Bull. Chem. Soc. Jpn., **70**, 997—1001 (1997)

Ordering the Isomeric Molecules through the Graph Spectrum: Generation of Two Topological Indices Depicting the Branch and Linear Characters (A Computational Method)

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(Received September 24, 1996)

Octane isomeric molecules have been ordered by using the graph spectrum of the vertex adjacency matrix and a Fortran-77 program. The program not only orders the isomeric molecules into various subgroups, but also generates topological descriptors, which primarily depict the branching and linear characters of the molecule. These descriptors are correlated with different physical properties, like standard entropy (S°_{298}), standard entropy of formation (ΔS°_{298}), heat of vaporization (H_v), octane number (MON), and *A* coefficient of Antoine equation. Good correlations of the descriptors with the above properties have been obtained.

The characteristic polynomial (CP) of the vertex adjacency matrix for all eighteen molecular graphs of octane isomers are considered. The eigenvalues of all these eighteen tree graphs are conjugated (i.e. $\pm\lambda_1$, $\pm\lambda_2$, $\pm\lambda_3$, $\pm\lambda_4$). Further, one can observe that $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq \lambda_5(-\lambda_4) \geq \lambda_6(-\lambda_3) \geq \lambda_7(-\lambda_2) \geq \lambda_8(-\lambda_1)$. The relationship between the eigenvalues and the path length has already been established.[1] The maximal eigenvalues of the graph spectrum has been suggested to be a topological index.[2—4] Trinajstić proposed that $+\lambda_1$ refers to the branching of the molecule.[1] Bonchev and Polansky,[5] while partitioning the octane isomeric molecules into various subgroups, have pointed out that octane possesses a 17% branch character and 2,2,3,3-tetramethylbutane also possesses 100% branch character. Further, they have noticed that the linear character decreases from octane to 2,2,3,3-tetramethylbutane. Hence, the branching and linear characters are inversely proportional to each other in one isomeric series. One can thus intuitively conclude that if $+\lambda_1$ is predominant in 2,2,3,3-tetramethylbutane and then $-\lambda_1$ is predominant in the octane case to explain the molecular-branching pattern.

1. Ordering the Isomeric Molecules (Octanes) Based on the Branch and Linear Characters Intuitively. It was pointed out earlier that no molecule in the octane isomeric series has a 100% linear character.[5] The most linear molecule (octane) has the minimum branch character. If one assigns ($+\lambda_4$) to depict the minimum branch character (which happens to be the lowest positive eigenvalue), then (λ_8 or $-\lambda_1$) depicts the maximum linear character. Hence, the octane is characterized through the ($+\lambda_4$, $-\lambda_1$) pair taking branch and linear characters simultaneously. Similarly, different pairs can be obtained while keeping $+\lambda_4$ fixed and varying the other eigenvalues. The following pairs are obtained to characterize the octane isomeric molecules: ($+\lambda_4$, $-\lambda_1$), ($+\lambda_4$, $-\lambda_2$), ($+\lambda_4$, $-\lambda_3$), ($+\lambda_4$, $-\lambda_4$), ($+\lambda_4$, $-\lambda_5$), ($+\lambda_4$, $-\lambda_6$), ($+\lambda_4$, $-\lambda_7$), and ($+\lambda_4$, $-\lambda_8$). The last pair is used to depict the 100% branching character. Hence, 2,2,3,3-tetramethylbutane is characterized by ($+\lambda_4$, $-\lambda_8$). If the first four pairs are analyzed, one can observe that the linear character decreases and the branch character increases. ($+\lambda_4$, $-\lambda_5$), ($+\lambda_4$, $-\lambda_6$), and ($+\lambda_4$, $-\lambda_7$) pairs depict the maximum branch character with very little linear character.

Here, in this brief report, we have adopted a very simple way to order the different isomeric molecules. The number of terminal methyl groups are considered for the subgrouping of the molecules. This is analogous to the Hosoya's ordering[6] of the isomeric molecules. In the case of octane we have two terminal vertices, and in the 2,2,3,3-tetramethylbutane we have six terminal vertices. Further, we have three terminal vertices in four molecules, four terminal vertices in eight molecules and five terminal vertices in four molecules. Eight molecules possessing four terminal vertices are disubstituted isomers. Out of the eight molecules, five molecules are having substitution at different positions, and three are having substitution at the same positions (quaternary center).

The ordering and the eigenvalue pair (describe the linearity and branching characters) are obtained using the program. For example, if in a particular subgroup four molecules with three terminal vertices are present, then a cubic factor (CF) is extracted from their CP and further extraction, of two more factors (one quadratic or two bilinear) gives the eigenvalue pair. Thus the eigenvalue pairs obtained give descriptors of that molecule. For the different subgroups, different factors (equal to the number of terminal centers) are extracted from their corresponding CP of the molecular graphs. After that, in each case two more linear factors (or a quadratic factor) are extracted which generate the descriptors (topological) for the respective isomeric molecule. In the present work we used a computer program based on the extraction of different factors, like linear (LF), quadratic (QF), cubic (CF), and

CP of the 2-methylheptane graph is given by,

$$\begin{tikzcd}
X^8 - 7X^6 + 14X^4 - 7X^2 \arrow[d, "QF_1\ (P_1 = -0.5,\ Q_1 = -1.45)"', "\begin{array}{l} X^2 - 0.6959X - 1.3569 \\ \text{(extracted factor)} \\ \lambda_2 \text{ and } -\lambda_3 \end{array}"] \\
\mathrm{DP} = X^6 + 0.6959X^5 - 5.1588X^4 - 2.6458X^3 + 5.1588X^2 \arrow[d, "p_3(1.913)"', "\begin{array}{l} (X + 1.9499) \\ \text{(extracted factor)} \\ -\lambda_1 \end{array}"] \\
\mathrm{DP} = X^5 - 1.254X^4 - 2.7138X^3 + 2.6458X^2
\end{tikzcd}$$

CP of 3-methylheptane is given by

$$\begin{tikzcd}
X^8 - 7X^6 + 14X^4 - 8X^2 + 1 \arrow[d, "\mathrm{QF}_1\ (P_1 = -0.5,\ Q_1 = -1.45)"', "\begin{array}{l} X^2 - 0.6728X - 1.2091 \\ \text{(extracted factor)} \\ \lambda_2 \text{ and } -\lambda_3 \end{array}"] \\
\mathrm{DP} = X^6 + 0.6728X^5 - 5.3383X^4 - 2.7782X^3 + 5.6765X^2 + 0.4603X - 0.8271 \arrow[d, "p_3\ (1.913)"', "\begin{array}{l} X + 1.9890 \\ \text{(extracted factor)} \\ -\lambda_1 \end{array}"] \\
\mathrm{DP} = X^5 - 1.3162X^4 - 2.7202X^3 + 2.6325X^2 + 0.4405X - 0.4158
\end{tikzcd}$$

CP of 4-methylheptane is given by

$$\begin{tikzcd}
X^8 - 7X^6 + 14X^4 - 8X^2 \arrow[d, "\mathrm{QF}_1\ (P_1 = -0.5,\ Q_1 = -1.45)"', "\begin{array}{l} X^2 - 0.4142X - 1.41421 \\ \text{(extracted factor)} \\ \lambda_2 \text{ and } -\lambda_3 \end{array}"] \\
\mathrm{DP} = X^6 - 0.41421X^5 - 5.41421X^4 - 1.65685X^3 + 5.65685X^2 \arrow[d, "p_3\ (1.913)"', "\begin{array}{l} X + 2.0000 \\ \text{(extracted factor)} \\ -\lambda_1 \end{array}"] \\
\mathrm{DP} = X^5 - 1.58578X^4 - 2.24264X^3 + 2.82842X^2
\end{tikzcd}$$

CP of 2-ethylhexane is given by

$$\begin{tikzcd}
X^8 - 7X^6 + 14X^4 - 9X^2 + 1 \arrow[d, "\mathrm{QF}_1\ (P_1 = -0.5,\ Q_1 = -1.45)"', "\begin{array}{l} X^2 - 0.32132X - 1.32132 \\ \text{(extracted factor)} \\ \lambda_2 \text{ and } -\lambda_3 \end{array}"] \\
\mathrm{DP} = X^6 - 0.32132X^5 - 5.57542X^4 - 1.366947X^3 + 6.19382X^2 + 0.184045X - 0.75681 \arrow[d, "p_3\ (1.913)"', "\begin{array}{l} X + 2.02852 \\ \text{(extracted factor)} \\ -\lambda_1 \end{array}"] \\
\mathrm{DP} = X^5 - 1.70719X^4 - 2.11233X^3 + 2.91797X^2 + 0.27465X - 0.37308
\end{tikzcd}$$

Scheme 1.

quartic (QrF), from one nth-order polynomial. The ordering of the molecules in one subgroup was tested through this computer program.

2. Method. Let $P_n(X)$ be a polynomial equation with degree 'n':

$$P_n(X) = X^n + a_1 x^{n-1} + a_2 X^{n-2} + \cdots + a_n. \tag{1}$$

Here, a_1, a_2, $\cdots$, a_n are real coefficients. If a quadratic factor (QF) of the type (X^2+PX+Q) is extracted from Eq. 1, one obtains, a quotient polynomial, $P_{n-2}(X)$, of degree $(n-2)$ with a remainder term, which is a polynomial of degree one, i.e. $(RX+S)$. On the other hand, if from polynomial (1) a linear factor (LF) of the type $(X+p_1)$ is extracted, one obtains a quotient polynomial, $P_{n-1}(X)$, of degree $(n-1)$ and remainder R. Now, we must solve the following equations with one iterative method:

$$R(p_1) = 0 \qquad \text{(linear case)} \tag{2}$$

and

$$R(P,Q) = 0; \qquad S(P,Q) = 0 \qquad \text{(quadratic case)}. \tag{3}$$

Let us consider 2m-7, where three terminal centers ocuur. Now, in this molecule three linear factors (LFs) or their equivalent factors depicting a CF is to be extracted. Since, a CF is to be extracted, two sets of (P,Q) values are chosen ($P_1=-0.5$, $Q_1=-1.45$ and $P_2=1.6$, $Q_2=-0.6$). QF$_1$ and p_3 are the operations which give the required CF (Scheme 1). After extracting of the CF, two more operations (p_3 and p_4) are performed to the deflated polynomial (DP) in the following way:

$$\begin{array}{c} \mathrm{DP} = X^5 - 1.254X^4 - 2.7138X^3 + 2.6458X^2 \\ p_3\,(1.913)\ \downarrow\ X + 1.5637\,(-\lambda_2) \\ \mathrm{DP} = X^4 - 2.8176X^3 + 1.692X^2 \\ p_4\,(-0.313)\ \downarrow\ X + 0\,(+\lambda_4) \\ \mathrm{DP} = X^3 - 2.81756X^2 + 1.69199X \end{array}$$

For the 3m-7 molecule after the extraction of the CF by QF and p_3, we performed the same operations in the following way:

$$\begin{array}{c} \mathrm{DP} = X^5 - 1.3162X^4 - 2.7202X^3 + 2.6325X^2 + 0.4405X - 0.4158 \\ p_3\,(1.913)\ \downarrow\ X + 1.4863\,(-\lambda_2) \\ \mathrm{DP} = X^4 - 2.8025X^3 + 1.4451X^2 + 0.4846X - 0.2798 \\ p_4\,(-0.313)\ \downarrow\ X - 0.4157\,(+\lambda_4) \\ \mathrm{DP} = X^3 - 2.38669X^2 + 0.45268X + 0.672817 \end{array}$$

Scheme 2.

Here, (P, Q) and p_1 are initial approximations. Similarly, any higher order factor, like cubic or quartic, can be extracted by using the above technique. One higher order factor can be extracted in different ways. For example, if a quartic factor (QrF) is to be extracted, one can extract two quadratic factors (QFs), one QF and two linear factors (LFs) or even four LFs. The extraction method of the desired factors from one nth-order polynomial has been described elsewhere.[7] In this method, the initial approximations (rough values) of P and Q are given in the program and the iteration continues.[8]

When one iteration is performed with an initial (p) value, it is called one linear operation; on the other hand, when an iteration is carried out with a set of (P, Q) initial values, it is a quadratic operation.[8]

3. Testing of the Ordering of the Isomeric Molecules in a Subgroup Using the Program. It was mentioned earlier (Section 1) that the number of factors to be extracted from the CP of the molecular graph is equal to the number of terminal vertices (methyl groups). Thus, if in a particular subgroup, four terminal vertices exist, one must extract a quartic factor or their equivalent from their corresponding CP. It may be noted that QF of the following type is equivalent to two LFs (two operations):

$$(X^2 + PX + Q) = (X + p_a)(X + p_b) \qquad (4)$$

Here, p_a and p_b are isolated from the P and Q values as $p_a+p_b=P$ and $p_a \cdot p_b=Q$.

In octane isomeric molecules we observed that the octane contains two terminal vertices. Here, a single set of (P, Q) values of the form (P_1, Q_1) is used for the extraction. The most branched 2,2,3,3-tetramethylbutane has six terminal vertices. Hence, three sets of (P_1, Q_1), (P_2, Q_2), and (P_3, Q_3) are used for the purpose. The linear initial approximations (p_1, p_2) are obtained from (P_1, Q_1), (p_3, p_4) are obtained from (P_2, Q_2) and finally (p_5, p_6) are generated from (P_3, Q_3).[7] The initial approximations are chosen while considering the following two aspects:

(i) For the extraction of a factor like QF, CF or QrF etc. from the CP using initial approximation(s) from a set of molecules present in a subgroup, the same type of operations following a particular order must be used in that subgroup. For example, if a QrF is to be extracted by taking one QF and two LF, like (QF$_1$; p_1; p_2), then for all of the molecules in that subgroup, QrF is extracted by (QF$_1$; p_1; p_2).

(ii) By using the initial approximations, while extracting a similar type of factor in a subgroup, each operation must generate similar eigenvalues of the different molecules in that subgroup.

Now, suppose a particular subgroup contains four molecules; then, necessarily, the extraction of the factors from their corresponding CPs must be done using the same order of operations. For example, 2-methylheptane (2m-7), 3-methylheptane (3m-7), 4-methylheptane (4m-7); and 2-ethylhexane (2e-6) belong to same subgroup containing three terminal vertices. The following operations are to be performed on their corresponding CPs with (P_1, Q_1) equal to $(-0.5, -1.45)$ and (P_2, Q_2) equal to $(1.6, -0.6)$ (Scheme 1).

Here, the same order of operations (QF$_1$; p_3) are used for the extraction of the CF. Table 1 depicts the number of operations and their similarity in different subgroups. It may be pointed out that in each molecule with the (QF$_1$; p_3) operations $(\lambda_2, -\lambda_3)$ and $-\lambda_1$ are extracted from their corresponding CPs in this subgroup.

4. The Topological Descriptors and Their Correlation with Different Properties. In Section 1 we pointed out that isomeric molecules are characterized through their branching and linear characters simultaneously. The eighteen isomeric molecules are divided into six subgroups (A—F). Further, we observed that octane (subgroup-A) is to be characterized through (λ_8 or $-\lambda_1$) and λ_4, whereas 2,2,3,3-tetramethylbutane (subgroup-F) is to be characterized through $+\lambda_1$ and $+\lambda_4$. The rest of the molecules are to be considered by varying the first entry in the pair of eigenvalues, which will lie in the range λ_2 to λ_7.

After ordering the isomeric molecules in a subgroup, the operations are continued. Two consecutive bilinear operations or a quadratic operation (after the extraction of the factor depicting the terminal center) will give the desired descriptors of the molecule. Choosing the two linear initial approximations or that of the QF must be done in such a way so as to extract λ_4 (minimum branching parameter) in all of the subgroups. If λ_4 is extracted in a linear operation, the other eigenvalue must be generated through its other component operation i.e. if p_1 generates λ_4, then p_2 must be used to obtain the other eigenvalue. The idea behind taking the other partner (p_2) is to complete one operation; i.e. QF$_1$ or (p_1, p_2) is a complete operation. Finally, by combining these two eigenvalues, λ_a and λ_b, we obtained $\Lambda_a=(\lambda_a+\lambda_b)$ and $\Lambda_b=\lambda_a\lambda_b$.

By analyzing Scheme 2, we observed that $(-\lambda_2$ and $\lambda_4)$

Table 1. Initial Approximations, Operations, and Descriptors of the Octane Isomeric Molecules

QF_1: $P_1=-0.5$, $Q_1=-1.45$, $p_1=0.9798$, and $p_2=-1.4798$
QF_2: $P_2=$ 1.6, $Q_2=-0.6$, $p_3=1.913$, and $p_4=-0.313$
QF_3: $P_3=$ 2.5, $Q_3=-1.0$, $p_5=2.58$, and $p_6=-0.35$

Sub group	Operations	Eigenvalues obtained through the operations depicting the descriptors	Descriptors Λ_a $(\lambda_a+\lambda_b)$	Λ_b $(\lambda_a\lambda_b)$
A				
Octane	→QF (QF_1)[b)]	$-\lambda_1, \lambda_4$	1.532	−0.652
B				
2m-7	→CF (p_3, p_4)	$-\lambda_2, \lambda_4$	1.564	0.000
3m-7	CF (p_3, p_4)	$-\lambda_2, \lambda_4$	1.070	−0.618
4m-7	CF (p_3, p_4)	$-\lambda_2, \lambda_4$	1.414	0.000
2e-6	CF (p_3, p_4)	$-\lambda_2, \lambda_4$	0.948	−0.492
C				
2,5m-6	→QrF (QF_2)	$-\lambda_3, \lambda_4$	0.618	0.000
2,4m-6	QrF (QF_2)	$-\lambda_3, \lambda_4$	0.720	0.000
2,3m-6	QrF (QF_2)	$-\lambda_3, \lambda_4$	0.835	0.000
3,4m-6	QrF $(QF_2)^*$[a)]	$-\lambda_3, \lambda_4$	0.261	−0.352
2m,3e-5	QrF (QF_2)	$-\lambda_3, \lambda_4$	1.000	0.000
D				
2,2m-6	QrF (QF_2)[b)]	$-\lambda_4, \lambda_4$	0.000	0.000
3,3m-6	QrF (QF_2)	$-\lambda_4, \lambda_4$	0.000	0.000
3m,3e-5	QrF (QF_2)	$-\lambda_4, \lambda_4$	0.000	−0.208
E				
2,2,3m-5	→PF (QF_2)	$-\lambda_5, \lambda_4$	0.000	0.000
2,2,4m-5	PF (QF_2)	$-\lambda_5, \lambda_4$	0.000	0.000
2,3,3m-5	PF (QF_2)	$-\lambda_5, \lambda_4$	0.000	0.000
2,3,4m-5	PF (QF_2)	$-\lambda_5, \lambda_4$	0.000	0.000
F				
2,2,3,3m-4	→HF (DP)	$-\lambda_8, \lambda_4$	−2.303	0.000

Note:

Subgroup	Factors	Corresponding operations to extract the factors	Eigenvalues extracted
A	→QF (Quadratic factor)	(QF_1)	$\lambda_2 \; -\lambda_3$
B	→CF (3rd order polynomial)	(QF_1, p_3)	$\lambda_2 \; -\lambda_3 \; -\lambda_1$
C	→QrF (4th order polynomial)	(p_3, p_3, p_2, p_2)	$-\lambda_1 \; -\lambda_2 \; \lambda_2 \; \lambda_3$
D		(p_1, p_2, p_3, p_3)	$-\lambda_3 \; \lambda_2 \; -\lambda_1 \; -\lambda_2$
E	→PF (5th order polynomial)	$(p_5, p_3, p_3, p_2, p_2)$	$-\lambda_1 \; -\lambda_2 \; -\lambda_3 \; \lambda_2 \; \lambda_3$
F	→HF (6th order polynomial)	(QF_1, QF_2, p_2, p_1)	$-\lambda_1 \; -\lambda_2 \; \lambda_3 \; \lambda_4 \; \lambda_2 \; -\lambda_3$

a) $(QF_2)^*$ bilinear operation of (QF_2). b) Operations for the generation of descriptors are given in parenthesis.

are the eigenvalues obtained after CF extraction. This extraction scheme matches our earlier qualitative assessment in Section 1 for the descriptors. A similar type of operations is performed for the other two molecules (3m-7 and 2e-6) of this subgroup, and the $(-\lambda_2, +\lambda_4)$ pair of eigenvalues is obtained with the p_3 and p_4 operations. Hence, for this subgroup the $(-\lambda_2, +\lambda_4)$ pair is taken for constructing of the descriptors (Λ_a and Λ_b).

It may be pointed out that for the first molecule (octane), after a QF is extracted the same QF gives the $(-\lambda_1, +\lambda_4)$ pair. Here, only one set of (P, Q) values is to be used, since a QF is to be extracted which matches the two terminal centers. A similar process is applied to detect the descriptors in the other subgroups; as well as the entire extraction scheme along with the order of operation; their eigenvalues and descriptors are given in Table 1.

For subgroups C and D, we observed that four terminal centers exist. Hence, after extracting a quartic factor (QrF), QF_2 (a quadratic operation) gives the eigenvalues pairs as $(-\lambda_3, +\lambda_4)$ and $(-\lambda_4, +\lambda_4)$, respectively. In the D subgroup a quaternary center is present, whereas in the C subgroup two tertiary groups are present. Hosoya and Narumi[6)] have pointed out that the branching effect of a quaternary carbon center is three-times greater than a tertiary carbon center.

Here, we have also noticed that though the same operation (QF_2) is used in C and D for the eigenvalues pairs, we obtained ($-\lambda_3$, λ_4) for C and ($-\lambda_4$, λ_4) for the D subgroup. We have already mentioned that $-\lambda_4$ has a less linear character than does $-\lambda_3$ (Section 2). After extracting of a fifth-order polynomial (PF) in subgroup E, the ($-\lambda_5$, λ_4) pair is obtained through QF_2 and for subgroup F, where only one 100% branched molecule is present, after the extraction of a sixth-order polynomial (HF) ($-\lambda_8$, λ_4) pair is obtained.

After generating Λ_a and Λ_b from the program, we tried to correlate them with such properties as the standard entropy (S°), entropy of formation (ΔS°), motor octane number (MON), heat of vaporization (H_v), and A coefficient of Antoine equation. All of the data were taken from the literature.[9—11] The two descriptors (Λ_a and Λ_b) are orthogonal to each other (R^2=0.1219). The following regression equations were obtained for the different properties:

$$S^\circ(\mathrm{cal\ deg^{-1}mol^{-1}})\ \text{at}\ 25^\circ\mathrm{C} = 102.91\,(\pm 0.26163) \\ +3.6303\,(\pm 0.26978)\Lambda_a - 5.3352\,(\pm 1.0371)\Lambda_b. \\ n = 18,\ R = 0.9752,\ s = 0.930457,\ F = 145.7.$$

$$\Delta S^\circ(\mathrm{kJ\ mol^{-1}\ K^{-1}}) \\ =791.71(\pm 1.4024) - 17.091(\pm 1.4461)\Lambda_a + 22.434(\pm 5.5590)\Lambda_b. \\ n=18,\ R=0.9669,\ s=4.994106,\ F=107.8.$$

$$\mathrm{MON} \\ = 95.042(\pm 3.9875) - 38.267(\pm 5.2216)\Lambda_a + 17.294(\pm 14.433)\Lambda_b \\ n=16,\ R=0.9080,\ s=11.10881,\ F=30.53.$$

$$A\ (\mathrm{mm\ Hg}) = 6.8393(\pm 0.00494) \\ +0.37992(\pm 0.00642)\Lambda_a - 0.4392(\pm 0.016116)\Lambda_b \\ n=17,\ R=0.9057,\ s=0.014102,\ F=31.96.$$

$$H_v\ (\mathrm{kJ\ mol^{-1}}) = 37.078\,(\pm 0.23938) \\ +1.6047\,(\pm 0.31079)\Lambda_a - 2.4886\,(\pm 0.78005)\Lambda_b \\ n = 17,\ R = 0.8971,\ s = 0.684139,\ F = 28.85.$$

Making use of the computer program, two important structural aspects of the isomeric molecules (octane) were obtained. The similarity of the isomeric molecules in a subgroup has been judged by the similar factors and their respective eigenvalues. For example, in the E subgroup $-\lambda_1$, $-\lambda_2$, $-\lambda_3$, λ_2, λ_3 are extracted by p_5, p_3, p_3, p_2, and p_2 operations in all of the molecules. After extracting such factors as QF, CF, QrF etc. two consecutive bilinear operations (or a quadratic operation) give the two descriptors. These two descriptors, Λ_a and Λ_b, depict the linear and branched characters of the molecule under consideration. In an earlier paper we pointed out that Λ_a and Λ_b are used to enumerate the total number of edges in a graph.[8]

We are thankful to Prof.M.Randić, Drake University, U.S.A. for his immense help and interest during this investigation. SMP thanks Council of Scientific and Industrial Research (CSIR), New Delhi, for one SRF position.

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