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Chemical Applicability of Second Ordered First and Second Gourava Indices

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ABSTRACT

In this note, we introduce the higher-ordered first and second Gourava indices of a molecular graph. In particular, we compute the second ordered first and second Gourava indices of some standard class of graphs and line graph of subdivision graph of 2D-lattice, nanotube and nanotorus of $TU\ C_4C_8[p,q]$. Furthermore, we study the linear regression analysis of the second ordered first and second Gourava indices with the entropy, acentric factor, enthalpy of vaporization and standard enthalpy of vaporization of an octane isomers.
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Keywords: Topological indices; Line graph; Subdivision graph; Nanostructure

1 INTRODUCTION

Chemical graph theory is a branch of mathematical chemistry, which has significant impact on the improvement of the chemical sciences. In molecular graph, graph is used to represent a molecule by considering the atoms as the vertices and molecular bonds as the edges. A topological index is a molecular descriptor that is determined based on the molecular graph of a chemical compound. For more details on topological indices refer [1–6]. Let $G=(V,E)$be such a graph with V as vertex set and E as edge set and $|V|=n, |E|=m$. The degree $d_G(v)$ of a vertex $v \in V(G)$ is the number of edges incident to it in G.

V. R. Kulli [7] introduced the first and second Gourava indices of a molecular graph as follows

$$GO_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v) + (d_G(u) \cdot d_G(v))] \tag{1.1}$$

$$GO_2(G) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v)) \cdot (d_G(u) \cdot d_G(v))] \tag{1.2}$$

Motivated by the chemical applications of higher-ordered connectivity index (or Randić index) [8], we introduce the higher-ordered first and second Gourava indices of Eqs. (1.1) and (1.2) as

$$^{\alpha}GO_1(G) = \sum_{u_1 u_2 \cdots u_{\alpha+1} \in E_\alpha(G)} [d_G(u_1) + d_G(u_2) \cdots + d_G(u_{\alpha+1})) \quad + (d_G(u_1) \cdot d_G(u_2) \cdots d_G(u_{\alpha+1}))] \tag{1.3}$$

$$^{\alpha}GO_2(G)=\sum_{u_1u_2\cdots u_{\alpha+1}\in E_\alpha(G)}\left[\left(d_G(u_1)+d_G(u_2)\cdots+d_G(u_{\alpha+1})\right)\quad\cdot\left(d_G(u_1)\cdot d_G(u_2)\cdots d_G(u_{\alpha+1})\right)\right]. \tag{1.4}$$

Here, E_α (G) denote the path of lengthα in a graph G, for example E_1 (G) and E_2 (G) are path of length 1 and 2 in a graph G respectively.

By putting $\alpha=2$ in Eqs. (1.3) and (1.4), we get the second ordered first and second Gourava indices as follows

$$^{2}GO_1(G)=\sum_{u_1u_nu_2\in E_n(G)}\left[d_G(u_1)+d_G(u_2)+d_G(u_3)\quad+\left(d_G(u_1)\cdot d_G(u_2)\cdot d_G(u_3)\right)\right] \tag{1.5}$$

$$^{2}GO_2(G)=\sum_{u_1u_nu_{\mathrm{R}}\in E_2(G)}\left[\left(d_G(u_1)+d_G(u_2)+d_G(u_3)\right)\quad\cdot\left(d_G(u_1)\cdot d_G(u_2)\cdot d_G(u_3)\right)\right]. \tag{1.6}$$

2 ESTIMATING THE SECOND ORDERED FIRST AND SECOND GOURAVA INDICES OF GRAPHS

In this section, we compute the second ordered first and second Gourava indices of path graph, wheel graph P_n, complete bipartite graph W_{n+1} and $K_{r,s}$ and r - regular graphs. Also, obtained bounds in terms of minimum vertex degree, size and order.

Remark 2.1. [9] For a graph G on m edges, the number of paths of length 2 in G is $-m+\frac{1}{2}M_1(G)$.

Theorem 2.1. Let P_n be the path on $n\geq 4$ vertices. Then

$^{2}GO_1(P_n)=14n-38$

$^{2}GO_2(P_n)=48n-152.$

Proof. For a path P_n on $n\geq 4$ vertices each vertex is of degree either 1 or 2. The partition of $E_2(P_n)$ is given as follows:

$$\left|E_{(1,2,2)}\right|=\left|u_1u_2u_3\in E_2(P_n):d_{p_n}(u_1)=1,d_{p_n}(u_2)=2,d_{p_n}(u_3)=2\right|=2,$$
$$\left|E_{(2,2,2)}\right|=\left|u_1u_2u_3\in E_2(P_n):d_{p_n}(u_1)=2,d_{p_n}(u_2)=2,d_{p_n}(u_3)=2\right|=(n-4).$$

From, partition of $E_2(P_n)$ and Eqs. (1.5) and (1.6), we get the desired result.

Theorem 2.2. Let W_{n+1} be the wheel on $n\geq 4$ vertices. Then

$$^{2}\mathrm{GO}_1(W_{n+1})=\frac{10n^3+36n^2+90n}{2}$$
$$^{2}\mathrm{GO}_2(W_{n+1})=\frac{9n^4+81n^3+162n^2+486n}{2}.$$

Proof. For a wheel W_{n+1} on $n\geq 3$ vertices each vertex is of degree either 3 or n. The partition of $E_2(W_{n+1})$ is given as follows:

$$\left|E_{(3,n,3)}\right|=\left|u_1u_2u_3\in E_2(W_{n+1}):d_{W_{n+1}}(u_1)=3,d_{W_{n+1}}(u_2)=n,d_{W_{n+1}}(u_3)=3\right|\quad=\frac{n^2+3n}{2}$$

$$\left|E_{(3,3,3)}\right|=\left|u_1u_2u_3\in E_2(W_{n+1}):d_{w_{n+1}}(u_1)=3,d_{W_{n+1}}(u_2)=3,d_{W_{n+1}}(u_3)=3\right|=n$$

From, partition of $E_2(W_{n+1})$ and Eqs. (1.5) and (1.6), we get the desired result.

Theorem 2.3. Let $K_{r,s}$ be the complete bipartite graph on $r\geq 2, s\geq 3$ vertices. Then

$$^{2}GO_1(K_{r,s})=r\binom{s}{2}\left(r^2s+2r+s\right)+s\binom{r}{2}\left(s^2r+2s+r\right),$$
$$^{2}GO_2(K_{r,s})=r^3s\binom{s}{2}(2r+s)+s^3r\binom{r}{2}(2s+r).$$

Proof. For a complete bipartite graph $K_{r,s}$ on $r\geq 2, s\geq 3$ vertices each vertex is of degree either 3 or *(n-1)*. The partition of $E_2(K_{r,s})$ is given as follows:

$$\left|E_{(r,s,r)}\right|=\left|u_1u_2u_3\in E_2(K_{r,s}):d_{K_{rs}}(u_1)=r,d_{K_{rs}}(u_2)=s,d_{K_{rs}}(u_3)=r\right|\quad=r\binom{s}{2},$$

$$\left|E_{(s,r,s)}\right| = |u_1u_2u_3 \in E_2(K_{r,s}) : d_{K_{rs}}(u_1) = s, d_{K_{rs}}(u_2) = r, d_{K_{rs}}(u_3) = s| \quad = s\binom{r}{2}.$$

From, partition of $E_2(K_{r,s})$ and Eqs. (1.5) and (1.6), we get the desired result.

Theorem 2.4. Let G be the r - regular graph on n vertices

$$^2GO_1(G) = \frac{nr(r-1)\left(r^3+3r\right)}{2}$$
$$^2GO_2(G) = \frac{3nr^5(r-1)}{2}.$$

Proof. Since G is the r - regular graph, the path of degrees (r, r, r) appears $\frac{nr(r-1)}{2}$ times in G. Therefore by Eqs. (1.5) and (1.6), we get the required result.

From Theorem 2.4, we obtain the following results.

Corollary 2.5. If C_n is a cycle on $n \geq 3$ vertices. Then

$$^2GO_1(C_n) = 14n$$
$$^2\mathrm{GO}_2(C_n) = 48n$$

Corollary 2.6. If K_n is a complete graph on $n \geq 4$ vertices. Then

$$^2GO_1(K_n) = \frac{n(n-1)(n-2)\left(n^3-3n^2+6n-4\right)}{2},$$
$$^2\mathrm{GO}_2(K_n) = \frac{3n(n-2)(n-1)^5}{2}.$$

Lemma 2.7. [10] Let G be the graph with n vertices and m edges $m > 0$. Then

$$M_1(G) \leq m\left(\frac{2m}{n-1}+n-2\right). \tag{2.1}$$

Lemma 2.8. [11] Let G be the graph with n vertices and m edges, $m > 0$. Then the equality

$$M_1(G) = m\left(\frac{2m}{n-1}+n-2\right).$$

holds if and only if G is isomorphic to star graph S_n or K_n or $K_{n-1} \cup K_1$.

Theorem 2.9. Let G be a graph of order n and size $m > 0$. Then

$$^2GO_1(G) \leq \left(n^3-3n^2+6n-4\right) \cdot m\left(\frac{m}{n-1}+\frac{n-4}{2}\right)$$

Equality holds if and only if G is isomorphic to K_n.

Proof: By using Eqn. (1.5)

$$\begin{aligned}
^2GO_1(G) = &\sum_{u_1u_nu_2 \in E_n(G)} [d_G(u_1)+d_G(u_2)+d_G(u_3) \\
&+ (d_G(u_1) \cdot d_G(u_2) \cdot d_G(u_3))] \\
&\leq \sum_{u_1u_nu_x \in E_n(G)} \left(n^3-3n^2+6n-4\right) \\
&= \left(n^3-3n^2+6n-4\right)\left(\frac{1}{2}M_1(G)-m\right)
\end{aligned}$$

By Eqn. (2.1) we get

$$\begin{aligned}&\leq \left(n^3-3n^2+6n-4\right)\left(\frac{1}{2}m\left(\frac{2m}{n-1}+n-2\right)-m\right)\\&=\left(n^3-3n^2+6n-4\right)\cdot m\left(\frac{m}{n-1}+\frac{n-4}{2}\right).\end{aligned}$$

Equality holds if and only if G is isomorphic to K_n.

Theorem 2.10. Let G be a graph of order n and size m. Then

$$^{2}GO_2(G)\leq 3m(n-1)^4\left(\frac{m}{n-1}+\frac{n-4}{2}\right).$$

Equality holds if and only if G is isomorphic to K_n.

Proof. The Proof follows exactly as mentioned in the Proof of Theorem 2.9.

Lemma 2.11. [11] Let G be a graph of order n and size m. Then

$$^{2}GO_2(G)\leq 3m(n-1)^4\left(\frac{m}{n-1}+\frac{n-4}{2}\right).$$

and the equality holds if and only if the difference of the degrees of any two vertices of graph G is at most one.

Theorem 2.12. Let G be a graph of order n, size m with minimum vertex degree δ. Then

$$^{2}GO_1(G)\geq 2mp\delta\left(3+\delta^2\right)-\frac{pn\delta\left(3+\delta^2\right)(p+1)}{2}\text{ where } p=\left\lfloor\frac{2m}{n}\right\rfloor$$

Equality holds if and only if G is a regular graph.

Proof: By using Eqn. (1.5)

$$\begin{aligned}{}^{2}GO_1(G)=&\sum_{u_1u_nu_\Omega\in E_n(G)}\left[d_G(u_1)+d_G(u_2)+d_G(u_3)\right.\\&\left.+\left(d_G(u_1)\cdot d_G(u_2)\cdot d_G(u_3)\right)\right]\\&\geq\sum_{u_1u_nu_2\in E_n(G)}\left(3\delta+\delta^3\right)\\&=\delta\left(3+\delta^2\right)\left(-m+\frac{M_1(G)}{2}\right)\end{aligned}$$

By Lemma 2.11, we get

$$\begin{aligned}&\geq\delta\left(3+\delta^2\right)\left(-m+m(2p+1)-\frac{pn(1+p)}{2}\right)\\&=2mp\delta\left(3+\delta^2\right)-\frac{pn\delta\left(3+\delta^2\right)(p+1)}{2}.\end{aligned}$$

Equality holds if and only if G is a regular graph.

Theorem 2.13. Let G be a graph of order n, size m with minimum vertex degree δ. Then

$$^{2}\mathrm{GO}_2(G)\geq 6mp\delta^4-\frac{3\delta^4pn(p+1)}{2}\text{ where } p=\left\lfloor\frac{2m}{n}\right\rfloor$$

Equality holds if and only if G is a regular graph.

Proof. The Proof follows exactly as mentioned in the Proof of Theorem 2.12.

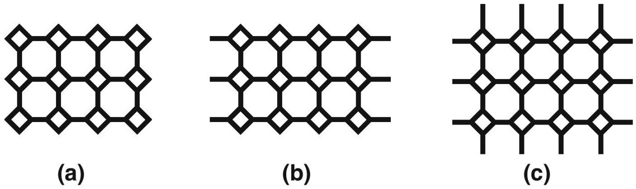

Figure 1: (a) 2D-lattice of $TU\ C_4C_8[4,3]$; (b) $TU\ C_4C_8[4,3]$nanotube; (c) $TU\ C_4C_8[4,3]$nanotorus.

Table 1: 1: Number of vertices and edges.

Graph	Number of vertices	Number of edges
2D-lattices of $TUC_4C_8[p,q]$	$4qp$	$6qp - q - p$
$TUC_4C_8[p,q]$ nanotube	$4qp$	$6qp - p$
$TUC_4C_8[p,q]$ nanotorus	$4qp$	$6qp$

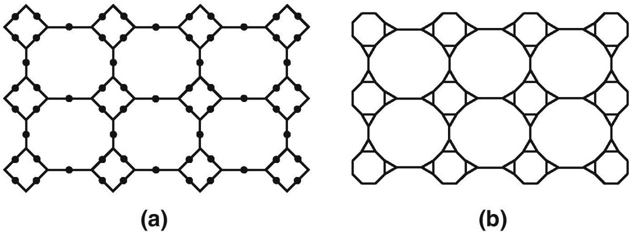

Figure 2: (a) Subdivision graph of 2D-lattice of $TU\ C_4C_8[4,3]$; (b) Line graph of the subdivision graph of 2D-lattice of $TU\ C_4C_8[4,3]$.

Table 2: Partition of paths of length 2 of the graph.

$(d_X(u), d_X(v), d_X(w))$ **where** $uvw \in E_2(X)$	**Number of paths of length 2 in X**
(2,2,2)	8
(2,2,3)	$4(p+q-2)$
(3,3,2)	$8(q+p-2)$
(3,3,3)	$(36qp-26p-26q+16)$

3 COMPUTING THE SECOND ORDERED FIRST AND SECOND GOURAVA INDICES OF SOME FAMILIES OF GRAPHS

In this section, we take into account the graph 2D-lattice, nanotube and nanotorus of $TU\ C_4C_8[p,q]$, where p is the number of squares in a row and $q$is the number of rows of squares [12–15]. These graphs are shown in Figure 1. The Table 1 shows the vertex set and edge set.

Lemma 3.1. [13] Let X be the line graph of the subdivision graph of 2D - Lattice of $TU\ C_4C_8[4,3]$. Then

$$M_1(X) = 108pq - 38p - 38q$$

Theorem 3.2 . Let X be the line graph of the subdivision graph of 2D - Lattice of $TU\ C_4C_8[4,3]$. Then

$$^2GO_1(X) = 1296pq - 652(p+q) + 120$$

$$^2\mathrm{GO}_2(X) = 8748pq - 4830(p+q) + 1296$$

Proof. From the Remark 2.1 and Lemma 3.1, it is clear that, total number of paths of length 2 in X is $36pq - 14p - 14q$. From Eqs. (1.5), (1.6) and Table 2, we deduce

$$^{2}GO_1(X) = \sum_{u_1u_nu_x \in E_n(G)} [d_G(u_1)+d_G(u_2)+d_G(u_3)+(d_G(u_1)\cdot d_G(u_2)\cdot d_G(u_3))]$$
$$= 8(6+8)+4(p+q-2)(7+12)+8(q+p-2)(8+18)$$
$$+(36qp-26p-26q+16)(9+27)$$
$$= 1296pq-652(p+q)+120$$
$$^{2}GO_2(X) = \sum_{u_1u_nu_n \in E_n(G)} [(d_G(u_1)+d_G(u_2)+d_G(u_3))\cdot(d_G(u_1)\cdot d_G(u_2)\cdot d_G(u_3))]$$
$$= 8(6\cdot 8)+4(p+q-2)(7\cdot 12)+8(q+p-2)(8\cdot 18)$$
$$+(36qp-26p-26q+16)(9\cdot 27)$$
$$= 8748pq-4830(p+q)+1296.$$

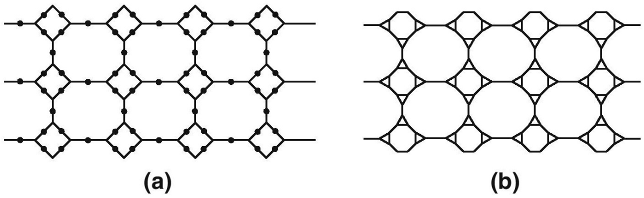

Figure 3: (a) Subdivision graph of of $TU\ C_4C_8[4,3]$ nanotube; (b) Line graph of the subdivision graph of $TU\ C_4C_8[4,3]$ of nanotube.

Lemma 3.3 . **[13]** Let Y be the line graph of the subdivision graph of $TU\ C_4C_8[4,3]$ nanotube. Then

$$M_1(Y) = 108pq-38p$$

Table 3: Partition of paths of length 2 of the graph.

$(d_Y(u), d_Y(v), d_Y(w))$ **where** $uvw \in E_2(Y)$	**Number of paths of length 2 in** Y
(2,2,3)	$4p$
(3,3,2)	$8q$
(3,3,3)	*(36pq - 26p)*

Theorem 3.4 . Let Y be the line graph of $TU\ C_4C_8[4,3]$ the subdivision graph of nanotube. Then

$$^{2}\mathrm{GO}_1(Y) = 1296pq-860p+208q,$$
$$^{2}\mathrm{GO}_2(Y) = 8748pq-5982p+1152q.$$

Proof. From the Remark 2.1 and Lemma 3.3, it is clear that, total number of paths of length 2 in Y is *36pq*. From Eqs. (1.5), (1.6) and Table 3, we get the required results.

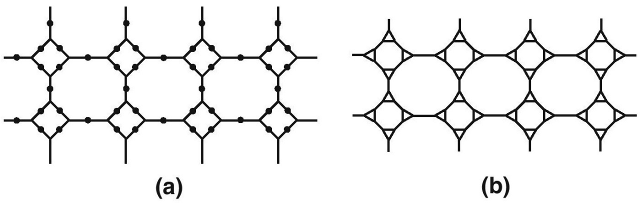

Figure 4: (a) Subdivision graph of $TU\ C_4C_8[4,3]$ of nanotorus; (b) Line graph of the subdivision graph of $TU\ C_4C_8[4,3]$ of nanotorus.

Theorem 3.5. Let Z be the line graph of the subdivision graph of $TU\ C_4C_8[p,q]$ nanotorus. Then

$$^{2}GO_1(Z) = 108n,$$
$$^{2}\mathrm{GO}_2(Z) = 729n.$$

Proof. The graph Z is 3-regular graph, by using Theorem 2.4, we obtain the desired result.

4 CHEMICAL APPLICABILITY OF THE SECOND ORDERED FIRST AND SECOND GOURAVA INDICES

In this section, we establish the linear regression analysis of the second ordered first and second Gourava indices with the entropy, acentric factor, enthalpy of vaporization and standard enthalpy of vaporization of an octane isomers.

A linear regression model with four physical characteristics based on the second ordered first and second Gourava indices is discussed in this section. Physical parameters of octane isomers, such as entropy (S), acentric factor (AF), enthalpy of vaporisation (HVAP), and standard enthalpy of vaporisation (DHVAP), have showed a strong relationship with the indices studied. The second ordered first and second Gourava indices is tested for the octane isomers, which can be found at https://www.moleculardescriptors.eu/dataset.htm. First and second Gourava indices are computed and tabulated in column 6 and 7 of Table 4. The linear regression models for *S, AF, HVAP* and *DHVAP* are fitted using the least squares approach utilising data from Table 4.

The fitted models for the second ordered first Gourava index $^{2}GO_1(G)$ are

$$S = 120.66037(\pm 3.36250) - 0.12079(\pm 0.02603)^{2}GO_1(G) \tag{4.1}$$

$$\text{Acentric Factor } = 0.4751946(\pm 0.0191537) - 0.0011054(\pm 0.0001483)^{2}GO_1(G) \tag{4.2}$$

$$\text{HVAP } = 75.05079(\pm 1.75198) - 0.04664(\pm 0.01356)^{2}GO_1(G) \tag{4.3}$$

$$DHVAP = 10.327506(\pm 0.310790) - 0.009516(\pm 0.002406)^{2}GO_1(G) \tag{4.4}$$

The fitted models for the second ordered second Gourava index $^{2}GO_2(G)$ are

$$S = 113.670043(\pm 2.948517) - 0.016511(\pm 0.005625)^{2}GO_2(G) \tag{4.5}$$

$$\text{Acentric Factor } = (4.176e-01)(\pm 1.915e-02) - (1.638e-04)(\pm 3.654e-05)^{2}\mathrm{GO}_2(G) \tag{4.6}$$

$$HVAP = 72.264706(\pm 1.425287) - 0.006203(\pm 0.002719)^{2}GO_2(G) \tag{4.7}$$

$$DHVAP = 9.7605648(\pm 0.2621262) - 0.0012685(\pm 0.0005001)^{2}GO_2(G) \tag{4.8}$$

Table 4: The corresponding values of the $^2GO_1(G)$ and $^2GO_2(G)$of octane isomers and experimental values of S, AF, $HVAP$ and $DHVAP$.

Alkane	*S*	*AF*	*HVAP*	*DHVAP*	$^2GO_1(G)$	$^2GO_2(G)$
n-Octane	111.700	0.398	73.190	9.915	74	232
2-Methylheptane	109.800	0.378	70.300	9.484	88	287
3-Methylheptane	111.300	0.371	71.300	9.521	97	344
4-Methylheptane	109.300	0.372	70.910	9.483	99	364
3-Ethylhexane	109.400	0.362	71.700	9.476	109	428
2,2-Dimethylhexane	103.400	0.339	67.700	8.915	122	436
2,3 -Dimethylhexane	108.000	0.348	70.200	9.272	122	488
2,4 -Dimethylhexane	107.000	0.344	68.500	9.029	113	423
2,5 -Dimethylhexane	105.700	0.357	68.600	9.051	102	342
3,3-Dimethylhexane	104.700	0.323	68.500	8.973	142	580
3,4-Dimethylhexane	106.600	0.340	70.200	9.316	132	558
2-Methyl-3-ethylpentane	106.100	0.332	69.700	9.209	135	585
3-Methyl-3-ethylpentane	101.500	0.307	69.300	9.081	162	720
2,2,3-Trimethylpentane	101.300	0.301	67.300	8.826	167	744
2,2,4-Trimethylpentane	104.100	0.305	64.870	8.402	140	543
2,3,3-Trimethylpentane	102.100	0.293	68.100	8.897	176	807
2,3,4 -Trimethylpentane	102.400	0.317	68.370	9.014	148	651
2,2,3,3 -Trimethylpentane	93.060	0.255	66.200	8.410	144	468

Table 5: Correlation coefficient and residual standard error regression model for the $^2GO_1(G)$ index.

Physical Property	Absolute Value of the correlation coefficient	Residual standard error
Acentric factor	0.8811943	0.01731
Entropy	0.7574559	3.039
HVAP	0.6519765	1.584
DHVAP	0.7031612	0.2809

Table 6: Correlation coefficient and residual standard error regression model for the $^2GO_2(G)$ index.

Physical Property	Absolute Value of the correlation coefficient	Residual standard error
Acentric factor	0.7462292	0.02438
Entropy	0.5916016	3.753
HVAP	0.4953769	1.814
DHVAP	0.5355184	0.3337

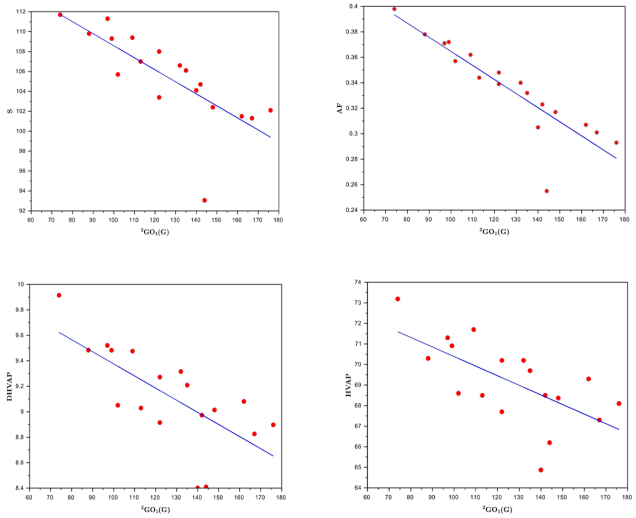

Figure 5: Scatter diagram of physical properties S, AF, $HVAP$ and $DHVAP$ with the ${}^2GO_1(G)$ index.

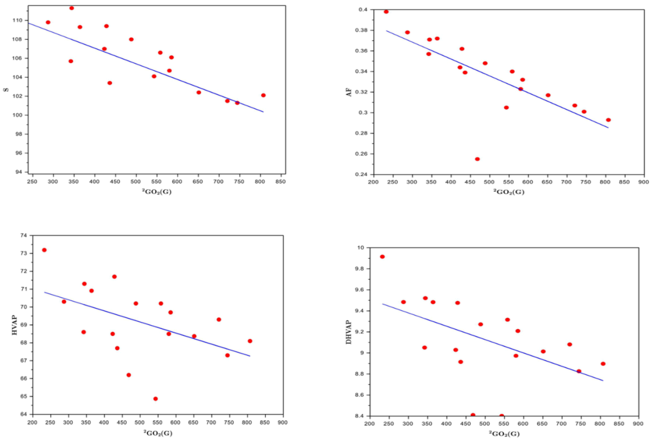

Figure 6: Scatter diagram of physical properties S, AF, $HVAP$ and $DHVAP$ with the ${}^2GO_2(G)$ index.

Note: The values in the brackets of equations (4.1)-(4.8), are the corresponding standard errors of the regression coefficients. Tables 5 and 6 and Figures 5 and 6 represents the residual standard error and correlation coefficient for the regression models of four physical properties with ${}^2GO_1(G)$ and ${}^2GO_2(G)$ indices. From Table 5 and Figure 5, we can observe that ${}^2GO_1(G)$ index correlates with the acentric factor and the good correlation coefficient $|r| = 0.8811943$. Also, the ${}^2GO_1(G)$index has correlation coefficient $|r| = 0.7574559$ with entropy, $|r| = 0.7031612$ with DHVAP and $|r| = 0.6519765$ with HVAP. From Table 6 and Figure 6, we can observe that ${}^2GO_2(G)$ index correlates with the acentric factor and the correlation coefficient $|r| = 0.7462292$. Also, the ${}^2GO_2(G)$ index has correlation coefficient $|r| = 0.5916016$ with entropy, $|r| = 0.5355184$ with DHVAP and $|r| = 0.4953769$ with HVAP. Among, second ordered first Gourava index ${}^2GO_1(G)$ and second ordered second Gourava index ${}^2GO_2(G)$, the second ordered first Gourava index ${}^2GO_1(G)$ has good correlation with the physical properties of octane isomers.

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