Chapter 4

On Randić index, Harmonic index and $\pi$-Electron Energy.

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4.1 Introduction

The Randić index is one of the most successful molecular descriptors in the studies of quantitative structure-property relationship (QSPR) and quantitative structure-activity relationships (QSAR). In view of its successful applications in QSPR and QSAR, some people gave physicochemical interpretation of this molecular descriptor [50, 72, 73, 99, 124]. The Randić index found countless chemical applications and became a popular topic of research in mathematics and mathematical chemistry [81, 82, 99].

The Randić index [109] denoted by $\mathcal{R}(G)$ is defined as the sum of the weights $(d_G(u)d_G(v))^{-1/2}$ over all edges $uv$ of graph $G$. That is,

$$
\mathcal{R}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}},
$$

where $d_G(u)$ denotes the degree of vertex $u$ in $G$ and $E(G)$ is an edge set of $G$.

Another variant of Randić index is called the harmonic index [40] and is defined as

$$
H(G) = \sum_{uv \in E(G)} \frac{2}{d_G(u) + d_G(v)}.
$$

The $\pi$-electron energy of a graph $G$ is defined as [54]

$$
\mathcal{E}_\pi(G) = \sum_{i=1}^{n} |\lambda_i|,
$$
where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of $G$.

The energy of a graph is closely related with the total $\pi$-electron energy of a nonsaturated hydrocarbons as calculated with the Hückel molecular orbital (HMO) method in quantum chemistry [59].

Driven by the work in [88], we study the association between harmonic index and Randić index. We attempt to quantify the association between harmonic index and Randić index by considering the same set of benzenoid hydrocarbons with the values for Randić index and energy from the work in [88] and we computed harmonic index of same benzenoid hydrocarbons. The Table 4.1, gives the list of 30 hydrocarbons along with their harmonic index, Randić index and Energy with the degree of each edge of benzenoid hydrocarbons.

### 4.2 Correlations Between Harmonic Index and Randić Index

We start with plotting the Randić index and harmonic index in a scatter plot so that we can get an idea on what type of correlation exists between harmonic and Randić index. The scatter plot as shown in Fig.4.1, clearly points out that the correlation is perfectly positive. After knowing that correlation between the two indices is perfectly positive, we verified it by computing Person’s co-efficient of correlation, which is equal to 1. In a situation like this we can always have
a linear relationship between harmonic index and Randić index of the form

\[ y = c_0 + c_1 x \]  \hspace{1cm} (4.1)

where, \( y \) is unknown (or the response); \( x \) is known (or the predictor) and \( c_0 \) and \( c_1 \) are regression coefficients. So that either of indices can be estimated when the other one is known. Proceeding, we obtain from the data given in Table 4.1, the linear relationship for Harmonic index and Randić index:

\[ H(G) = 0.052(\pm 0.030) + 0.986(\pm 0.003)R(G). \]  \hspace{1cm} (4.2)

For the model (4.2) both regression co-efficients \( c_0 \) and \( c_1 \) are significant. The co-efficient of determination \( (R^2) \), which accounts for the proportion of variance in the response variable that is predicted from a known variable is found to be 1. According to the theory, an \( R^2 = 1 \) indicates that the predictors used in the model predicts all variance in the response variable. In other words, an \( R^2 = 1 \) means that the predictor(s), predicts the response without any error. The Fig. 4.1 establishes this assertion.

### 4.3 Correlations Between Indices and Energy

Here we investigate the inter correlations between harmonic index, Randić index and energy. We plot scatter plots for Harmonic index v/s Energy (Fig. 4.2) and Randić index v/s Energy (Fig. 4.3). The scatter
plots suggest that both the combinations shows a perfect correlation among themselves. The coefficient of correlation is 0.999 for both the cases.

Hence energy can be expressed as being in a linear relationship of the form Eq. (4.1) with either of the indices. Eq. (4.3) and Eq. (4.4) are the models for energy based on harmonic index and Randić index respectively.

\[
\mathcal{E}_\pi = -1.233(\pm 0.206) + 2.986(\pm 0.020)H(G) \quad (4.3)
\]

\[
\mathcal{E}_\pi = -1.080(\pm 0.223) + 2.944(\pm 0.022)R(G) \quad (4.4)
\]

The co-efficient of determination \((R^2)\) for the Eq. (4.3) and Eq. (4.4) is 0.9999. So we can deduce that both the models account as
Figure 4.2: Correlation between Harmonic index and Energy along with the Regression line.

Figure 4.3: Correlation between Randić index and Energy along with the regression line.
much as 99.99 of the variation in energy and hence are equally efficient for estimating the energy.

4.4 Estimating energy using number of edges

As the molecular graphs of benzenoid hydrocarbons consists of hexagons, there are only two types of vertices present in their structure. They are the vertices of degree 2 and degree 3. That is benzenoids contain 3 types of edges $e_{22}$ (edges which connect vertices of degree 2); $e_{23}$ (edges which connect vertices of degree 2 and 3) and $e_{33}$ (edges which connect the vertices of degree 3).

We obtained a model which will estimate the energy of a molecule based on the number of edges of the type $e_{22}$, $e_{23}$ and $e_{33}$. We computed the number of these edges based on Eqs. (4.5), (4.6, (4.7) and tabulated in Table 4.1.

\[
e_{22} = n - 2h - r + 2 \quad (4.5)
\]
\[
e_{23} = 2r \quad (4.6)
\]
\[
e_{33} = 3h - r - 3 \quad (4.7)
\]

Proceeding we obtained an equation of the form:

\[
E_\pi = c_0 + c_1 e_{22} + c_2 e_{23} + c_3 e_{33} \quad (4.8)
\]

where, $c_0$, $c_1$, $c_2$ and $c_3$ are the regression coefficients and are estimated using least squares method. After substituting the values for
the regression coefficients in (4.8) we get

\[ E_\pi = -0.027(\pm 0.064) + 1.341(\pm 0.008)e_{22} + 1.146(\pm 0.003)e_{23} + 1.060(\pm 0.003)e_{33}. \]  

(4.9)

The constant \( c_0 \) is found to be insignificant when tested for significance of the regression co-efficients using t-test. In such a case we can omit the insignificant constant and rewrite the model (4.9) as:

\[ E_\pi = 1.341(\pm 0.008)e_{22} + 1.146(\pm 0.003)e_{23} + 1.060(\pm 0.003)e_{33} \]  

(4.10)

4.5 Randić index and harmonic index of some class of trees.

Theorem 4.5.1. If \( T_1 \) is a tree with \( n \) vertices as shown in Fig. 4.4., then
\[ R(T_1) = \frac{x}{\sqrt{x+1}} + \frac{n-x-2}{\sqrt{n-x-1}} + \frac{1}{\sqrt{(x+1)(n-x-1)}}. \]

**Proof.** Without loss of generality, consider the vertices \( a, b \) as shown in Fig.4.4, where \( d_{T_1}(a) = x+1, d_{T_1}(b) = n-x-1 \). Partition the edge set \( E(T_1) \) into 3 subsets \( E_1, E_2 \) and \( E_3 \) such that \( E_1 = \{uv|d_{T_1}(u) = 1 \text{ and } d_{T_1}(v) = x+1\} \), \( E_2 = \{uv|d_{T_1}(u) = 1 \text{ and } d_{T_1}(v) = z+1\} \), \( E_3 = \{ab\} \). It is easy to see that \( |E_1| = x, |E_2| = n-x-2, |E_3| = 1 \). Therefore,

\[ R(T_1) = \sum_{uv \in E(T_1)} \frac{1}{\sqrt{d_{T_1}(u)d_{T_1}(v)}} \]

\[ = \sum_{uv \in E_1(T_1)} \frac{1}{\sqrt{d_{T_1}(u)d_{T_1}(v)}} + \sum_{uv \in E_2(T_1)} \frac{1}{\sqrt{d_{T_1}(u)d_{T_1}(v)}} \]

\[ + \sum_{uv \in E_3(T_1)} \frac{1}{\sqrt{d_{T_1}(u)d_{T_1}(v)}} \]

\[ = \sum_{uv \in E_1(T_1)} \frac{1}{\sqrt{(x+1)(1)}} + \sum_{uv \in E_2(T_1)} \frac{1}{\sqrt{(n-x-2+1)(1)}} + \]

\[ \sum_{uv \in E_3(T_1)} \frac{1}{\sqrt{(x+1)(n-x-2+1)}} \]

\[ = \frac{x}{\sqrt{(x+1)(1)}} + (n-x-2)\frac{1}{\sqrt{(n-x-2+1)(1)}} + \]

\[ \frac{1}{\sqrt{(x+1)(n-x-2+1)}} \]

\[ = \frac{x}{\sqrt{x+1}} + \frac{n-x-2}{\sqrt{n-x-1}} + \frac{1}{\sqrt{(x+1)(n-x-1)}}. \]
Theorem 4.5.2. If \( T_2, T_3, T_4 \) is a graph with \( n \) vertices as shown in Fig. 4.4, then,

(i) \( R(T_2) = \frac{x}{\sqrt{x+1}} + \frac{n-x-3}{\sqrt{n-x-2}} + \frac{1}{\sqrt{2(x+1)}} + \frac{1}{\sqrt{2(n-x-2)}}. \)

(ii) \( R(T_3) = \frac{1}{2} + \frac{x}{\sqrt{x+1}} + \frac{n-x-4}{\sqrt{n-x-3}} + \frac{1}{\sqrt{2(x+1)}} + \frac{1}{\sqrt{2(n-x-3)}}. \)

(iii) \( R(T_4) = 1 + \frac{x}{\sqrt{x+1}} + \frac{n-x-5}{\sqrt{n-x-4}} + \frac{1}{\sqrt{2(x+1)}} + \frac{1}{\sqrt{2(n-x-4)}}. \)

(iv) \( H(T_2) = \frac{2x}{x+2} + \frac{2(n-x-3)}{n-x-1} + \frac{2}{x+3} + \frac{2}{n-x}. \)

(v) \( H(T_3) = \frac{1}{2} + \frac{2x}{x+2} + \frac{2(n-x-4)}{n-x-2} + \frac{2}{x+3} + \frac{2}{n-x-1}. \)

(vi) \( H(T_3) = 1 + \frac{2x}{x+2} + \frac{2(n-x-5)}{n-x-3} + \frac{2}{x+3} + \frac{2}{n-x-2}. \)
Proof. The proof of Theorem 4.5.2 is analogous to the proof of the Theorem 4.5.1.

Theorem 4.5.3. If $T_5$ is a tree with $n$ vertices as shown in Fig. 4.5., then

$$R(T_5) = \frac{x}{\sqrt{x+1}} + \frac{y}{\sqrt{y+2}} + \frac{n-x-y-3}{\sqrt{n-x-y-2}} + \frac{1}{\sqrt{(x+1)(y+2)}} + \frac{1}{\sqrt{(y+2)(n-x-y-2)}}.$$ 

Proof. Without loss of generality, consider the vertices $a$, $b$, $c$ as shown in 4.5., where $d_{T_5}(a) = x + 1$, $d_{T_5}(b) = y + 2$, $d_{T_5}(c) = z + 1$ Partition the edge set $E(T_5)$ into 5 subsets $E_1$, $E_2$, $E_3$, $E_4$ and $E_5$ such that

$E_1 = \{uv|d_{T_5}(u) = 1 \text{ and } d_{T_5}(v) = x + 1\}$, $E_2 = \{uv|d_{T_5}(u) = 1 \text{ and } d_{T_5}(v) = y + 2\}$, $E_3 = \{uv|d_{T_5}(u) = 1 \text{ and } d_{T_5}(v) = z + 1\}$, $E_4 = \{ab\}$, $E_5 = bc$. It is easy to see that $|E_1| = x$, $|E_2| = y$, $|E_3| = z$, $|E_4| = 1$, $|E_5| = 1$. 

Figure 4.5: $T_5, T_6, T_7$ and $T_8$ Trees
\[ |E_4| = |E_5| = 1. \text{ Therefore,} \]

\[
\mathcal{R}(T_5) = \sum_{uv \in E(T_5)} \frac{1}{\sqrt{d_{T_5}(u)d_{T_5}(v)}}
\]

\[
= \sum_{uv \in E_1(T_5)} \frac{1}{\sqrt{d_{T_5}(u)d_{T_5}(v)}} + \sum_{uv \in E_2(T_5)} \frac{1}{\sqrt{d_{T_5}(u)d_{T_5}(v)}}
\]

\[
+ \sum_{uv \in E_3(T_5)} \frac{1}{\sqrt{d_{T_5}(u)d_{T_5}(v)}} + \sum_{uv \in E_4(T_5)} \frac{1}{\sqrt{d_{T_5}(u)d_{T_5}(v)}}
\]

\[
+ \sum_{uv \in E_5(T_5)} \frac{1}{\sqrt{d_{T_5}(u)d_{T_5}(v)}}
\]

\[
= \sum_{uv \in E_1(T_5)} \frac{1}{\sqrt{(x+1)(1)}} + \sum_{uv \in E_2(T_5)} \frac{1}{\sqrt{(y+2)(1)}} + \sum_{uv \in E_3(T_5)} \frac{1}{\sqrt{(z+1)(1)}}
\]

\[
+ \sum_{uv \in E_4(T_5)} \frac{1}{\sqrt{(x+1)(y+2)}} + \sum_{uv \in E_5(T_5)} \frac{1}{\sqrt{(y+2)(z+1)}}
\]

\[
= \frac{x}{\sqrt{(x+1)}} + \frac{y}{\sqrt{y+2}} + \frac{\sqrt{n-x-y-3}}{\sqrt{n-x-y-2}} + \frac{1}{\sqrt{(x+1)(y+2)}} + \frac{1}{\sqrt{(y+2)(z+1)}}
\]

Here we have \( n=x+y+z+3 \). By replacing \( z=n-x-y-3 \), the above equation reduces to

\[
\mathcal{R}(T_5) = \frac{x}{\sqrt{x+1}} + \frac{y}{\sqrt{y+2}} + \frac{\sqrt{n-x-y-3}}{\sqrt{n-x-y-2}} + \frac{1}{\sqrt{(x+1)(y+2)}} + \frac{1}{\sqrt{(y+2)(n-x-y-2)}}
\]
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\[
H(T_5) = \sum_{uv \in E(T_5)} \frac{2}{d_{T_5}(u) + d_{T_5}(v)}
\]

\[
= \sum_{uv \in E_1(T_5)} \frac{2}{d_{T_5}(u) + d_{T_5}(v)} + \sum_{uv \in E_2(T_5)} \frac{2}{d_{T_5}(u) + d_{T_5}(v)} + \sum_{uv \in E_3(T_5)} \frac{2}{d_{T_5}(u) + d_{T_5}(v)} + \sum_{uv \in E_4(T_5)} \frac{2}{d_{T_5}(u) + d_{T_5}(v)} + \sum_{uv \in E_5(T_5)} \frac{2}{d_{T_5}(u) + d_{T_5}(v)}
\]

\[
= \sum_{uv \in E_1(T_5)} \frac{2}{(x+1)(1)} + \sum_{uv \in E_2(T_5)} \frac{2}{(y+2)(1)} + \sum_{uv \in E_3(T_5)} \frac{2}{(z+1)(1)}
\]

\[
= x \frac{2}{x+2} + y \frac{2}{y+3} + z \frac{2}{z+2} + \frac{2}{x+y+3} + \frac{2}{y+z+3}
\]

\[
= \frac{2x}{x+2} + \frac{2y}{y+3} + \frac{2(n-x-y-3)}{n-x-y-1} + \frac{2}{x+y+3} + \frac{2}{n-x}.
\]

\[\square\]

**Theorem 4.5.4.** If \(T_6, T_7\) and \(T_8\) is a graph with \(n\) vertices as shown in Fig. 4.5., then,

(i) \(\mathcal{R}(T_6) = \frac{x}{\sqrt{x+1}} + \frac{y}{\sqrt{y+1}} + \frac{n-x-y-4}{\sqrt{n-x-y-3}} + \frac{1}{\sqrt{3(x+1)}} + \frac{1}{\sqrt{3(y+1)}} + \frac{1}{\sqrt{3(n-x-y-3)}}.\)

(ii) \(\mathcal{R}(T_7) = \frac{x}{\sqrt{x+1}} + \frac{y}{\sqrt{y+2}} + \frac{n-x-y-5}{\sqrt{n-x-y-4}} + \frac{1}{\sqrt{2(x+1)}} + \frac{2}{\sqrt{2(y+2)}} + \frac{1}{\sqrt{2(n-x-y-4)}}.\)

(iii) \(\mathcal{R}(T_8) = \frac{x}{\sqrt{x+1}} + \frac{y}{\sqrt{y+2}} + \frac{n-x-y-4}{\sqrt{n-x-y-3}} + \frac{1}{\sqrt{(x+1)(y+2)}} + \frac{2}{\sqrt{2(y+2)}} + \frac{1}{\sqrt{2(n-x-y-3)}}.\)
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\[(iv) \quad H(T_6) = \frac{2x}{x+2} + \frac{2y}{y+2} + \frac{2(n-x-y-4)}{n-x-y-2} + \frac{2}{n-x-y} + \frac{2}{x+4} + \frac{2}{y+4}.
\]

\[(v) \quad H(T_7) = \frac{2x}{x+2} + \frac{2y}{y+3} + \frac{2(n-x-y-5)}{n-x-y-3} + \frac{2}{n-x-y-2} + \frac{2}{x+3} + \frac{4}{y+4}.
\]

\[(vi) \quad H(T_8) = \frac{2x}{x+2} + \frac{2y}{y+3} + \frac{2(n-x-y-4)}{n-x-y-2} + \frac{2}{n-x-y-1} + \frac{2}{x+y+3} + \frac{2}{y+4}.
\]

**Proof.** The proof of Theorem 4.5.4 is analogous to the proof of the Theorem 4.5.3. \( \square \)

### 4.6 Algorithm

**Step 1:** START

**Step 2:** Declare, \( a[25][25], d[25], m \) as integers and \( \text{sum1}, s[25], \text{sum}, \text{ts}=0 \) as floating points.

**Step 3:** Read \( m, a[i][j] \)

**step 4:** Compute: Degree of each vertex of given graph

\[ \text{for } i \text{ to } m \]
\[ \quad d[i] \leftarrow 0 \]
\[ \text{for } j \text{ to } m \]
\[ \quad d[i] \leftarrow d[i]+a[i][j] \]

Display: Degree \( d[i] \) of vertex \( i \)

**Step 5:** Check the condition, if \( a[i][j]=1 \) is true

Display: Vertex \( i \) is adjacent to vertex \( j \)
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Figure 4.6:

\[
\text{sum} \leftarrow d[i]+d[j]
\]

**Step 6:** Display the sum of adjacent vertices degree

\[
\text{ts} \leftarrow \text{ts}+(2/\text{sum})
\]

**Step 7:** Display the sum of Harmonic Index by deviding total sum ts by 2

**Step 8:** STOP

We represent the graph \( G \) by adjacency matrix \( A(G) \). The vertices of graph \( G \) are \( v_1, v_2, v_3, v_4 \). The element 1 in \( A(G) \) represents the adjacency between the vertices of graph \( G \) and 0 represents the non-adjacency between the vertices of graph \( G \). Addition of elements of each row gives the degree of a corresponding vertex in \( G \), i.e., we get 3 by adding all the elements of a first row of adjacency matrix \( A(G) \).
which is degree of vertex \( v_1 \) in graph \( G \). Similarly we get other vertex degrees by adding the elements of corresponding row. Using this we calculate degree of each vertex and store it in \( d[i] \) by using for loop.

The outer loop iterates \( i \) times and the inner loop iterates \( j \) times, the statements inside the inner loop will be executed a total of \( i \times j \) times. It is because, inner loop will iterate \( j \) times for each of the \( i \) iterations of the outer loop. This means the outer and inner loop are dependent on the problem size, that is, here we considered size \( n \). The statement in the whole loop will be executed \( O(n^2) \) times. In the loop int \( i = 0 \), this will be executed only once. The time is actually calculated to \( i = 0 \) and not the declaration, \( i < n \) this will be executed \( n + 1 \) times, \( i ++ \) will be executed \( n \) times, \( a[i][j] = 1 \), This will be executed \( n \) times (in worst case scenario).

By the definition of Randić index, we multiply the degree of vertices which are adjacent, by adjacency matrix \( A(G) \), we check the adjacency of one vertex to another by using if condition, then we multiply the degree of those adjacency vertices using \( d[i] \), (This loop follows same procedure as explained for above loop so this also executed \( O(n^2) \) times). Then we sum the multiplied value of each adjacent vertices and each time we store the resulting value in one variable say \( ts \) as per the definition of Randić index, that is, \( 1/\sqrt{\text{sum}} \). So for the above example we get final value of total sum \( ts = 3.9266 \). We obtain the Randić index by dividing \( ts \) by 2. Therefore the Randić index of this
graph is 1.9633.

4.7 Conclusion

In this chapter we studied the relations between Randić index, harmonic index and π-Electron energy. Also we obtained Randić index and harmonic index of certain class of trees.
Table 4.1: 30 lower Benzenoid hydrocarbons with degrees of edges, harmonic index, Randić index and Energy

<table>
<thead>
<tr>
<th>Molecule</th>
<th>$e_{22}$</th>
<th>$e_{23}$</th>
<th>$e_{33}$</th>
<th>Harmonic Index</th>
<th>Randić Index</th>
<th>Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td>6</td>
<td>0</td>
<td>0</td>
<td>3</td>
<td>3</td>
<td>8</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>6</td>
<td>4</td>
<td>1</td>
<td>4.9333</td>
<td>4.9663</td>
<td>13.6832</td>
</tr>
<tr>
<td>Anthracene</td>
<td>6</td>
<td>8</td>
<td>2</td>
<td>6.8666</td>
<td>6.9326</td>
<td>19.3137</td>
</tr>
<tr>
<td>Phenanthrene</td>
<td>7</td>
<td>6</td>
<td>3</td>
<td>6.8999</td>
<td>6.9494</td>
<td>19.4483</td>
</tr>
<tr>
<td>Tetracene</td>
<td>6</td>
<td>12</td>
<td>3</td>
<td>8.7999</td>
<td>8.8989</td>
<td>24.9308</td>
</tr>
<tr>
<td>Benzo[c]phenanthrene</td>
<td>8</td>
<td>8</td>
<td>5</td>
<td>8.8666</td>
<td>8.9326</td>
<td>25.1875</td>
</tr>
<tr>
<td>Benzo[a]anthrene</td>
<td>7</td>
<td>10</td>
<td>4</td>
<td>8.8333</td>
<td>8.9158</td>
<td>25.1012</td>
</tr>
<tr>
<td>Chrysene</td>
<td>8</td>
<td>8</td>
<td>5</td>
<td>8.8666</td>
<td>8.9326</td>
<td>25.1922</td>
</tr>
<tr>
<td>Triphenylene</td>
<td>9</td>
<td>6</td>
<td>6</td>
<td>8.8999</td>
<td>8.9494</td>
<td>25.2745</td>
</tr>
<tr>
<td>Pyrene</td>
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<td>8</td>
<td>5</td>
<td>7.8666</td>
<td>7.9326</td>
<td>22.5055</td>
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<tr>
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<td>4</td>
<td>10.7333</td>
<td>10.8653</td>
<td>30.544</td>
</tr>
<tr>
<td>Benzo[a]tetracene</td>
<td>7</td>
<td>14</td>
<td>5</td>
<td>10.7666</td>
<td>10.8821</td>
<td>30.7255</td>
</tr>
<tr>
<td>Dibenzo[a,h]anthracene</td>
<td>8</td>
<td>12</td>
<td>6</td>
<td>10.7999</td>
<td>10.8989</td>
<td>30.8805</td>
</tr>
<tr>
<td>Dibenzo[a,j]anthracene</td>
<td>8</td>
<td>12</td>
<td>6</td>
<td>10.7999</td>
<td>10.8989</td>
<td>30.8795</td>
</tr>
<tr>
<td>Pentaphene</td>
<td>7</td>
<td>14</td>
<td>5</td>
<td>10.7666</td>
<td>10.8821</td>
<td>30.7627</td>
</tr>
<tr>
<td>Benzo[g]chrysene</td>
<td>10</td>
<td>8</td>
<td>8</td>
<td>10.8666</td>
<td>10.9326</td>
<td>30.999</td>
</tr>
<tr>
<td>Pentahelicene</td>
<td>9</td>
<td>10</td>
<td>7</td>
<td>10.8333</td>
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