph* if and only if the edge set *E*(*G*) is the union of disjoint orthogonal cuts: $C_1 \cup C_2 \cup ... \cup C_k = E$ and $C_i \cap C_j = \emptyset$ for $i \neq j$, $i, j = 1,2,...,k$.

If the graph is a cyclic one, the codistant edges to the both endpoints of any edge are not counted in calculating the *PI* index.

2D 3D

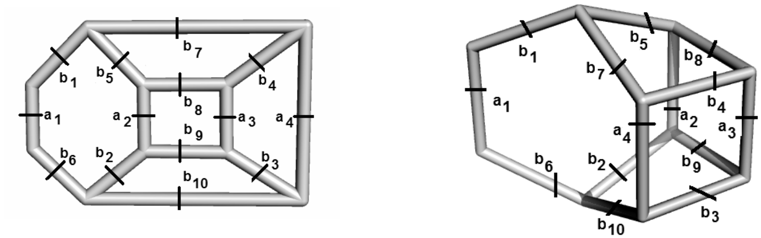

Figure 1. Codistant edges in a graph, *cf* relations (2 to 4): {a} is an *oc* strip; {b} does not have all elements codistant to each other (*e.g.*, b_1&b_5; b_7&b_{10}), so that {b} is a *qoc* strip (see text).

If *G* is a co-graph, the number of edges $m(G) = |E(G)|$ can be expressed as:

$$m(G) = n_1(e) + n_2(e) + m(C(e)) \tag{5}$$

with $m(C(e)) = |C(e)|$ being the cardinality or the *length* of the orthogonal cut $C(e) = \{e_i, e_j, ..., e_k\}$. Clearly, in a co-graph there exist more than one orthogonal cut edge sets. Eq (1) becomes:

$$PI(G) = \sum_{e \in E(G)} \{m(G) - m(C(e))\} = \sum_{e \in E(G)} m(G) - \sum_{e \in E(G)} m(C(e)) \tag{6}$$

$$PI(G) = m^2(G) - \sum_{C \in \underline{C}(G)} m^2(C) \tag{7}$$

where $\underline{C} = \underline{C}(G)$ is the set of all orthogonal cuts in *G*. Calculation of the *PI* index is exemplified on the phenylenic strip in Figure 2 (Note that the phenylenic strip is a co-graph).

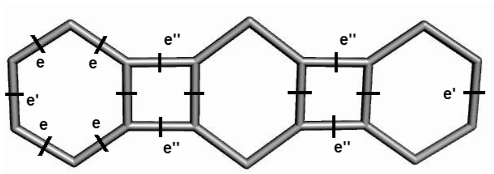

Figure 2. A phenylenic strip

The total number of edges is: $m = 8h - 2$, h being the number of hexagons. In the above example, $m(C(e)) = 2h\times(2)$, $m(C(e'\,)) = 1\times(2h)$ and $m(C(e''\,)) = (h\text{-}1)\times(2)$. This gives:

$$PI = (8h\text{-}2)^2 - [2h\times 2^2 + 1\times(2h)^2 + (h\text{-}1)\times 2^2] = 60h^2 - 44h + 8$$

CI INDEX

If any two consecutive edges of a cut edge sequence are codistant (obeying the relations (2) and (3)) and belong to one and the same face of the covering, such a sequence is called a *quasi-orthogonal cut "qoc"* strip. This means that the transitivity relation (4) is not necessarily obeyed.

A *qoc* strip starts and ends either out of *G* (at an edge with endpoints of degree lower than 3, if *G* is an open lattice) or in the same starting polygon (if *G* is a closed lattice). Any *oc* strip is a *qoc* strip but the reverse is not always true.

A new index, *CI* (Cluj-Ilmenau), eventually equal to *PI* in bipartite graphs embedded in the plane, is calculable, by a formula similar to that in (7), on the ground of the above *qoc* restriction, as:

$$CI(G) = m^2(G) - \sum_{Q\in \underline{Q}(G)} m^2(Q) \qquad (8)$$

with $\underline{Q} = \underline{Q}(G)$ being the set of all *qoc* strips in *G*. The index calculation for the graph in Figure 1 is:

$$\begin{aligned} CI(G) &= m^2 - times\times|\{a\}|^2 - times\times|\{b\}|^2 \\ &= 14^2 - 1\times 4^2 - 1\times 10^2 = 80 \end{aligned}$$

Note that the index *CI* equals the value of *PI* for the graph in Figure 2 ($CI = PI = 416$, for h=3) but not for that in Figure 1 ($PI = 138$).

CI INDEX IN POLYHEX TUBES AND TORI

(a) Armchair Tubes

In armchair tubes, as given in Figure 3a, the index is calculable by relation (9):

$$CI(TUV[2p,q]) = m^2(G) - C(G) - R(G) \qquad (9)$$

For all polyhex armchair tubes the circular term $C(G)$ (C-cut runs along the dark edges, in Figure 3a) is the same:

$$C(G) = 2p(q-1)^2 \qquad (10)$$

The radial term $R(G)$ varies function of the tube structure:

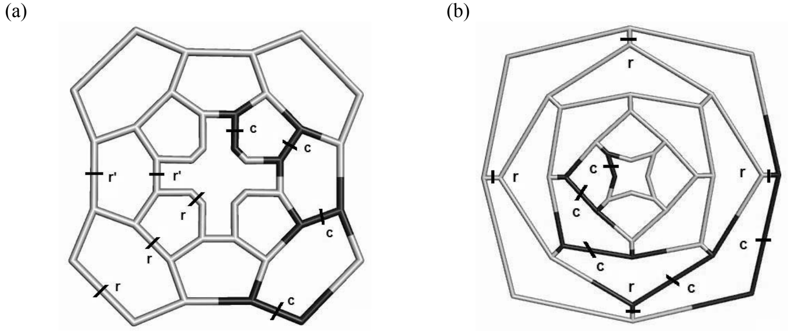

Figure 3. (a) Armchair tube TUV[2*p*,*q*]; *p*=4; *q*=5 (b) zig-zag tube TUH[2*p*,*q*]; *p*=4; *q*=5.

q = even:

$$R(G) = 2p(q/2)^2 = pq^2/2 \tag{11}$$

$$CI(TUV[2p,q_e]) = p^2(3q-2)^2 - 2p(q-1)^2 - pq^2/2$$
$$= 9p^2q^2 - 12p^2q + 4p^2 - (5/2)pq^2 + 4pq - 2p$$

q = odd:

$$R(G) = p((q+1)/2)^2 + p((q-1)/2)^2 = (p/2)(q^2+1) \tag{12}$$

$$CI(TUV[2p,q_o]) = p^2(3q-2)^2 - 2p(q-1)^2 - (p/2)(q^2+1) \tag{13}$$

$$= 9p^2q^2 - 12p^2q + 4p^2 - (5/2)pq^2 + 4pq - (5/2)p$$

With the number of edges being:

$$m(G) = p(3q-2) \tag{14}$$

(b) Tori H[*q*,2*p*]

Such tori correspond to "armchair" tubes, in the Schlegel-like projection,[5] resulting by identifying the points located on the central and peripheral levels ((Figure 3a, p=4; q=4). In such cases, q is always even; q-winding around the tube while p around the central hollow of the torus.

The radial term is the same for all the cases:

$$R(G) = 2p \cdot (q/2)^2 \tag{15}$$

and the circular term C vary as follows:

$$C(G) = k \cdot (2pq/k)^2 \tag{16}$$

with k being the greatest common divisor of q and $2p$.

The index is calculated as:

$$CI(H[q,2p]) = 9p^2q^2 - k(2pq/k)^2 - 2p(q/2)^2 = (18kp^2q^2 - 8p^2q^2 - kpq^2)/(2k) \quad (17)$$

with the number of edges:

$$m(\mathrm{H}[q,2p]) = 3pq \quad (18)$$

(c) Zig-zag Tubes

For zig-zag tubes, as given in Figure 3b, the index is calculable by relation (19):

$$CI(TUH[2p,q]) = m^2(G) - C(G) - R(G) \quad (19)$$

$$C(G) = (q-1)p^2 \quad (20)$$

$$R(G) = 2pq^2 \quad (21)$$

$$CI(TUH[2p,q]) = p^2(3q-1)^2 - (q-1)p^2 - 2pq^2 = 9p^2q^2 - 7p^2q + 2p^2 - 2pq^2 \quad (22)$$

with the number of edges being:

$$m(G) = p(3q-1) \quad (23)$$

(d) Tori V[*q*,2*p*]

The toroidal objects of this class correspond to "zig-zag" tube, in the Schlegel-like projection, from which are designed by identification of the points located on the central and peripheral levels (Figure 3b, p=4; q=4). The circular term is the same for all the cases:

$$C(G) = q \cdot p^2 \quad (24)$$

and the radial term R varies as follows:

$$R(G) = k \cdot (2pq/k)^2 \quad (25)$$

with k being as above.

The index is calculated as:

$$CI(V[q,2p]) = 9p^2q^2 - k(2pq/k)^2 - p^2q = (9kp^2q^2 - 4p^2q^2 - kp^2q)/k \quad (26)$$

With the number of edges:

$$m(\mathrm{V}[q,2p]) = 3pq \quad (27)$$

For the symbols of tubes and tori herein used, the reader is invited to consult refs. 6, 7.

CONCLUSIONS

A new index *CI* (Cluj-Ilmenau) was proposed to account for the opposite cuts in a bipartite lattice. It is related to the well-known *PI* index, with the main difference in definition of the quasi-orthogonal cut edge strips. These indices can be useful in correlating properties with molecular structures.[8]

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