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Prediction of Physical properties of Primary amines using Molecular structures by Multi linear Regression Analysis

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Abstract:

In this research paper, the interrelation of the additive connectivity degree based topological invariants with the boiling point for the primary amines has been investigated. To obtain the model for predicting the properties we have used correlation, linear regression analysis and multi linear regression analysis. The results obtained in this research have tabulated for the twelve descriptors considered under this research. The results include the values of the correlation coefficients, the percentage error with the regression values obtained. This representation will help successfully for modeling and predicting the standard hotness of boiling points of twenty primary amines considered in this work. The obtained correlation coefficient between the Boiling Point and topological invariants values validates the study. This will be the best model for predicting the physical properties of molecular structures.

Keywords: Molecular graphs, Topological Invariants, Primary amines, Multiple linear regression analysis.

Mathematics Subject Classification: 05C05, 05C12

Introduction:

In the fields of chemical graph theory, molecular topology, and mathematical chemistry, a topological index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. Topological indices are used for example in the development of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure. Topological descriptors are derived from hydrogen-suppressed molecular graphs, in which the atoms are represented by vertices and the bonds by edges. The connections between the atoms can be described by various types of topological matrices (e.g., distance or adjacency matrices), which can be mathematically manipulated so as to derive a single number, usually known as graph invariant, graph-theoretical index or topological index. As a result, the topological index can be defined as two-dimensional descriptors that can be easily calculated from the molecular graphs, and do not depend on the way the graph is depicted or labeled and no need of energy minimization of the chemical structure. Quantitative structure-activity relationship models (QSAR models) are regression or classification models used in the chemical and biological sciences and engineering. Like other regression models, QSAR regression models relate a set of "predictor" variables (X) to the potency of the response variable (Y), while classification QSAR models relate the predictor variables to a categorical value of the response variable.

Additionally, when physicochemical properties or structures are expressed by numbers, one can find a mathematical relationship, or quantitative structure-activity relationship, between

the two. The mathematical expression, if carefully validated can then be used to predict the modeled response of other chemical structures.

The main objective of this research is to give the usefulness of the topological indices and the prediction of the physical properties of molecules. Here, the primary amines are considered and its boiling point is compared with the regression values.

BASIC INCEPTIONS:

Linear Correlations:

The term correlation refers to the relationship between the variables. Simple correlation refers to the relationship between two variables. There may be fluctuation or co variation between the variables of the variables. The direction of change and the closeness of the relationship are found. When the values of two variables change in the same direction, there is positive correlation between the two variables. When the values of two variables change in the opposite directions , there is negative correlation between the two variables.

$$r = \frac{N \sum XY - \sum X \sum Y}{\sqrt{N \sum X^2 - (\sum X)^2} \sqrt{N \sum Y^2 - (\sum Y)^2}}$$

Linear Regressions:

Regression equation gives the value of the dependent variable corresponding to any specified value of the independent variable.

Regression equations:

$$Y - \bar{Y} = b_{YX} (X - \bar{X})$$

$$X - \bar{X} = b_{XY} (Y - \bar{Y})$$

Percentage error:

The **mean percentage error (MPE)** is the computed average of percentage errors by which forecasts of a model differ from actual values of the quantity being forecast.

The formula for the mean percentage error is:

$$MPE = \frac{100\%}{n} \sum_{t=1}^n \frac{a_t - f_t}{a_t}$$

where a_t is the actual value of the quantity being forecast, f_t is the forecast, and n is the number of different times for which the variable is forecast.

Because actual rather than absolute values of the forecast errors are used in the formula, positive and negative forecast errors can offset each other; as a result the formula can be used as a measure of the bias in the forecasts.

MULTIPLE REGRESSION ANALYSIS:

Whenever we are interested in studying the joint effect of a group of variables upon a variable not included in that group, is that of multiple regression analysis. The equation of the multiple regression of Y on X_1 and X_2 is represented by

$$Y = b_{12.3}X_1 + b_{13.2} + X_2,$$

Here, we considered two variables are X_1 and X_2 where X_1 is Harmonic invariants and X_2 is second modified Zagreb invariants and Y as the Boiling Point, where $b_{12.3}$ and $b_{13.2}$ are

coefficients of the required equation of the multiple regression of Y on X₁ and X₂. The coefficients of the multiple regression are given by

$$b_{12.3} = \frac{\sigma_1}{\sigma_2} \frac{\begin{vmatrix} r_{12} & r_{23} \\ r_{13} & 1 \end{vmatrix}}{\begin{vmatrix} 1 & r_{23} \\ r_{23} & 1 \end{vmatrix}}, \quad b_{13.2} = \frac{\sigma_1}{\sigma_3} \frac{\begin{vmatrix} 1 & r_{12} \\ r_{23} & r_{13} \end{vmatrix}}{\begin{vmatrix} 1 & r_{23} \\ r_{23} & 1 \end{vmatrix}}$$

$$\sigma_i^2 = \frac{1}{N} \sum X_i^2 \text{ and } r_{ij} = \frac{Cov(X_i, X_j)}{\sigma_i \sigma_j}, \text{ where } Cov(X_i, X_j) = \frac{1}{N} \sum X_i X_j .$$

Computation of Additive connectivity topological invariants of Molecular structures:

Case: 1 (n- propylamine)

The number of edges with end degrees (1,2) is equal to 2, the number of edges with end degrees (2,2) is equal to 1.

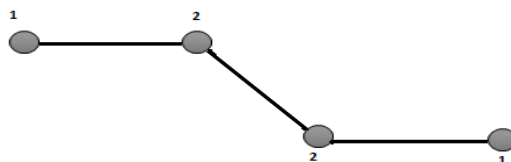


Fig: MS(G₁)

Case: 2(2-aminopropane)

The number of edges with end degrees (1,3) is equal to 3.

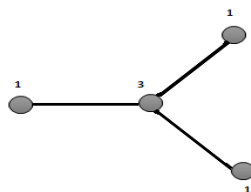


Fig: MS(G₂)

Case: 3(2-amino-2methylpropane)

The number of edges with end degrees (1,4) is equal to 4.

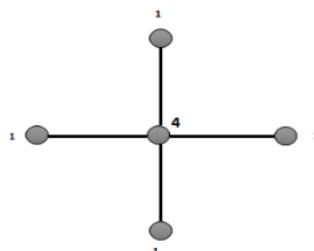


Fig: MS(G₃)

Case: 4(2-merthylpropylamine)

The number of edges with end degrees (1,3) is equal to 2, the number of edges with end degrees (1,2) is equal to 1, the number of edges with end degrees (2,3) is equal to 1.

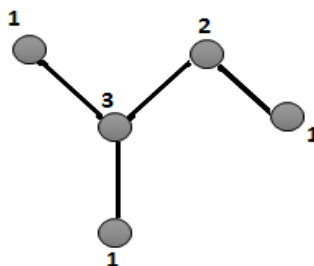


Fig: MS(G₄)

Case: 5(n- butylamine)

The number of edges with end degrees (1,2) is equal to 2, the number of edges with end degrees (2,2) is equal to 2.

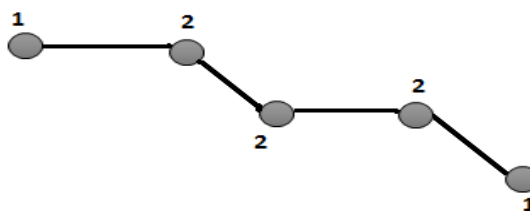


Fig: MS(G₅)

Case: 6(2-amino-2-methylbutane)

The number of edges with end degrees (1,2) is equal to 1, the number of edges with end degrees (1,4) is equal to 3, the number of edges with end degrees (2,4) is equal to 1.

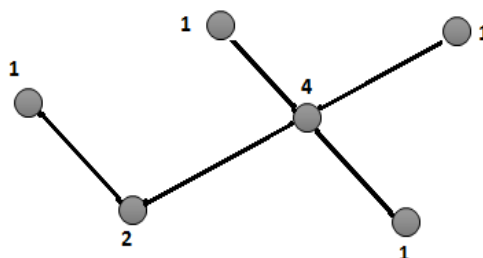


Fig: MS(G₆)

Case: 7(2-aminopentane)

The number of edges with end degrees (1,2) is equal to 2, the number of edges with end degrees (1,3) is equal to 1, the number of edges with end degrees (2,3) is equal to 2.

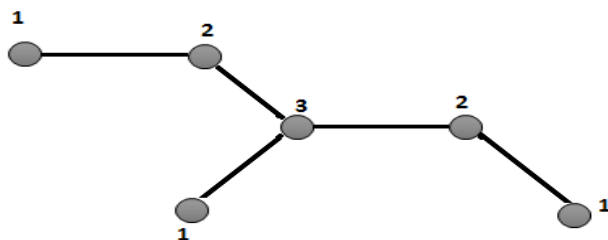


Fig: MS(G₇)

Case: 8(3-methylbutylamine)

The number of edges with end degrees (1,3) is equal to 2, the number of edges with end degrees (2,2) is equal to 1, the number of edges with end degrees (1,2) is equal to 1, the number of edges with end degree (2,3) is equal to 1.

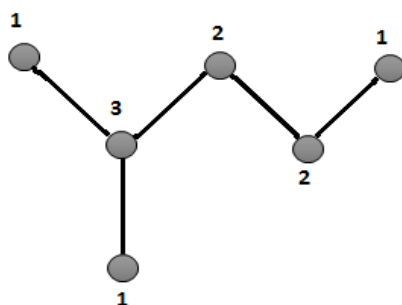


Fig: MS(G₈)

Case: 9 (2-methylbutylamine)

The number of edges with end degrees (1,2) is equal to 2, the number of edges with end degrees (2,3) is equal to 2, the number of edges with end degrees (1,3) is equal to 1.

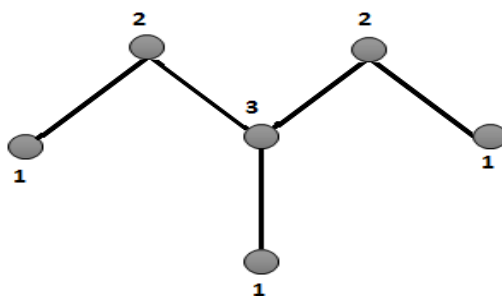


Fig: MS(G₉)

Case: 10 (n- pentylamine)

The number of edges with end degrees (1,2) is equal to 2, the number of edges with end degrees (2,2) is equal to 3.

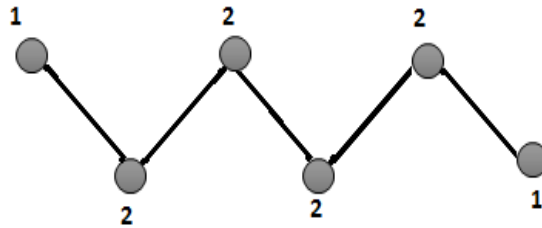


Fig: MS(G_{10})

Case: 11 (4- methylpentylamine)

The number of edges with end degrees (1,2) is equal to 2, the number of edges with end degrees (1,3) is equal to 1, the number of edges with end degrees (2,3) is equal to 1, the number of edges with end degrees (2,2) is equal to 1.

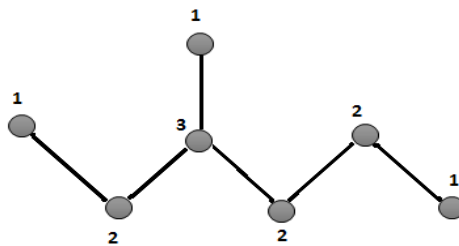


Fig: MS(G_{11})

Case: 12(n- hexylamine)

The number of edges with end degrees (1,2) is equal to 2, the number of edges with end degrees (2,2) is equal to 4.

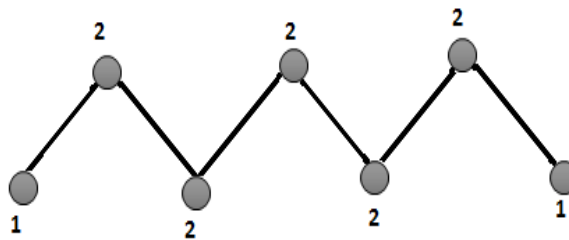


Fig: MS(G_{12})

Case: 13 (3- methylpentylamine)

The number of edges with end degrees (1,2) is equal to 2, the number of edges with end degrees (2,2) is equal to 1, the number of edges with end degrees (2,3) is equal to 2, the number of edges with end degrees (1,3) is equal to 1.

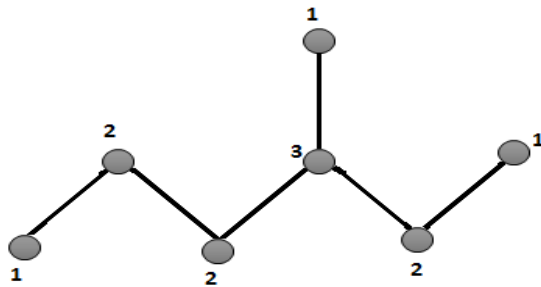


Fig: MS(G_{13})

Case: 14(4- aminoheptane)

The number of edges with end degrees (1,2) is equal to 2, the number of edges with end degrees (2,2) is equal to 2, the number of edges with end degrees (2,3) is equal to 2, the number of edges with end degrees (1,3) is equal to 1.

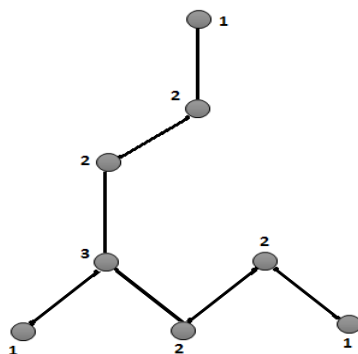


Fig: MS(G_{14})

Case: 15 (2- aminopentane)

The number of edges with end degrees (1,2) is equal to 1, the number of edges with end degrees (2,2) is equal to 3, the number of edges with end degrees (1,3) is equal to 2, the number of edges with end degrees (2,3) is equal to 1.

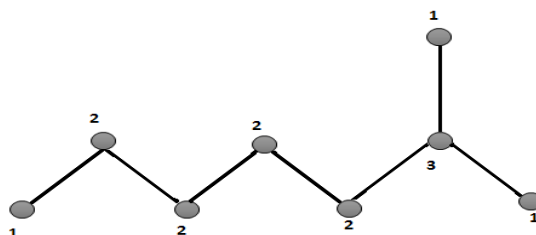


Fig: MS(G_{15})

Case: 16 (n- heptylamine)

Let the number of edges with end degrees (1,2) is equal to 2, the number of edges with end degrees (2,2) is equal to 5.

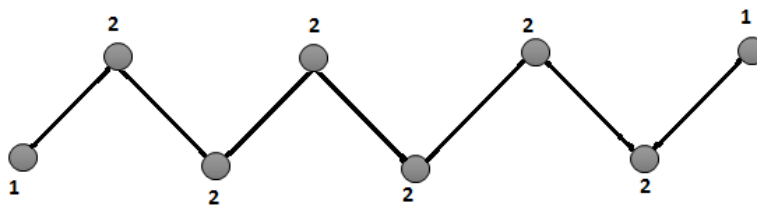


Fig: MS(G_{16})

Case: 17 (n- octylamine)

The number of edges with end degrees (1,2) is equal to 2, the number of edges with end degrees (2,2) is equal to 6.

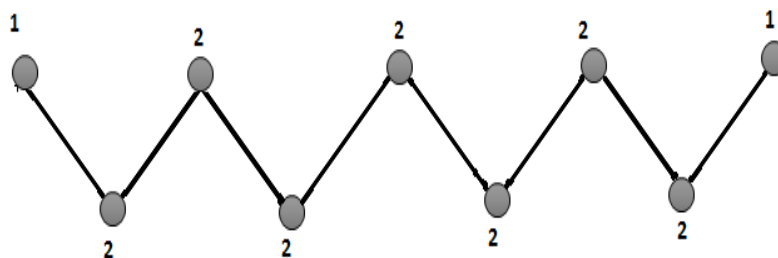


Fig: MS(G_{17})

Case: 18 (Cyclooctane)

The number of edges with end degrees (2,2) is equal to 8.

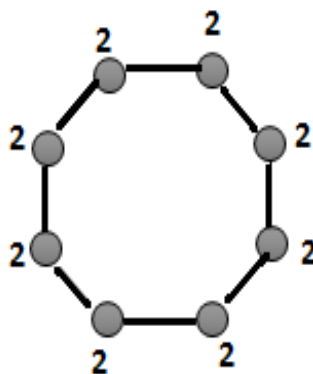


Fig: MS(G_{18})

Case: 19 (2-aminoundecane)

The number of edges with end degrees (1,3) is equal to 4, the number of edges with end degrees (3,3) is equal to 1, the number of edges with end degrees (2,2) is equal to 2, the number of edges with end degrees (2,3) is equal to 6.

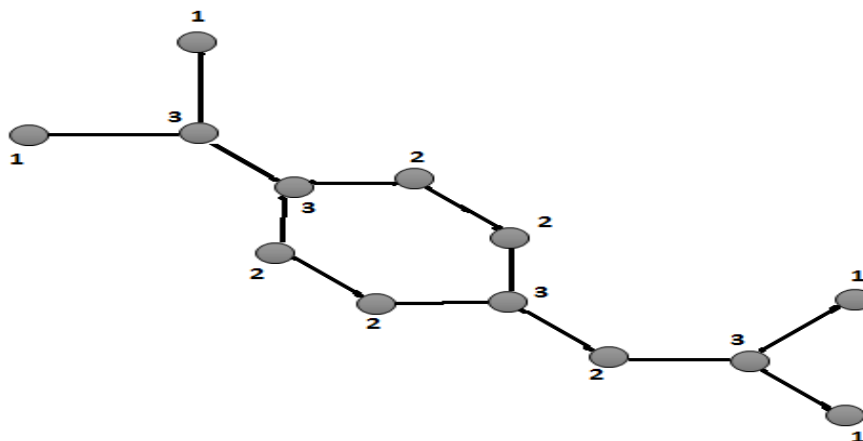


Fig: MS(G₁₉)

Case: 20 (3-aminopentane)

The number of edges with end degrees (1,2) is equal to 2, the number of edges with end degrees (2,2) is equal to 2.

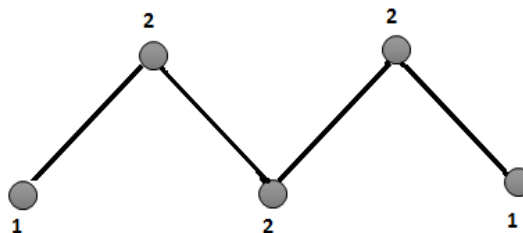


Fig: MS(G₂₀)

Table: 1 : Formulae for Additive connectivity of Degree based Topological invariants :

TOPOLOGICAL INVARIANTS	NOTATION	FORMULAE
Randic index	$\chi(G)$	$\sum_{e \in E(G)} \frac{1}{\sqrt{ij}}$
Geometric-Arithmetic	$GA(G)$	$\sum_{e \in E(G)} \frac{2\sqrt{ij}}{i+j}$
Sum-Connectivity	$SCI(G)$	$\sum_{e \in E(G)} \frac{1}{\sqrt{i+j}}$
Harmonic	$HI(G)$	$\sum_{e \in E(G)} \frac{2}{i+j}$
First Zagreb	$M_1(G)$	$\sum_{e \in E(G)} i+j$

Second Zagreb	$M_2(G)$	$\sum_{e \in E(G)} ij$
Second Modified Zagreb	$M_3(G)$	$\sum_{e \in E(G)} \frac{1}{ij}$
Inverse sum	$IS(G)$	$\sum_{e \in E(G)} \frac{ij}{i+j}$
Alberston	$Alb(G)$	$\sum_{e \in E(G)} i-j $
Atom – Bond connectivity	$ABC(G)$	$\sum_{e \in E(G)} \sqrt{\frac{i+j-2}{ij}}$
Symmetric Division Index	$SD(G)$	$\sum_{e \in E(G)} \frac{i^2 + j^2}{ij}$
Augmented Zagreb	$AZI(G)$	$\sum_{e \in E(G)} \left(\frac{ij}{i+j-2}\right)^3$

Table :2

The additive connectivity degree based topological invariants obtained and its corresponding boiling point of Primary amines.

Primary amines	Additive connectivity degree based of Topological Invariants						Boiling Point
	$\chi(G)$	GA(G)	SCI(G)	HI(G)	$M_1(G)$	$M_2(G)$	
n-Propylamine	1.914	2.885	0.920	1.830	10	8	58.68
2-aminopropane	0.577	2.598	1.500	1.500	12	9	31.11
2-amino-2methylpropane	2.000	3.2	1.788	1.600	20	16	40.68
2-methylpropylamine	2.269	3.653	2.024	2.067	16	14	61.54
n-butylamine	2.414	3.885	2.414	2.330	14	12	75.25
2-amino-2 methylbutane	2.560	4.284	2.326	2.200	24	22	75.25
2-aminopentane	2.807	4.710	2.548	2.630	20	19	92.88

3-methylbutylamine	2.769	4.653	2.524	2.567	20	18	92.88
2 – methylbutylamine	2.807	4.710	2.548	2.630	20	19	88.02
n-pentylamine	2.914	4.885	2.654	2.500	18	16	108.78
4-methylpentylamine	3.308	5.710	3.049	3.133	24	23	123.09
n-hexylamine	3.414	5.885	3.155	3.333	22	20	139.31
3-methylpentylamine	3.049	5.711	3.049	3.133	24	23	123.09
4-aminoheptane	3.808	6.712	3..549	3.633	28	27	150.37
2-aminopentane	3.331	6.655	3.524	3.567	28	26	156.11
n-heptylamine	3.914	6.886	3.655	3.833	26	24	167.63
n-octylamine	4.414	7.884	4.155	4.333	30	28	188..47
Cyclooctane	4.000	8.000	4.000	4.000	32	32	202.26
2-aminoundecane	6.092	12.343	6.016	5.733	60	65	206.52
3-aminopentane	2.414	3.885	2.155	2.333	14	12	88.02

Table : 3 :

The additive connectivity degree based topological invariants obtained and its corresponding boiling point of Primary amines.

Primary amines	Additive connectivity of topological invariants						Boiling Point
	$M_3(G)$	IS(G)	Alb(G)	ABC(G)	SD(G)	AZI(G)	
n-Propylamine	1.250	3.330	2	2.120	7	24.000	58.68
2-aminopropane	1.000	2.250	6	2.449	10	6.750	31.11
2-amino-2methylpropane	1.000	3.200	12	3.464	17	9.480	40.68
2-methylpropylamine	1.334	3.367	6	3.041	11.34	18.750	61.54
n-butylamine	1.500	3.333	2	2.828	9	32.000	75.25
2-amino-2 methylbutane	1.375	4.400	12	4.012	17.75	18.370	75.25
2-aminopentane	1.667	4.483	6	3.644	12.667	35.375	92.88

3-methylbutylamine	1.584	4.370	6	3.753	13.34	30.750	92.88
2 – methylbutylamine	1.667	4.490	6	3.644	12.660	35.375	88.02
n-pentylamine	1.750	4.334	2	3.535	11.000	40.000	108.78
4- methylpentylamine	1.916	5.483	6	4.351	14.667	43.375	123.09
n-hexylamine	3.000	5.333	2	4.242	13.000	48.000	139.31
3- methylpentylamine	1.916	5.083	6	4.351	14.667	43.375	123.09
4-aminoheptane	2.166	6.484	6	5.058	16.667	51.375	150.37
2-aminopentane	2.084	7.117	6	5.167	17.334	46.750	156.11
n-heptylamine	2.250	6.334	2	4.949	15	56.000	167.63
n-octylamine	2.500	7.333	2	5.656	17	64.000	188.47
Cyclooctane	2.000	8.000	0	5.656	16	64.000	202.26
2-aminoundecane	2.944	13.700	14	9.587	32.333	88.891	206.52
3-aminopentane	1.500	3.383	2	2.828	9	32.000	88.02

Table :4:

The correlation coefficient between the additive connectivity degree based topological invariants and boiling point of primary amines.

Topological Invariants	Correlated coefficient(r)
Randic	0.920341769
Geometric - Arithmetic	0.924170328
Sum connectivity	0.921790412
Harmonic	0.956729366
First Zagreb	0.787782829
Second Zagreb	0.778881496
Second Modified Zagreb	0.870389181
Inverse sum	0.871539361
Alberston	-0.15397724
Atom- bond connectivity	0.845502294
Symmetric – Division	0.628727905
Augmented Zagreb	0.960973088

Correlation coefficient between Boiling point and Topological invariants of primary amines:

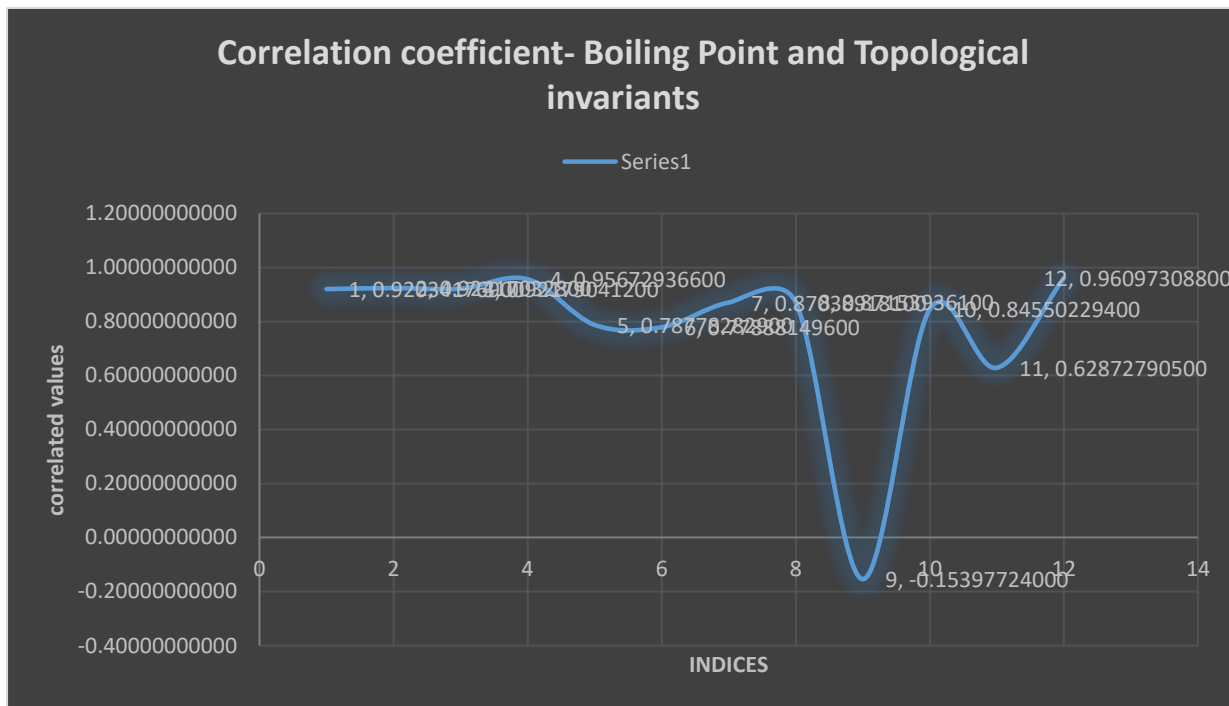


Figure :1

Table:5:

Linear Regression equations of the additive connectivity degree based topological invariants $TI_M(G)$ on boiling point B_p :

Topological Invariants	Regression equation of B_p on $TI_M(G)$	Regression equation of $TI_M(G)$ on B_p
Randic	$B_p = 42.849 TI_M(G) - 16.721$	$TI_M(G) = 0.020 B_p + 0.769$
Geometric - Arithmetic	$B_p = 21.196 TI_M(G) - 2.170$	$TI_M(G) = 0.039 B_p + 1.031$
Sum connectivity	$B_p = 43.430 TI_M(G) - 11.493$	$TI_M(G) = 0.020 B_p + 0.608$
Harmonic	$B_p = 48.255 TI_M(G) - 28.566$	$TI_M(G) = 0.019 B_p + 0.788$
First Zagreb	$B_p = 3.898 TI_M(G) + 23.451$	$TI_M(G) = 0.159 B_p + 5.054$
Second Zagreb	$B_p = 3.376 TI_M(G) + 91.847$	$TI_M(G) = 0.180 B_p + 1.221$
Second Modified Zagreb	$B_p = 81.258 TI_M(G) - 34.393$	$TI_M(G) = 0.009 B_p + 0.799$
Inverse sum	$B_p = 18.068 TI_M(G) + 17.953$	$TI_M(G) = 0.042 B_p + 4.313$
Alberston	$B_p = - 2.120 TI_M(G) + 124.733$	$TI_M(G) = -0.011 B_p + 6.548$
Atom- bond connectivity	$B_p = 27.301 TI_M(G) - 1.631$	$TI_M(G) = 0.026 B_p + 1.266$
Symmetric – Division	$B_p = 6.254 TI_M(G) - 23.621$	$TI_M(G) = 0.063 B_p + 7.221$
Augmented Zagreb	$B_p = 2.527 TI_M(G) + 13.855$	$TI_M(G) = 0.366 B_p - 2.109$

Table : 6

The regression values of Boiling Point (B_p) based on Topological invariants $TI_M(G)$.

Primary amines	Additive connectivity of degree based Topological invariants					
	$\chi(G)$	GA(G)	SCI(G)	HI(G)	$M_1(G)$	$M_2(G)$
n-Propylamine	65.292	58.980	28.463	59.741	62.431	118.855
2-aminopropane	8.003	52.897	53.652	43.817	70.227	122.231
2-amino-2methylpropane	68.977	65.657	66.160	48.642	101.411	145.863
2-methylpropylamine	80.503	75.259	76.409	71.177	85.819	139.111
n-butylamine	86.716	80.176	93.347	83.868	78.023	132.359
2-amino-2 methylbutane	92.972	88.634	89.525	77.595	117.003	166.119
2-aminopentane	103.556	97.663	99.167	98.345	101.411	155.991
3-methylbutylamine	101.928	96.455	98.124	95.305	101.411	152.615
2 – methylbutylamine	103.556	97.663	99.167	98.345	101.411	155.991
n-pentylamine	108.141	101.372	103.770	92.072	93.615	145.863
4-methylpentylamine	125.023	118.859	120.925	122.617	117.003	169.495
n-hexylamine	129.565	122.568	125.529	132.268	109.207	159.367
3-methylpentylamine	113.926	118.880	120.925	122.617	117.003	169.495
4-aminoheptane	146.448	140.098	142.640	146.744	132.595	182.999
2-aminopentane	126.009	138.889	141.554	143.560	132.595	179.623
n-heptylamine	150.990	143.786	147.244	156.395	124.799	172.871
n-octylamine	172.414	164.939	168.959	180.523	140.391	186.375
Cyclooctane	154.675	167.398	162.227	164.454	148.187	199.879
2-aminoundecane	244.315	259.452	249.782	248.080	257.331	311.287
3-aminopentane	86.716	80.176	82.099	84.013	78.023	132.359

Table : 7

The regression values of Boiling Point (B_p) based on Topological Invariants $TI_M(G)$

Primary amines	Additive connectivity of degree based topological invariants					
	$M_3(G)$	IS(G)	Alb(G)	ABC(G)	SD(G)	AZI(G)
n-Propylamine	67.180	78.119	120.493	56.247	20.157	74.503
2-aminopropane	46.865	58.606	112.013	65.229	38.919	30.912
2-amino-2methylpropane	46.865	75.771	99.293	92.940	82.697	37.811
2-methylpropylamine	74.005	78.788	112.013	81.391	47.299	61.236
n-butylamine	87.494	78.174	120.493	75.576	32.665	94.719
2-amino-2 methylbutane	77.337	97.452	99.293	107.901	87.388	60.276
2-aminopentane	101.064	98.952	112.013	97.854	55.598	103.248
3-methylbutylamine	94.320	96.910	112.013	100.830	59.807	91.560
2 – methylbutylamine	101.064	99.078	112.013	97.854	55.555	103.248
n-pentylamine	107.809	96.260	120.493	94.878	45.173	114.935
4-methylpentylamine	121.297	117.020	112.013	117.156	68.106	123.464
n-hexylamine	209.381	114.310	120.493	114.180	57.681	135.151
3-methylpentylamine	121.297	109.793	112.013	117.156	68.106	123.464
4-aminoheptane	141.612	135.106	112.013	136.457	80.614	143.680
2-aminopentane	134.949	146.543	112.013	139.433	84.786	131.992
n-heptylamine	148.438	132.396	120.493	133.482	70.189	155.367
n-octylamine	168.752	150.446	120.493	152.783	82.697	175.583
Cyclooctane	128.123	162.497	124.733	152.783	76.443	175.583
2-aminoundecane	204.831	265.485	95.053	260.104	178.590	238.483
3-aminopentane	87.494	79.077	120.493	75.576	32.665	94.719

Table : 8

The Regression values of Topological invariants $TI_M(G)$ based on boiling point (B_p).

Molecular graphs of Primary amines	Actual Boiling Point (B_p)	Additive connectivity of degree based topological invariants					
		$\chi(G)$	GA(G)	SCI(G)	HI(G)	$M_1(G)$	$M_2(G)$
n-Propylamine	58.68	1.943	3.320	1.782	1.903	14.384	11.783
2-aminopropane	31.11	1.391	2.244	1.230	1.379	10.000	6.821
2-amino-2methylpropane	40.68	1.583	2.618	1.422	1.561	11.522	8.543
2-methylpropylamine	61.54	2.000	3.431	1.839	1.958	14.839	12.298
n-butylamine	75.25	2.274	3.966	2.113	2.218	17.019	14.757
2-amino-2 methylbutane	75.25	2.274	3.966	2.113	2.218	17.019	14.757
2-aminopentane	92.88	2.627	4.653	2.466	2.553	19.822	17.939
3-methylbutylamine	92.88	2.627	4.653	2.466	2.553	19.822	17.939
2 – methylbutylamine	88.02	2.529	4.464	2.368	2.460	19.049	17.065
n-pentylamine	108.78	2.945	5.273	2.784	2.855	22.350	20.801
4-methylpentylamine	123.09	3.231	5.832	3.070	3.127	24.625	23.377
n-hexylamine	139.31	3.555	6.464	3.394	3.435	27.204	26.297
3-methylpentylamine	123.09	3.231	5.832	3.070	3.127	24.625	23.377
4-aminoheptane	150.37	3.776	6.895	3.615	3.645	28.963	28.288
2-aminopentane	156.11	3.891	7.119	3.730	3.754	29.917	29.321
n-heptylamine	167.63	4.122	7.569	3.961	3.973	31.707	31.394
n-octylamine	188.47	4.538	8.381	4.377	4.369	35.027	35.146
Cyclooctane	202.26	4.814	8.919	4.653	4.631	37.213	37.628
2-aminoundecane	206.52	4.899	9.085	4.738	4.712	37.891	38.395
3-aminopentane	88.02	2.529	4.464	2.368	2.460	19.049	17.065

Table : 9

The Regression values of Topological invariants $TI_M(G)$ based on boiling point (B_p).

Molecular graphs of Primary amines	Actual Boiling point (B_p)	Additive connectivity of topological invariants					
		$M_3(G)$	IS(G)	Alb(G)	ABC(G)	SD(G)	AZI(G)
n-Propylamine	58.68	1.327	6.778	5.903	2.792	10.918	19.368
2-aminopropane	31.11	1.079	5.620	6.206	2.075	9.181	9.277
2-amino-2methylpropane	40.68	1.165	6.022	6.101	2.324	9.784	12.780
2-methylpropylamine	61.54	1.353	6.898	5.871	2.866	11.098	20.415
n-butylamine	75.25	1.476	7.474	5.720	3.223	11.962	25.433
2-amino-2 methylbutane	75.25	1.476	7.474	5.720	3.223	11.962	25.433
2-aminopentane	92.88	1.635	8.214	5.526	3.681	13.072	31.885
3-methylbutylamine	92.88	1.635	8.214	5.526	3.681	13.072	31.885
2 – methylbutylamine	88.02	1.591	8.010	5.580	3.555	12.766	30.106
n-pentylamine	108.78	1.778	8.882	5.351	4.094	14.074	37.704
4-methylpentylamine	123.09	1.907	9.483	5.194	4.466	14.976	42.942
n-hexylamine	139.31	2.053	10.164	5.016	4.888	15.998	48.878
3-methylpentylamine	123.09	1.907	9.483	5.194	4.466	14.976	42.942
4-aminoheptane	150.37	2.152	10.629	4.894	5.176	16.694	52.926
2-aminopentane	156.11	2.204	10.870	4.831	5.325	17.056	55.027
n-heptylamine	167.63	2.308	11.353	4.704	5.624	17.782	59.244
n-octylamine	188.47	2.495	12.229	4.475	6.166	19.095	66.871
Cyclooctane	202.26	2.619	12.808	4.323	6.525	19.963	71.918
2-aminoundecane	206.52	2.658	12.987	4.276	6.636	20.232	73.477
3-aminopentane	88.02	1.591	8.010	5.580	3.555	12.766	30.106

Table : 10

The Percentage of error value on Topological invariants $TI_M(G)$ and its Regression values.

Topological Invariants	Percentage error value
Randic	14.8837
Geometric - Arithmetic	14.1026
Sum connectivity	18.2457
Harmonic	5.1028
First Zagreb	22.5430
Second Zagreb	26.9190
Second Modified Zagreb	7.0324
Inverse sum	92.4141
Alberston	67.4709
Atom- bond connectivity	13.0436
Symmetric – Division	21.9689
Augmented Zagreb	20.9070

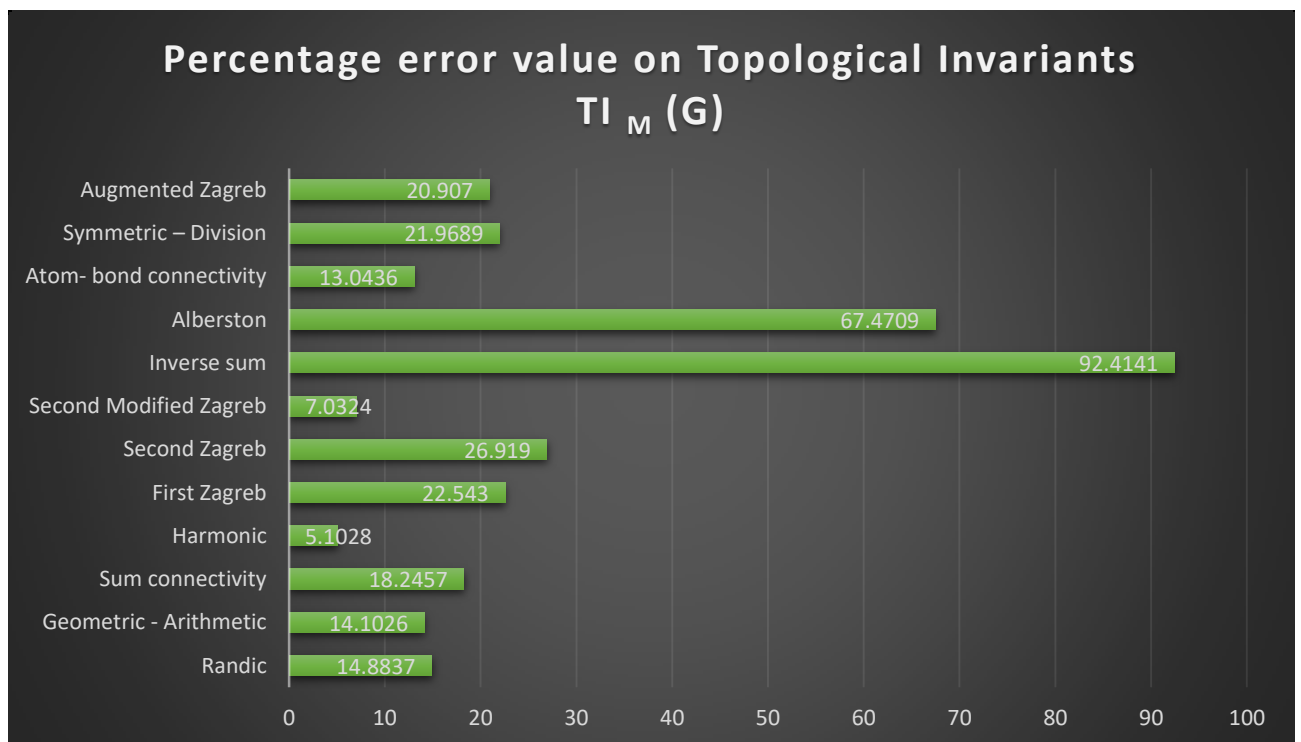


Figure: 2

Table : 11 : The Percentage of error value on Boiling Point (B_p) and its Regression values.

Topological Invariants	Percentage error value
Randic	18.1917
Geometric - Arithmetic	18.7356
Sum connectivity	22.7925
Harmonic	9.9300
First Zagreb	29.6340
Second Zagreb	75.2233
Second Modified Zagreb	13.9139
Inverse sum	24.1055
Alberston	50.0524
Atom- bond connectivity	27.4648
Symmetric – Division	48.4022
Augmented Zagreb	14.8362

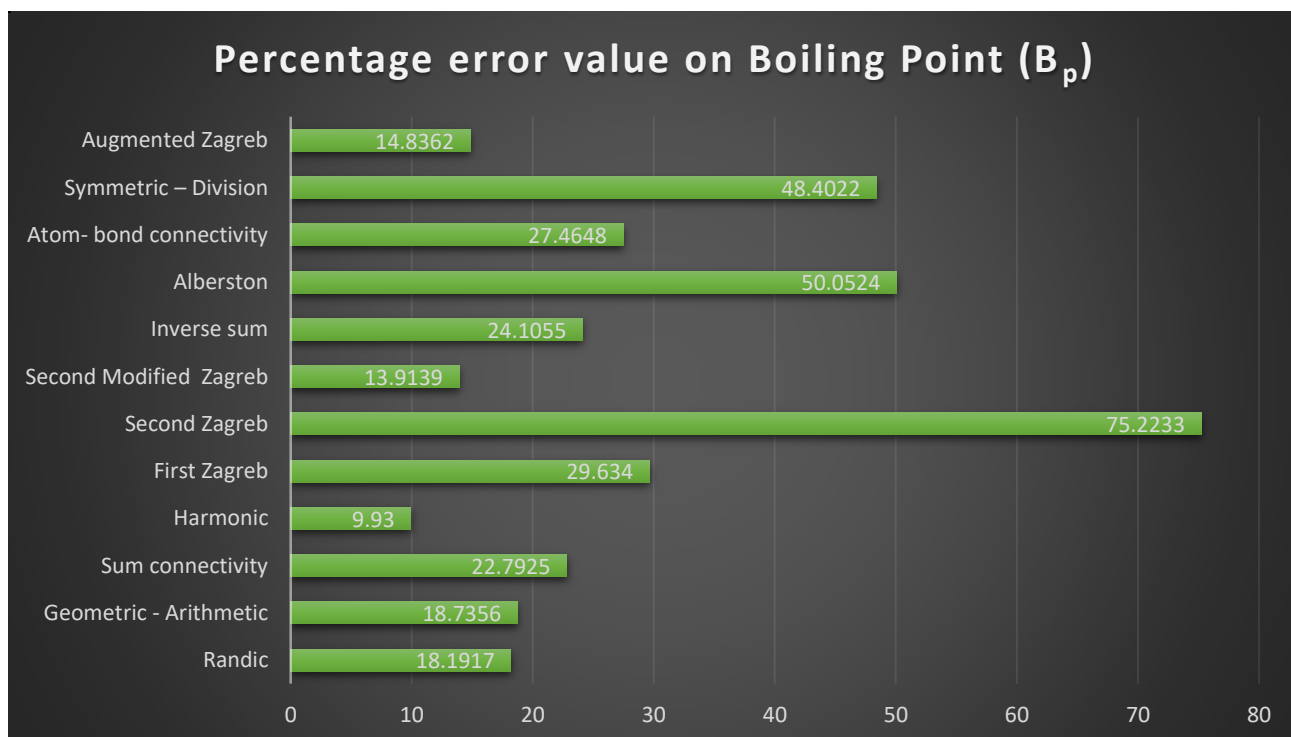


Figure : 3

Table : 12 :

Multiple Regression Analysis computation table:

The values obtained from multiple regression analysis are given below,

Primary amines	(Y)	(X ₁)	(X ₂)	(Y) ²	(X ₁) ²	(X ₂) ²	(YX ₁)	(X ₁ X ₂)	(YX ₂)
n-Propylamine	58.68	1.830	1.250	3443.34	3.3489	1.5625	107.3844	2.2875	73.350
2-aminopropane	31.11	1.500	1.000	967.832	2.2500	1.0000	46.6650	1.5000	31.110
2-amino-2methylpropane	40.68	1.600	1.000	1654.86	2.5600	1.0000	65.0880	1.6000	40.680
2-methylpropylamine	61.54	2.067	1.334	3787.17	4.2725	1.7796	127.2032	2.7574	82.0944
n-butylamine	75.25	2.330	1.500	5662.56	5.4289	2.2500	175.3325	3.4950	112.8750
2-amino-2 methylbutane	75.25	2.200	1.375	5662.56	4.8400	1.8906	165.550	3.0250	103.4688
2-aminopentane	92.88	2.630	1.667	8626.69	6.9169	2.7789	244.2744	4.3842	154.8310
3-methylbutylamine	92.88	2.567	1.584	8626.69	6.5895	2.5091	238.423	4.0661	147.1219
2 – methylbutylamine	88.02	2.630	1.667	7747.52	6.9169	2.7789	231.4926	4.3842	146.7293
n-pentylamine	108.78	2.500	1.750	11833.088	6.2500	3.0625	271.950	4.3750	190.3650
4-methylpentylamine	123.09	3.133	1.916	15151.148	9.8157	3.6711	385.641	6.0028	235.8404
n-hexylamine	139.31	3.333	3.000	19407.276	11.1089	9.0000	464.3202	9.9990	417.9300
3-methylpentylamine	123.09	3.133	1.916	15151.148	9.8157	3.6711	385.641	6.0028	235.8404
4-aminoheptane	150.37	3.633	2.166	22611.137	13.1987	4.6916	546.2942	7.8691	325.7014
2-aminopentane	156.11	3.567	2.084	24370.332	12.7235	4.3431	556.8444	7.4336	325.3332
n-heptylamine	167.63	3.833	2.250	28099.817	14.6919	5.0625	642.5258	8.6243	377.1675
n-octylamine	188.47	4.333	2.500	35520.941	18.7749	6.2500	816.6405	10.8325	471.1750
Cyclooctane	202.26	4.000	2.000	40909.108	16.000	4.0000	809.040	8.0000	404.5200
2-aminoundecane	202.52	5.733	2.944	41014.350	32.8673	8.6671	1161.0472	16.8780	596.2189
3-aminopentane	88.02	2.333	1.500	7747.520	5.44289	2.2500	205.3507	3.4995	132.0300
Total	2265.940	58.8850	36.4030	307995.11	193.8130	72.2183	7646.7079	117.016	4604.382

$$r_{12} = 0.989717, r_{13} = 0.976283, r_{23} = 0.989077$$

$$b_{12.3} = 44.21487, b_{13.2} = -7.88532$$

$$\sigma_1 = 124.0958, \sigma_2 = 3.112981, \sigma_3 = 1.900242$$

Hence, the required equation of the multiple regression is given by

$$Y = 44.21487 X_1 - 7.88532 X_2$$

Table : 13 : Computation of percentage of error based on Multi Regression analysis

REGRESSION VALUE OF HARMONIC INDICES	REGRESSION VALUE OF SECOND MODIFIED ZAGREB	MULTI REGRESSION EQUATION	ACTUAL VALUE BOILING POINT (B_p) OF PRIMARY AMINES	PERCENTAGE ERROR OF (B_p) WITH MULTI REGRESSION	PERCENTAGE ERROR OF (B_p) WITH HARMONIC INDICES	PERCENTAGE ERROR OF (B_p) WITH SECOND MODIFIED ZAGREB
59.741	67.18	71.05657	58.68	0.210916	0.018081	0.144853
43.817	46.865	58.43699	31.11	0.878399	0.408454	0.506429
48.642	46.865	62.85848	40.68	0.545194	0.195723	0.15204
71.177	74.005	80.87313	61.54	0.314155	0.156597	0.202551
83.868	87.494	91.19268	75.25	0.211863	0.114525	0.162711
77.595	77.337	86.43041	75.25	0.148577	0.031163	0.027734
98.345	101.064	103.1403	92.88	0.110468	0.058839	0.088114
95.305	94.32	101.0092	92.88	0.087524	0.026109	0.015504
98.345	101.064	103.1403	88.02	0.171782	0.117303	0.148194
92.072	107.809	96.73787	108.78	0.110702	0.153594	0.008926
122.617	121.297	123.4169	123.09	0.002656	0.003843	0.014567
132.268	209.381	123.7122	139.31	0.111965	0.050549	0.502986
122.617	121.297	123.4169	123.09	0.002656	0.003843	0.014567
146.744	141.612	143.553	150.37	0.045335	0.024114	0.058243
143.56	134.949	141.2814	156.11	0.094988	0.080392	0.135552
156.395	148.438	151.7336	167.63	0.09483	0.067023	0.11449
180.523	168.752	171.8697	188.47	0.088079	0.042166	0.104621
164.454	128.123	161.0889	202.26	0.203556	0.186918	0.366543
248.08	204.831	230.2695	202.52	0.137021	0.224965	0.011411
84.013	87.494	91.32532	88.02	0.037552	0.045524	0.005976

Result and discussion: Table one gives the formulae considered in this research for additive connectivity invariants of degree based topological invariants. In table two, the obtain the results of the values of the additive connectivity of degree based topological invariants its corresponding boiling point of primary amines from Randic invariants to second Zagreb invariants are made known. In table three, the obtained the results of the values of the additive connectivity of degree based topological invariants its corresponding boiling point of primary amines from second modified Zagreb to Augmented Zagreb are tabulated.

In table four and five, the correlation coefficient is presented and the Regression equations between the topological invariants and boiling point of Primary amines are given away. In table six and seven, the corresponding regression values of Boiling point based on Topological invariants and vice-versa are revealed. In table eight and nine, the corresponding linear regression analysis value of topological invariants based on boiling point and vice-versa are tabulated. In table ten and eleven, the percentage error on topological invariants and boiling point are exposed. In table twelve, the multiple regression analysis using the Invariants Harmonic and second modified Zagreb with its corresponding values of Primary amines are performed. Finally, based on the analysis we sampled twelve variance results which are also called as indices. On applying error percentage, the indices having the lowest error values are considered for the multiple regression analysis. First close result is harmonic and the second value is second modified Zagreb. By comparing both of the indices harmonic value results gives the closest match and gives higher yield or performance.

Conclusion: The present study is an attempt to explore correlating ability of a newly proposed topological index, in predicting physical properties and biological activities. With regard to various physical properties, linear analysis has been performed on all the datasets. It has been found that linear regression analysis could give better correlation coefficients. The obtained Mean percentage error as compared to linear regression analysis, it is showing that the harmonic index value results is the most least value if it is compared with remaining topological invariants.

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