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A Study of Graph Invariants of Aramids

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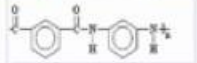
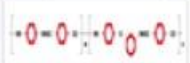
Aramids

- aromatic polyamide
- synthetic polymers formed from aromatic monomers

Examples:

Aramid	Kevlar	Nomax	Technora
Fiber			
Formation			

Applications:

- ✓ Ballistic protective applications
- ✓ Protective apparel
- ✓ motorcycle protective clothing
- ✓ Industrial and automotive applications
- ✓ Aircraft body parts
- ✓ Fibre optic and electromechanical cables
- ✓ Friction linings
- ✓ Gaskets for high temperature and pressure applications
- ✓ Adhesives and sealants
- ✓ Sails for boats

Objectives

- To derive M-Polynomials of aramids (Kevlar, Nomax and Technora) and derive First, Second and Modified Zagreb Indices (topological indices) of these aramids.
- To derive a formula for predicting melting points of aramids on the basis of calculated topological indices.

Experimental and Results/Discussion

Theorem

The M-polynomial of the Kevlar $k_{m,n}$ and Nomex $N_{m,n}$, $m \geq 2, n \geq 2$ are calculated and found to be the same. The M-polynomial expression found is given as follows:

$$M\left(k_{m,n}\right) = M\left(N_{m,n}\right) =$$

$$(3n + 3mn - m + 1)x^2y^2 + (6mn - 6n + 2m - 2)x^2y^3 + (3mn - 4m - 3n + 4)x^3y^3.$$

Proposition

The first, second and modified of Kevlar are computed from the M-polynomial as follows:

$$M_1 = 60mn - 36n - 18m + 18.$$

$$M_2 = 75mn - 51n - 28m + 28.$$

$$MM_2 = \left(\frac{25}{12}mn - \frac{7}{12}n - \frac{13}{36}m + \frac{13}{36}\right).$$

Theorem

The M-polynomial of the Technora are calculated as follows: $T_{m,n}$, $m \geq 3, n \geq 1$.

$$M\left(T_{m,n}\right) = (3n + 14mn - 4m + 1)x^2y^2 + (30mn - 4n + 8m - 54)x^2y^3 + (12mn - 16m - 3n + 4)x^3y^3.$$

Proposition

The first, second and modified Zagreb indices of Technora are computed from the M-polynomial as follows:

$$M_1 = 278mn - 26n - 72m - 242.$$

$$M_2 = 344mn - 39n - 112m - 284.$$

$$MM_2 = \left(\frac{59}{6}mn - \frac{21}{12}n - \frac{13}{9}m - \frac{299}{36}\right).$$

The M-polynomial and Topological indices of Kevlar, Nomex and Technora by using chemical graph.

Then Hosoya polynomial of Kevlar and Nomex.

Melting point of aramids using Zagreb indicies

The equation to predict melting points of Aramids using Zagreb indices becomes

$\alpha z_1 + \beta z_2 + \gamma z_m$ = Melting point

Melting point of Kevlar, Nomex and Technora are 350℃ ,500 ℃ and 250 ℃ putting value in above equation and solving the system of equation leads to the values of coefficient α, β and γ.

$\alpha = -325.593, \beta = 15.24, \gamma = 190.2.$

Melting points of other aramids can be obtained substituting Zagreb indices of that aramid in the formula:

$$-325.593M_1 + 15.24M_2 + 190.2MM_2$$

Ayesha Sattar, A Study of Topological Indices of Aramids, Thesis, National Textile Univsity, 2020.