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On Adriatic Indices and its Application to Some Properties of Alkanes

Ishwar Baidari[1], Preeti Savant[1,*] and Ashwini Yalnaik[2]

1 Department of Computer Science, Karnatak University, Dharwad, Karnataka, India.

2 Department of Mathematics, Karnatak University, Dharwad, Karnataka, India.

Abstract: The adriatic indices like max-min and min-max deg indices are defined by V.Damir and G.Marija. In this paper we have given certain generalization for some graphs and presented few bounds for these two indices. Along with that some graph operations has been performed like join and corona product. Lastly some chemical applications of max-min and min-max degree indices for alkanes are explored.

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Keywords: Adriatic indices, Heat of Atomization, Heat of Formation, Chemical trees.

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1. Introduction

Mathematical chemistry is the branch of theoretical chemistry in which mathematics is applied for mathematical modelling of chemical marvels. It is also called Computer chemistry and the main conceptions it involves are, molecular graph and topological index. One of the sub area of mathematical chemistry is chemical graph theory, which applies graph theory concepts to chemical phenomena, which has enormous applications in QSPR (Quantitative Structure-Property Relationships) [1]. Topological index is a numerical quantity acquired from graphical structure of chemical compound to assess the physico-chemical properties of these compounds where, assorted research in this area is done with respect to QSAR/QSPR study [2] [3]. There are many bond-additive descriptors, but our work is focused on two such descriptors known as, max-min degree index and min-max degree index. The max-min deg index of a graph $\mu_1(G)$ is defined as, [4]

$$\mu_1(G) = \sum_{uv\in E(G)} \frac{max\{d_u, d_v\}}{min\{d_u, d_v\}}.$$

The min-max deg index of a graph $\mu_2(G)$, is defined as,

$$\mu_2(G) = \sum_{uv\in E(G)} \frac{min\{d_u, d_v\}}{max\{d_u, d_v\}},$$

where d_u and d_v are degree of vertices u and v, (uv) is an edge belongs to edge set of graph $(E(G))$. The graphs considered here are simple, undirected and connected graphs. The *graph G* can be defined as collection of vertices and edges. Set

* *E-mail: savant.priti5@gmail.com*

of vertices and edges are represented by $V(G)$ and $E(G)$ respectively. The *degree* or *valancy* of vertex is the number of vertices that are incident to it. If each degree of a graph is same then it is known as *regular graph*. A graph whose all vertices degree is $n-1$ is called *Complete graph*, K_n. The *path*, P_n is a tree whose vertex degrees are either 1 or 2. The diameter of *star* is always 2 and central vertex has degree $n-1$ other are leaf nodes. Let G_1 and G_2 be two graphs, denoted by $G_1 + G_2$ the join of two graphs, which is obtained from G_1 and G_2 by joining every vertex of G_1 to that of G_2. The corona of two graphs G_1 and G_2 is the graph $G = G_1 \circ G_2$ formed from one copy of G_1 and $|V(G_1)|$ copies of G_2 where the i^{th} vertex of G_1 is adjacent to every vertex in the i^{th} copy of G_2 [5]. Here we consider the corona of $G \circ y(K_1)$, in particular, is the graph constructed from a copy of G and for each vertex $v \in V(G)$, the new vertices $u^{'}, v^{'}, \ldots, k^{'}$ and the pendent edge $vu^{'}, vv^{'}, \ldots, vk^{'}$ are added.

2. Adriatic Indices of Alkanes

In this article we present the association between max-min deg index and min-max deg index for some Alkanes. Alkanes belongs to the class of aliphatic hydrocarbons, whose structure is similar to tree structure in graph theory. So the structure can be classified into three types: path, star and general tree structure. The chemical tree involves four kinds of valancies 1, 2, 3, and 4. Let m and n be the number of edges and vertices respectively, and in tree $m = n-1$ [6]. And possible edges are: $E(G) = \{(m_{1,1}), (m_{1,2}), (m_{1,3}), (m_{1,4}), (m_{2,2}), (m_{2,3}), (m_{2,4}), (m_{3,3}), (m_{3,4}), (m_{4,4})\}$.

2.1. Max-min deg index

In the *path* the number of pendent edges are 2 and the number of non-pendent edges are $m-2$. The value of max-min deg index of pendent edges is 2 and non-pendent edges is $2/2 = 1$. Hence the max-min deg index of path can be generalized as, $\mu_1(P_n) = 4 + m - 2 = m + 2$. *Star* has vertices with degrees 1 and m, Therefore the max-min deg index of star is given as, $\mu_1(S_n) = m^2$. For chemical trees ten different kinds of edges are possible, which are mentioned above, whose vertex degrees are not more than 4. Hence this index for chemical trees can be generalized as follows:

$$\begin{aligned}\mu_1(T_n) &= \frac{4}{4}m_{4,4} + \frac{4}{3}m_{4,3} + \frac{4}{2}m_{4,2} + \frac{4}{1}m_{4,1} + \frac{3}{3}m_{3,3} + \frac{3}{2}m_{3,2} + \frac{3}{1}m_{3,1} + \frac{2}{2}m_{2,2} \\ &\quad + \frac{2}{1}m_{2,1} + \frac{1}{1}m_{1,1} \\ &= 1 \cdot (m_{4,4} + m_{3,3} + m_{2,2} + m_{1,1}) + 2 \cdot (m_{4,2} + m_{2,1}) + 4m_{4,1} + 3m_{3,1} \\ &\quad + 1.33m_{4,3} + 1.5m_{3,2}.\end{aligned}$$

2.2. Min-max deg index

The min-max deg index μ_2 of path graph is given as, $\mu_2(P_n) = m - 1$. One can observe that min-max deg index of Star is, $\mu_2(S_n) = 1$. Similarly like previous index, μ_2 for chemical trees can be given as,

$$\begin{aligned}\mu_2(T_n) &= 1m_{1,1} + 0.5m_{1,2} + 0.33m_{1,3} + 0.25m_{1,4} + 1m_{2,2} + 0.66m_{2,3} + 0.5m_{2,4} + 1m_{3,3} \\ &\quad + 0.75m_{3,4} + 1m_{4,4} \\ &= 1(m_{1,1} + m_{2,2} + m_{3,3} + m_{4,4}) + 0.5(m_{1,2} + m_{2,4}) + 0.33m_{1,3} + 0.25m_{1,4} \\ &\quad + 0.66m_{2,3} + 0.75m_{3,4}.\end{aligned}$$

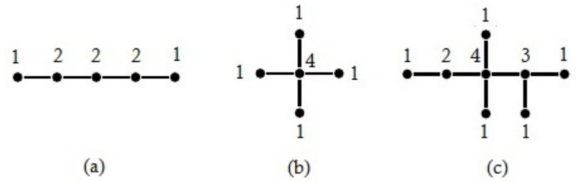


Figure 1: Types of tree structures in Alkane: (a) path, (b) star (c) chemical tree, with degree of each vertex.

3. Main Results

Theorem 3.1. *Let T be tree then,*

$$M_2(P_n) - 3(m-2) \leq \mu_1(T) \leq m^2. \tag{1}$$

$$1 \leq \mu_2(T) \leq M_2(P_n) - 3m + 3. \tag{2}$$

Proof. We know that in trees, $m = n+1$ is true, for equation (1), $M_2(P_n)$ and $\mu_1(P_n)$ end edge values are same and every other values differ by 3 so, path of max min degree in terms of second Zagreb index is given as $M_2(P_n) - 3(m-2)$. As the complexity of connectivity increases, $\mu_1(T)$ raises, therefore left side inequality holds. Where as for S_n, μ_1 is m times m hence its values is always greater than other trees, this satisfies right inequality. For equation (2), the left inequality holds if $n > 3$ because $\mu_2(S_n)$ is always one and $\mu_2(T)$ varies due to distinct degrees of vertices in a graph. In P_n, pendent edge value is twice $1/2$ and 2, for alternative edge values are 1 and 4 for μ_2 and M_2 respectively. The right inequality holds due to greater degrees of trees than path. For both equations equality restriction holds if $n = 2$ and 3. □

Theorem 3.2. *For any regular graph G,*

$$\mu_1 = \mu_2 = \frac{nr}{2}$$

Proof. The degrees in regular graphs is same so, from definition (1) and (2) we get mentioned results. □

Corollary 3.3. *For cycle and complete graph μ_1 and μ_2 is,*

$$\mu_1(C_n) = \mu_2(C_n) = n.$$
$$\mu_1(K_n) = \mu_2(K_n) = \frac{n(n-1)}{2}.$$

Theorem 3.4. *Let P_{n_1} and P_{n_2} be two paths with $n_1 > n_2 \geq 2$. then join of these is given as,*

$$\mu_1(P_{n_1} + P_{n_2}) = \frac{a^3b^2 + a^3b + 4a^2b^2 + 6a^2b + ab^3 + 4ab^2 + 7ab - 4a + b^3 + 3b^2 + 8b}{(a+1)\cdot(b+1)\cdot(b+2)}.$$

$$\mu_2(P_{n_1} + P_{n_2}) = \frac{a^3b + 2a^3 + a^2b^3 + 5a^2b^2 + 7a^2b + ab^3 + 7ab^2 + 8ab - 10a - 10b - 24}{(a+2)\cdot(b+2)\cdot(a+1)}.$$

Proof. Consider paths P_{n_1} and P_{n_2}, where $|P_{n_1}| = a$, $|P_{n_2}| = b$ and each vertex set consists of 2 pendent vertices and $n-2$ non pendent vertices. For P_{n_1} degree of 2 vertices is $b+1$ rest are $b+2$. similarly for P_{n_2} degree of 2 vertices is $a+1$

rest are $a+2$. For max-min deg index,

$$\mu_1(P_{n_1}+P_{n_2}) = 2\cdot\frac{(a+2)}{(a+1)} + (a-3)\cdot\frac{(a+2)}{(a+2)} + 2\cdot\frac{(b+2)}{(b+1)} + (b-3)\cdot\frac{(b+2)}{(b+2)} + 4\cdot\frac{(a+1)}{(b+1)}$$

$$+ (a-2)\cdot(b-2)\cdot\frac{(a+2)}{(b+2)} + 2\cdot(b-2)\frac{(a+2)}{(b+1)} + 2\cdot(a-2)\cdot\frac{(a+1)}{(b+2)}$$

$$= \frac{(2a+4)}{(a+1)} + a - 3 + \frac{(2b+4)}{(b+1)} + b - 3 + \frac{4a+4}{(b+1)} + \frac{(a+2)\cdot(a-2)\cdot(b-2)}{(b+2)}$$

$$+ \frac{2\cdot(a+2)\cdot(b-2)}{(b+1)} + \frac{2\cdot(a-2)\cdot(a+1)}{(b+2)}$$

$$= \frac{a^2b+ab^2+a+b^2+b+2}{(a+1)\cdot(b+1)} + \frac{4\cdot(a+1)}{b+1} + \frac{(a+2)\cdot(a-2)\cdot(b-2)}{b+2}$$

$$+ \frac{2\cdot(a+2)\cdot(b-2)}{(b+1)} + \frac{2\cdot(a-2)\cdot(a+1)}{(b+2)}$$

$$= \frac{a^3b^2 - a^3b - 2a^3 + 4a^2b^2 + 6a^2b + ab^3 + 4ab^2 + 13ab + 2a + b^3 + 3b^2 + 12b + 4}{(a+1)\cdot(b+1)\cdot(b+2)}$$

$$+ \frac{2\cdot(a-2)\cdot(a+1)}{(b+2)}$$

$$= \frac{a^3b^2 + a^3b + 4a^2b^2 + 6a^2b + ab^3 + 4ab^2 + 7ab - 4a + b^3 + 3b^2 + 8b}{(a+1)\cdot(b+1)\cdot(b+2)}.$$

For min-max deg index,

$$\mu_2(P_{n_1}+P_{n_2}) = \frac{2\cdot(a+1)}{(a+2)} + (a-3) + \frac{2\cdot(b+1)}{(b+2)} + (b-3) + \frac{4\cdot(b+1)}{(a+1)} + \frac{(a-2)\cdot(b-2)\cdot(b+2)}{(a+2)}$$

$$+ \frac{2\cdot(b-2)\cdot(b+1)}{(a+2)} + \frac{2\cdot(a-2)\cdot(b+2)}{(a+1)}$$

$$= \frac{2a+2}{(a+2)} + a - 3 + \frac{2b+2}{(b+2)} + b - 3 + \frac{4b+4}{(a+1)} + \frac{(a-2)\cdot(b-2)\cdot(b+2)}{(a+2)}$$

$$+ \frac{2\cdot(b+1)\cdot(b-2)}{(a+2)} + \frac{2\cdot(a-2)\cdot(b+2)}{(a+1)}$$

$$= \frac{a^3b + 2a^3 + a^2b^3 + 3a^2b^2 - a^2b - 8a^2 + ab^3 + 7ab^2 + 8ab - 10a + 8b^2 + 22b + 8}{(a+2)\cdot(b+2)\cdot(a+1)}$$

$$+ \frac{2\cdot(a-2)(b+2)}{(a+1)}$$

$$= \frac{a^3b + 2a^3 + a^2b^3 + 5a^2b^2 + 7a^2b + ab^3 + 7ab^2 + 8ab - 10a - 10b - 24}{(a+2)\cdot(b+2)\cdot(a+1)}.$$

□

Theorem 3.5. *Let P_{n_1} and R_n be path and regular graph then join of these becomes,*

$$\mu_1(P_n+R_n) = \frac{b^4 + 2b^3 + 2b^2a^2 + 2b^2ar + 2b^2a - 3b^2 + 2ba^2 + 2bar + 10ba + 4br - 4b + 4a + 4}{2\cdot(b+1)\cdot(b+2)}.$$

$$\mu_2(P_n+R_n) = \frac{3b^3a + b^3r + 9b^2a + b^2r - 4b^2 + 2ba^2 + 2abr + 4ab - 4br - 8b + 4a^2 + 4ar - 8a - 8r}{2\cdot(b+2)\cdot(a+r)}.$$

Proof. The $|P_n| = a$, $|R_n| = b$ and r be the regularity, the degrees vertices in P_n are $b+1$ for pendent vertices, $b+2$ for non pendent vertices and for R_n is $r+a$. Hence max-min deg index becomes,

$$\begin{aligned}\mu_1(P_n+R_n) &= \frac{2\cdot(b+2)}{b+1}+a-3+\frac{b\cdot(b-1)}{2}+\frac{2b\cdot(r+a)}{b+1}+\frac{b(a-2)\cdot(r+a)}{b+2}\\ &= \frac{b^3+2ba-3b+2a+2}{2\cdot(b+1)}+\frac{2b\cdot(a+r)}{b+1}+\frac{b\cdot(a-2)\cdot(a+r)}{b+2}\\ &= \frac{b^4+2b^3+2b^2a^2+2b^2ar+2b^2a-3b^2+2ba^2+2bar+10ba+4br-4b+4a+4}{2\cdot(b+1)\cdot(b+2)}.\end{aligned}$$

For min-max deg index

$$\begin{aligned}\mu_2(P_n+R_n) &= \frac{2\cdot(b+1)}{b+2}+a-3+\frac{b\cdot(b-1)}{2}+\frac{2b\cdot(b+1)}{r+a}+\frac{b\cdot(a-2)\cdot(b+2)}{r+a}\\ &= \frac{ba-b+2a-4}{b+2}+\frac{b\cdot(b+1)}{2}+\frac{2b\cdot(b+1)}{a+r}+\frac{b\cdot(a-2)\cdot(b+2)}{a+r}\\ &= \frac{3b^3a+b^3r+9b^2a+b^2r-4b^2+2ba^2+2abr+4ab-4br-8b+4a^2+4ar-8a-8r}{2\cdot(b+2)\cdot(a+r)}.\end{aligned}$$

□

Corollary 3.6. *Let P_n and C_n be path and cycle. Then*

$$\mu_1(P_n+C_n)=\frac{b^3+b^2a^2+3b^2a+2b^2+ba^2+7ab+5b+2a+2}{(b+1)\cdot(b+2)}$$

$$\mu_2(P_n+C_n)=\frac{b^3a+5b^2a+ba^2+7ba-2b+2a^2-8}{(b+2)\cdot(a+2)}$$

Corollary 3.7. *Let P_n and K_n be path and complete graph. Then*

$$\mu_1(P_n+K_n)=\frac{b^4+2b^3a+2b^3+2a^2b^2+2b^2a+b^2+2a^2b+8ab+4a-8b+4}{2\cdot(b+1)\cdot(b+2)}$$

$$\mu_2(P_n+K_n)=\frac{b^4+3b^2a+11b^2a-9b^2+2a^2b+6ab-12b+4a^2-12a+8}{2\cdot(b+2)\cdot(a+b-1)}$$

Theorem 3.8. *Let R be a regular graph then, μ_1 and μ_2 of corona of R and y times K_1 is,*

$$\mu_1(R\circ y(K_1))=\frac{nr+2ny(r+y)}{2}.$$

$$\mu_2(R\circ y(K_1))=\frac{nr^2+2ny+nry}{2(r+y)}.$$

Proof. Let r be a degree of R and K_1 be the trivial graph. The leaf nodes are represented by ny and degree of its adjacent vertices is $r+y$, where $nr/2$ is number of edges in R. Therefore,

$$\begin{aligned}\mu_1(R\circ y(K_1)) &= ny(r+y)+\frac{nr}{2}\\ &= \frac{nr+2ny(r+y)}{2}.\\ \mu_2(R\circ y(K_1)) &= \frac{ny}{r+y}+\frac{nr}{2}\\ &= \frac{nr^2+2ny+nry}{2(r+y)}.\end{aligned}$$

□

Corollary 3.9. *For μ_1 and μ_2 of corona of C_n and $y(K_1)$ is,*

$$\mu_1(C_n \circ y(K_1)) = n(y+1)^2.$$

$$\mu_2(C_n \circ y(K_1)) = \frac{2n(y+1)}{y+2}.$$

Corollary 3.10. *For μ_1 and μ_2 of corona of K_n and $y(K_1)$ is,*

$$\mu_1(K_n \circ y(K_1)) = \frac{n(2y^2 - 2y + 2ny + n - 1)}{2}.$$

$$\mu_2(K_n \circ y(K_1)) = \frac{n(n^2 + y + ny - 2n + 1)}{2(n+y-1)}.$$

4. Correlation Between μ_1, μ_2 with Properties of Alkanes

This section comprises of linear regression analysis of μ_1 and μ_2 with π-electronic energy E_π, Heat of Atomization ΔH_a and Heat of Formation ΔH_t. Table 1 represents experimental values of E_π, ΔH_a, ΔH_t and index values μ_1, μ_2 and also the product of two indices ($\mu_2 * \mu_2$) of alkanes are listed. Table 2 and 3 depicts the statistical outcome like, coefficient of determination (R^2); standard error of the estimate (S) and regression expression, of linear regression analysis of figure 2 and 3 respectively.

Molecule	μ_1	μ_2	$\mu_1 * \mu_2$	E_π	ΔH_a	ΔH_t
Propane	4	1	4	2.828427	955.49	24.82
2-Methylbutane	9.5	1.83	17.385	5.226252	1518.57	36.92
2,3-Dimethylbutane	13	2.33	30.29	6	1799.63	42.49
2,4-Dimethylpentane	15	2.67	40.05	6.828427	2080.92	48.3
3,3-Diethylpentane	16	4	64	10.472136	2639.05	55.81
3,3-Dimethylpentane	16	2.5	40	7.595865	2080.81	48.17
2,5-Dimethylhexane	16	3.67	58.72	8.472136	2361.33	53.21
2,2-Dimethylpentane	17	2.75	46.75	6.720566	2081.91	49.29
2,2,3-Trimethylpentane	17	3.5	59.5	8.519258	2360.73	52.61
2,3,3-Trimethylpentane	19.33	2.92	56.4436	8.375131	2359.85	51.73
3,3-Dimethylhexane	19.83	3	59.49	8.261125	2360.73	52.61

Table 1: Max-min deg index (μ_1), min-max deg index (μ_2), product of values of these two indices ($\mu_2 * \mu_2$), $\pi-$ electronic energy (E_π), heat of atomization (ΔH_a), heat of formation (ΔH_t) of alkanes.

The values of $\pi-$electrnic energy is evaluated using MathChem, an open source Python package for calculating topological indices [7] and Heat of Atomization, Heat of Formation are taken from the book Molecular Connectivity in Chemistry and Drug Research [8].

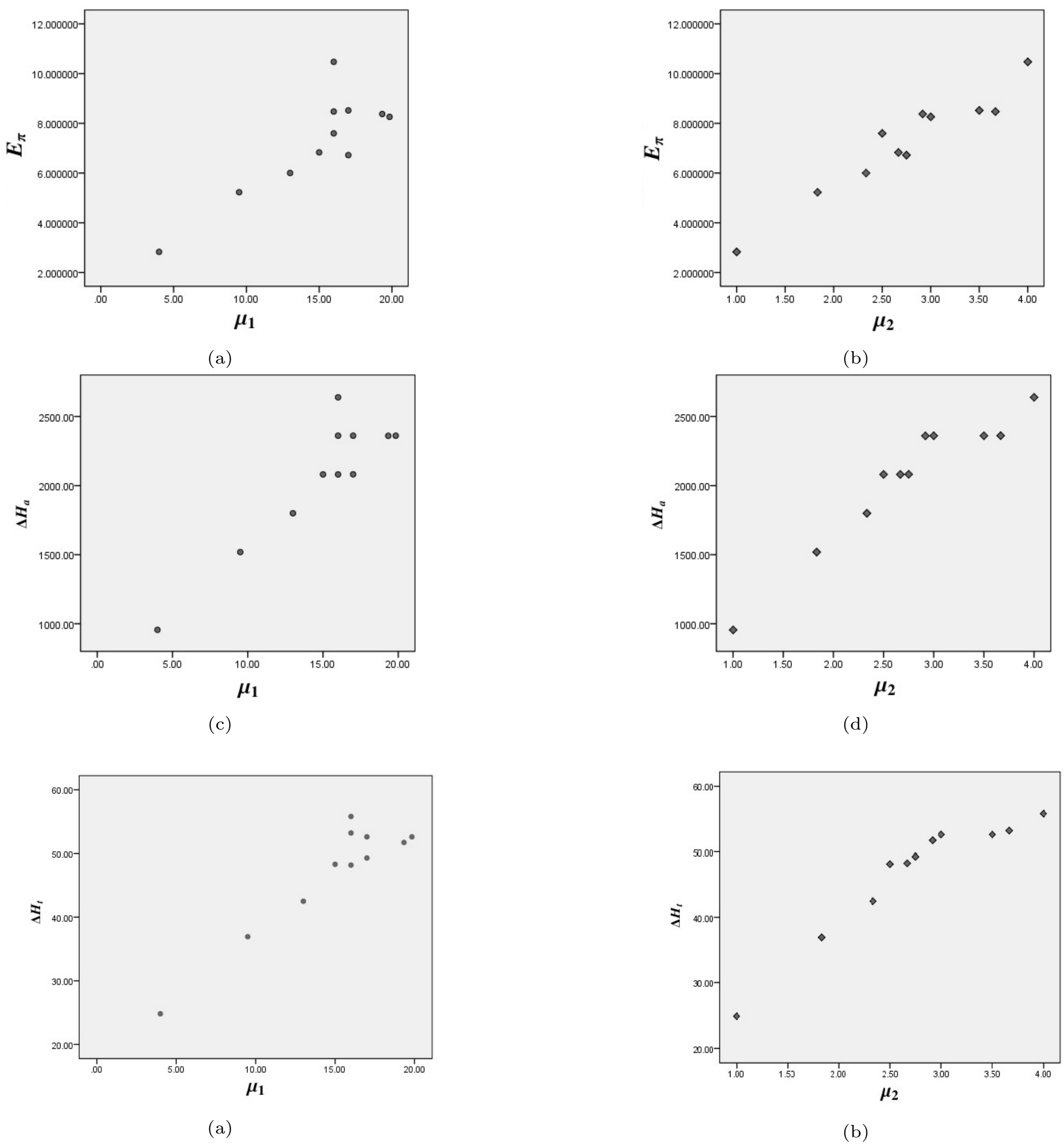
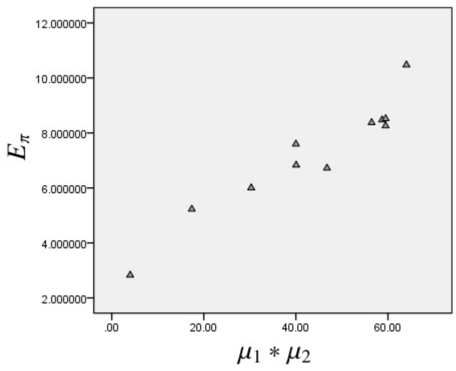


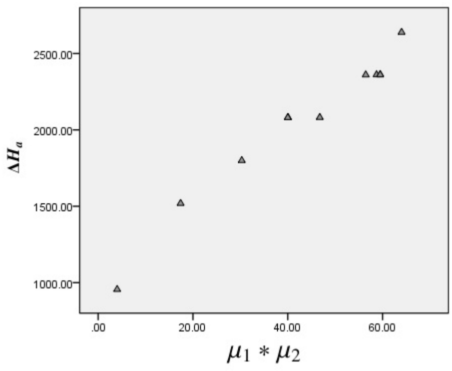
Figure 2: Illustration of the linear regression analysis of π-electronic energy, E_π; heat of atomization, ΔH_a and heat of formation, ΔH_t with max-min μ_1 and min-max μ_2 deg index.

Figure	Index	Property	R^2	S	Expression
(a)	μ_1	E_π	0.708	1.16	$E_\pi = (0.376 \pm .080)\mu_1 + (1.646 \pm 1.241)$
(b)	μ_2	E_π	0.921	0.603	$E_\pi = (2.305 \pm .0.225)\mu_2 + (0.887 \pm 0.643)$.
(c)	μ_1	ΔH_a	0.839	202.0	$\Delta H_a = (95.888 \pm 14.011)\mu_1 + (636.470 \pm 215.954)$
(d)	μ_2	ΔH_a	0.918	144.14	$\Delta H_a = (538.974 \pm 53.719)\mu_2 + (576.362 \pm 153.597)$
(e)	μ_1	ΔH_t	0.878	3.335	$\Delta H_t = (1.865 \pm 0.231)\mu_1 + (19.319 \pm 3.566)$
(f)	μ_2	ΔH_t	0.889	33.18	$\Delta H_t = (10.086 \pm 1.185)\mu_2 + (19.245 \pm 3.389)$

Table 2: Regression analysis details of figure 2.



(a)



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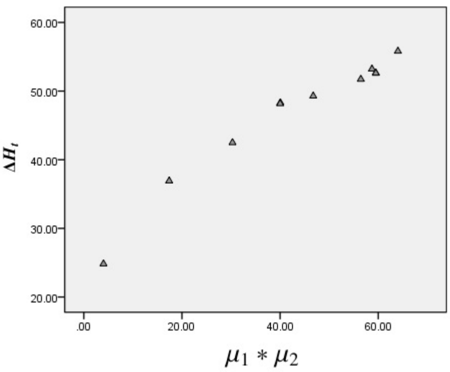

(c)

Figure 3: Illustration of correlation of E_π, ΔH_a, ΔH_t with product of values of two indices i.e ($\mu_1 * \mu_2$) of alkanes.

Index	Property	R^2	S	Expression
$\mu_1 * \mu_2$	E_π	0.910	0.644	$E_\pi = (0.10 \pm 0.01)(\mu_1 * \mu_2) + (2.877 \pm 0.494)$
$\mu_1 * \mu_2$	ΔH_a	0.963	97.43	$\Delta H_a = (24.08 \pm 1.584)(\mu_1 * \mu_2) + (1011.02 \pm 74.669)$
$\mu_1 * \mu_2$	ΔH_t	0.942	2.294	$\Delta H_t = (0.453 \pm 0.37)(\mu_1 * \mu_2) + (27.276 \pm 1.759)$

Table 3: Report of linear regression analysis of figure 3.

5. Conclusion

In this work we made an attempt to correlate two degree based adriatic indices with π electronic energy, heat of atomization and heat of formation of alkanes. The bounds and explicit formulas for their values under some graph operations are presented.

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