Topological Indices of Line Graph of Metal Organic Compound

Muhammad Talha Farooq[1,2] and Pawaton Kaemawichanurat [1,2]

[1]Mathematics and Statistics with Applications (MaSA),

[2]Department of Mathematics, King Mongkut's University of Technology Thonburi, Bangkok, Thailand

Abstract:

The transition metal is a planar metallic organic structure, and tetra-cyano-benzene is one of the most studied networks of *3d* series of transition metal. Tetra-cyano-benzene behaved as a useful object in the alloy synthesis industry due to its excellency of hardness. Interestingly, the *TM –TCNB* systems are metallic in any event in one turn heading and show long-run ferromagnetic coupling on the off chance that for attractive structures, which speak to perfect applicants and a fascinating possibility of uncommon applications in spintronics. To study this, tetra-cyano-benzene structure we use an authentic mathematical tool known as vertex-edge and edge-vertex base topological indicators and shows some physical and chemical properties in numerical form, to understand the structure deeply. The topological indices are the numerical invariants of a molecular graph and are very useful for predicting their physical properties. Here, we calculate the degree based topological indices of line and paraline graph of Transition Metal Tetracyanobenzene $C_{10}H_2N_4[m,n]$ for $(m \times n)$ chain *2D* structure like general Randic index R_α for different values of $\alpha = (1,-1,1/2,-1/2)$, Geometric Arithmetic index, Forgotten topological index, first, second and third Zagreb index, Atom-bond connectivity index, first and second multiplicative Zagreb index, Symmetric division index, Sum-connectivity index, Reduced Reciprocal Randic index, first and second Gourava index, first and second Hyper-gourava index, first, second and third Reduced Zagreb index and Balban index for transition metal tetra-cyano benzene based on vertex-edge and edge-vertex degree.

Introduction:

The metal-organic networks transition metal of the three-dimensional series: *Ti, V, Cr, Fe, Co, Ni, Cu* or *Zn(TM)* tetracyanobenzene *(TCNB)* has a high melting and boiling point with low band energy which assist the electrical and thermal conductivity. Due to the finer size of $TM-TCNB$, it has more physical and mechanical qualities, such as good hardness, as a result, it is mostly employed in the alloy synthesis industry to refine high-temperature stability. Line graphs have been used in chemistry since the very beginning of structural chemistry. Bertz [1] was the first to suggest the use of line graphs of molecular graphs and their invariants for representing organic molecules physicochemical characteristics and also he established the first topological index based on a line graph in 1981, and further the idea of molecular branching and complexity. There are several topological indices based on the molecular graph's line graph. Line graphs were rarely employed in various mutually unrelated disciplines of chemistry.

Topological indices are generally classified into three categories degree-based, distance-based and spectrum-based. Wiener conceived the idea of first topological indices in 1947 while he determined the boiling point of paraffin [2]. After this he named this index "Wiener index". Then came the topological index theory. Now a days there are several topological indexes available like Randi´c Index, atom bond connectivity index, geometric arithmetic index and Zagreb index. The first Randi´c index of a chemical graph G is introduced by Randi´c in [3] 1975 this is the first and oldest degree based topological indices. Gutman [4] presented the first and second Zagreb indices in 1972.

References

1. *Bertz, S. H. (1981). The bond graph. Journal of the Chemical Society, Chemical Communications, (16), 818-820*
2. *Wiener, H. (1947). Structural determination of paraffin boiling points. Journal of the American chemical society, 69(1), 17-20.*
3. *Randic, M. (1975). Characterization of molecular branching. Journal of the American Chemical Society, 97(23), 6609-6615.*
4. *Gutman, I., & Trinajstic, N. (1972). Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons. Chemical physics letters, 17(4), 535-538.*