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Correlation between the Arithmetic-Geometric Indices of n-Heptane Alkane Isomers

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Abstract:*In this paper, the correlation abilities of nine vertex-degree-based AG (Arithmetic-Geometric) indices occurring in the physico-chemical properties of boiling point , density and refractive index of n-heptane alkane isomers is presented.*

Keywords:*Arithmetic-Geometric Index, graph theory, n-heptane alkane isomers.*

I. Introduction

Let G be a simple graph with n vertices and m edges, with vertex set V(G)={v_1,v_2,…..,v_n} and edge set E(G). The edge connecting the vertices v_i and v_j will be denoted by v_iv_j. The degree of the vertex v_i, denoted by d_i, is the number of first neighbors of v_i in the underlying graph.

A topological index is a structural descriptor (derived from molecular graph) that represents an efficient way to express in a numerical form the size, shape, cyclicity and branching. The topological indices of molecular graphs are widely used for establishing correlations between the structure of a molecular compound and its physico-chemical properties or biological activity[5].

II. Arithmetic-Geometric Index

One of the important degree based topological indices is Arithmetic-Geometric (AG) index of G

: $AG(G)=\sum_{uv\in E(G)} \frac{du+dv}{2\sqrt{du.dv}}$ ……(1)

Where, AG index is considered for distinct vertices.
The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of u and v. where du (or dv) denote the degree of the vertex u (or v)[6,7,8].

III. Data Sources

Boiling point , Density and Refractive index of n-Heptane alkane isomers are taken from Lecture 6(Structural Isomers).

IV. Figures and Tables

Table1. The values of Boiling point , Density , Refractive index and AG index of n-Heptane alkane isomers.

S.No.	C_7H_{16} alkane isomers name	Boiling point (^{0}C) Y_1	Density(g/cm^3)Y_2	RefractiveIndexY_3	AG(G)
I.	Heptane	98	0.684	1.3878	6.3034
II.	2-methylhexane	90	0.677	1.3848	6.3367
III.	3-methylhexane	92	0.686	1.3887	6.3365
IV.	2,2-dimethylpentane	79	0.674	1.3822	6.3713
V.	3,3-dimethylpentane	86	0.694	1.3909	6.3713
VI.	2,3-dimethylpentane	90	0.695	1.3919	6.3700
VII.	2,4-dimethylpentane	81	0.673	1.3815	6.3700
VIII.	3-ethylpentane	94	0.698	1.3934	6.3367
IX.	2,2,3-trimethylbutane	81	0.690	1.3894	6.4047

Table2. Comparison between experimental and predicted values of boiling point with respect to n-heptane alkane isomers.

S.No.	C_7H_{16} alkane isomers name	Experimental boiling point (^{0}C) Y_1	Predicted boiling point(^{0}C) Y_1^1
I.	Heptane	98	97.2523
II.	2-methylhexane	90	91.282
III.	3-methylhexane	92	91.3179
IV.	2,2-dimethylpentane	79	85.0786

V.	3,3-dimethylpentane	86	85.0786
VI.	2,3-dimethylpentane	90	85.3117
VII.	2,4-dimethylpentane	81	85.3117
VIII.	3-ethylpentane	94	91.282
IX.	2,2,3-trimethylbutane	81	79.0904

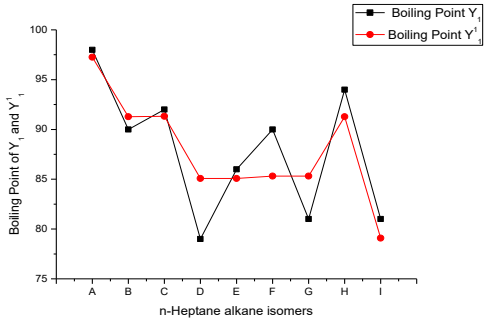

Figure1. The graph showing the n-Heptane alkane isomers versus Boiling point Y_1 and Y_1^1 values.

Table3. Comparison between experimental and predicted values of Density with respect to n-heptane alkane isomers.

S.No.	**C_7H_{16} alkane isomers name**	**Experimental Density(g/cm^3)Y_2**	**Predicted Density(g/cm^3)Y_2^1**
I.	Heptane	0.684	0.687
II.	2-methylhexane	0.677	0.686
III.	3-methylhexane	0.686	0.686
IV.	2,2-dimethylpentane	0.674	0.685
V.	3,3-dimethylpentane	0.694	0.685
VI.	2,3-dimethylpentane	0.695	0.685
VII.	2,4-dimethylpentane	0.673	0.686
VIII.	3-ethylpentane	0.698	0.686
IX.	2,2,3-trimethylbutane	0.690	0.683

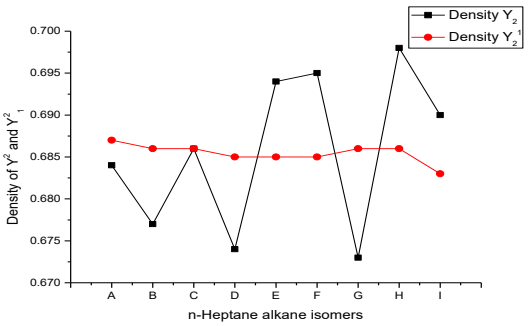

Figure2 The graph showing the n-Heptane alkane isomers versus Density Y_2 and Y_2^1 values.

Table4. Comparison between experimental and predicted values of Refractive index with respect to n-heptane alkane isomers.

S.No.	**C_7H_{16} alkane isomers name**	**Experimental Refractive Index Y_3**	**Predicted Refractive Index Y_3^1**
I.	Heptane	1.3878	1.3921
II.	2-methylhexane	1.3848	1.3895
III.	3-methylhexane	1.3887	1.3895
IV.	2,2-dimethylpentane	1.3822	1.3867
V.	3,3-dimethylpentane	1.3909	1.3867
VI.	2,3-dimethylpentane	1.3919	1.3868
VII.	2,4-dimethylpentane	1.3815	1.3868
VIII.	3-ethylpentane	1.3934	1.3895
IX.	2,2,3-trimethylbutane	1.3894	1.3841

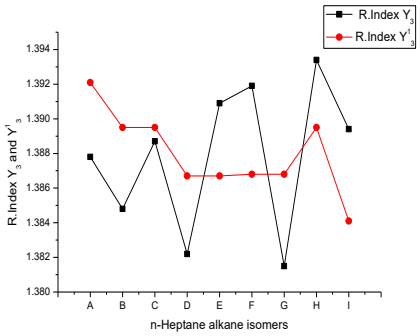

Figure3. The graph showing the n-Heptane alkane isomers versus Refractive index Y_3 andY_3^1 values.

Table5. Comparison between predicted values of Refractive index and Density with respect to n-heptane alkane isomers.

S.No.	C_7H_{16} alkane isomers name	Y_3^1	Y_2^1
I.	Heptane	1.3921	0.687
II.	2-methylhexane	1.3895	0.686
III.	3-methylhexane	1.3895	0.686
IV.	2,2-dimethylpentane	1.3867	0.685
V.	3,3-dimethylpentane	1.3867	0.685
VI.	2,3-dimethylpentane	1.3868	0.685
VII.	2,4-dimethylpentane	1.3868	0.686
VIII.	3-ethylpentane	1.3895	0.686
IX.	2,2,3-trimethylbutane	1.3841	0.683

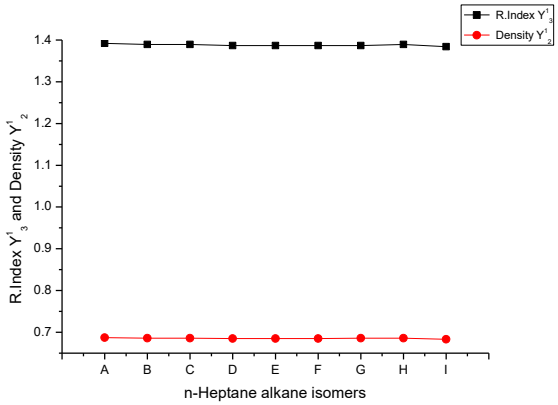

Figure4. The graph showing the n-Heptane alkane isomers versus predicted Refractive index (Y_3^1) and Density (Y_2^1) values.

V. Conclusion

Fig.1.n-Heptane alkane isomers are considered here to evaluate the correlation of boilingpoint and a comparison with the experimental value is carried out. Y_1 is the experimental boiling point and Y_1^1 is the boiling point determined using AG index. It can be seen that the both compound values (Y_1 and Y_1^1) are near to each other.

The above observation shows that the AG index derived can be used to determine the boiling point of n-heptane alkane isomers.

Fig.2: n-Heptane alkane isomers are considered here to evaluate the correlation of density and a comparison with the experimental value is carried out. Y_2 is the experimental density and Y_2^1 is the density determined using AG index. It can be seen that the both compound values (Y_2 and Y_2^1) are near to each other.

The above observation shows that the AG index derived can be used to determine the density of n-heptane alkane isomers.

Fig.3: n-Heptane alkane isomers are considered here to evaluate the correlation of refractive index and a comparison with the experimental value is carried out. Y_3 is the experimental refractive index and Y_3^1 is the refractive index determined using AG index. It can be seen that the both compound values (Y_3 and Y_3^1) are near to each other.

The above observation shows that the AG index derived can be used to determine the refractive index of n-heptane alkane isomers.

Fig.4: n-Heptane alkane isomers are considered here to evaluate the correlation of refractive index and a comparison with the density value is carried out. Y_3^1 is the refractive index and Y_2^1 is the density determined using AG index.It can be seen that the both compound values (Y_3^1 and Y_2^1) difference is nearly 0.7.

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