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Application of the Tosha Index in QSPR Modeling of Lower Alkanes

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ABSTRACT: In this article, a Quantitative Structure-Property Relationship (QSPR) analysis was performed to show that the Tosha index is an effective molecular descriptor for predicting the physicochemical properties of lower alkanes. Logarithmic regression models were employed to establish quantitative correlations between the Tosha index and various physical properties of lower alkanes, including boiling points (bp) $^{\circ}C$, molar volumes (mv) cm^3, molar refractions (mr) cm^3, heats of vaporisation (hv) kJ, critical temperatures (ct) $^{\circ}C$, critical pressures (cp) atm, and surface tensions (st) dyne cm^{-1}. The analysis shows that the Tosha index is a reliable and statistically significant predictive framework for these compounds. This emphasizes its potential applications in theoretical chemistry and molecular property estimation. Overall, the study emphasizes the significance of graph-theoretical indices in cheminformatics and encourages the creation of effective predictive models for simple hydrocarbon systems such as lower alkanes.

Key Words: Geodesic, tension on an edge, topological index.

Contents

1. Introduction

Mathematical chemistry studies molecular structures using mathematical methods. These methods solve a wide range of chemistry problems. Chemical graph theory connects chemistry and graph theory, and it uses graph theory to solve many of mathematical chemistry's most difficult problems. A topological index of a chemical structure (graph) is a number that relates the chemical structure to its reactivity or physical properties. Topological indices of big chemical structures, like metal-organic frameworks, are very helpful for understanding these structures and figuring out their physical and chemical properties, which would be hard to calculate for such large networks important in reticular chemistry. Topological indices are numbers that show the structural features of molecules by using ideas from graph theory on large networks important in reticular chemistry. As a result, every topological index defined on graphs using degrees, distances, shortest paths, and so on must account for some chemical properties of molecules. As a result, there is potential for developing new topological indices for graphs.

For standard terminology and notion in graphs, we refer the reader to the text-book of Harary [4]. The non-standard will be given in this paper as and when required.

Throughout this paper, $G = (V, E)$ denotes a graph (finite, undirected and simple) and $V = V(G)$ and $E = E(G)$ denote vertex set and edge set of G, respectively. Two non-distinct edges in a graph are adjacent if they are incident on a common vertex. We consider that an edge in a graph is not adjacent to itself. The degree of a vertex v in a graph G is the number of edges associated with it and is denoted by $d(v)$.

The distance between two vertices u and v in G, denoted by $d(u, v)$ is the number of edges in a shortest path (also called a graph geodesic) connecting them. We say that a graph geodesic P is passing through

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an edge e in G if e is an edge in P. The number of geodesics in G is denoted by f.

The notion of tension on edge in a graph has been studied recently by K. Bhargava, N.N. Dattatreya, and R. Rajendra in their paper [3]. Let G be a graph and e be an edge in G. The tension on e, denoted by $\tau_G(e)$ or simply $\tau(e)$, is defined as the number of geodesics in G passing through e. A graph G is said to be k-tension-regular if all its edges are of tension k.

The total tension of G, denoted by $N_\tau(G)$, is defined as:

$$N_\tau(G) = \sum_{e \in E} \tau(e). \tag{1.1}$$

The Tosha index $T(G)$ [22] of a graph G is defined by

$$T(G) = \sum_{e \in E(G)} \tau(e)^2. \tag{1.2}$$

For stress/tension based topological indices, we suggest the reader to refer the papers [1,2,6-13,15-26,29-31].

The experimental values for the physical properties - boiling points (bp) $^\circ C$, molar volumes (mv) cm^3, molar refractions (mr) cm^3, heats of vaporization (hv) kJ, critical temperatures (ct) $^\circ C$, critical pressures (cp) atm, and surface tensions(st) $dyne\ cm^{-1}$ of considered lower alkanes are presented in the following Table 1. For QSPR analysis for $T(G)$ of molecular graphs with the physical properties of lower alkanes we use this data. For the experimental data of numerical values in columns 2 to 8 of the Table 1 one can refer [14] or [32].

Table 1: The experimental numerical values of the physical properties of low alkanes

Alkane	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
Pentane	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	27.9	116.4	25.29	24.6	187.8	32.9	15
2,2-Dimethylpropane	9.5	122.1	25.72	21.8	160.6	31.6	
Hexane	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylhexane	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	115.6	160.4	38.98	38.8	293	26.6	20.99

2,4-Dimethylhexane	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	141.6	169.9	43.2	41.8	334.5	26.85	23.31

2. Tosha Index as a Molecular Descriptor

Any graph representing a molecular structure can be given a mathematical formula known as a topological index, also called a molecular descriptor. Using this topological index, one can investigate various physicochemical features of molecules and assess mathematical values. Consequently, it is a practical method for evading labor-intensive and expensive laboratory tests.

To build regression models and investigate correlations between the physical attributes and the structure of the compounds, quantitative structure-property relationship (QSPR) investigations are employed to convert the physical properties of chemical compounds into numerical data. Several topological indices have been investigated using QSPR.

We perform a QSPR study for $T(G)$ of molecular graphs of lower alkanes with their physical characteristics in this part. The $T(G)$ of molecular graphs were calculated using Eq.(1.2). Table 2 lists the calculated $T(G)$ values of molecular graphs. QSPR analysis is performed using the experimental values of the physical properties of the considered lower alkanes listed in Table 1, such as boiling points (bp) $^{\circ}C$, molar volumes (mv) cm^3, molar refractions (mr) cm^3, heats of vaporisation (hv) kJ, critical temperatures (ct) $^{\circ}C$, critical pressures (cp) atm, and surface tensions (st) $dyne\ cm^{-1}$.

Table 2: $T(G)$ of Lower Alkanes

Alkane	T_G	Alkane	T_G
Pentane	104	2-Methyloctane	1836
2-Methylbutane	84	3-Methyloctane	1708
2,2-Dimethylpropane	64	4-Methyloctane	1632
Hexane	259	3-Ethylheptane	1504
2-Methylpentane	220	4-Ethylheptane	1428
3-Methylpentane	203	2,2-Dimethylheptane	1576
2,3-Dimethylbutane	164	2,3-Dimethylheptane	1500
2,2-Dimethylbutane	181	2,4-Dimethylheptane	1500
Heptane	560	2,5-Dimethylheptane	1576
2-Methylhexane	496	2,6-Dimethylheptane	1704
3-Methylhexane	452	3,3-Dimethylheptane	1372
3-Ethylpentane	408	3,4-Dimethylheptane	1372
2,3-Dimethylpentane	388	3,5-Dimethylheptane	1448
2,4-Dimethylpentane	388	4,4-Dimethylheptane	1296
2,2-Dimethylpentane	432	3-Ethyl-2-methylhexane	1296
3,3-Dimethylpentane	344	4-Ethyl-2-methylhexane	1372
2,3,3-Trimethylbutane	324	3-Ethyl-3-methylhexane	1168
Octane	1092	3-Ethyl-4-methylhexane	1504
2-Methylheptane	997	2,3,3-Trimethylhexane	1164
3-Methylheptane	916	2,3,4-Trimethylhexane	1240
4-Methylheptane	885	2,3,5-Trimethylpentane	1368
4-Ethylhexane	804	2,4,4-Trimethylhexane	1240
2,2-Dimethylhexane	821	3,3,4-Trimethylhexane	1112
2,3-Dimethylhexane	790	2,2,3-Trimethylhexane	1240
2,4-Dimethylhexane	821	2,2,4-Trimethylhexane	1316
2,5-Dimethylhexane	902	2,2,5-Trimethylhexane	1444
3,3-Dimethylhexane	709	3,3-Diethylpentane	1040
3,4-Dimethylhexane	740	2,2-Diethyl-3-ethylpentane	1112
3-Ethyl-3-methylpentane	709	2,3-Diethyl-3-ethylpentane	1036
3-Ethyl-2-methylpentane	628	2,4-Diethyl-3-ethylpentane	1164
2,3,3-Trimethylpentane	645	2,2,3,3-Tetramethylpentane	980
2,3,4-Trimethylpentane	726	2,2,3,4-Tetramethylpentane	1108
2,2,3-Trimethylpentane	614	2,2,4,4-Tetramethylpentane	1184
2,2,4-Trimethylpentane	695	2,3,3,4-Tetramethylpentane	1032
Nonane	1968		

3. Logarithmic Regression Model

Regression analysis is a statistical technique that models a dependent variable and one or more independent variables and examines the relationship between them. In a variety of fields, including economics, finance, the social sciences, and engineering, it is widely used to understand how independent factors affect the dependent variable and to produce forecasts or estimates.

Finding the line or curve that most accurately depicts the relationship between the variables is the basic

tenet of regression analysis. The dependent variable (also known as the response variable) is the one we are trying to predict or explain. Independent variables, also called predictor variables or explanatory variables, are the variables that are projected to have an effect on the dependent variable.
We used the SPSS program for these analyses. While there are many different types of regression analysis, the most popular kind is basic linear regression, which requires only one independent variable. Basic linear regression assumes that there is a linear relationship between the variables. The line's equation is displayed as:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \cdots + \beta_z X_z + \varepsilon$$

where Y is the dependent variable, β_0 is the Y-intercept, β_i is the coefficient of the independent variable for $i = 1, \ldots, z$, X is the independent variable, and ε is the error term.
By estimating the values of β_0 and β_1, regression analysis seeks to minimize the sum of squared differences between the observed values of Y and the expected values from the model. This estimation procedure frequently employs the least squares method. Additionally, regression analysis provides a number of statistical metrics to assess the quality of the model, including the coefficient of determination (R^2), which indicates the proportion of the variance of the dependent variable that can be explained by the independent variables.
Regression analysis is a powerful tool for determining the relationships between variables, creating predictions, and examining cause-and-effect relationships. It is extensively utilized in numerous fields for research, data analysis, and decision-making.
A statistical technique called logarithmic regression analysis, logarithmic transformation, or log-linear regression is used to model the relationship between a dependent variable and one or more independent variables when a logarithmic scale may more accurately symbolize the relationship. The logarithmic model is expressed as:

$$Y = \beta_0 + \beta_1 \log X_1 + \beta_2 \log X_2 + \beta_3 \log X_3 + \cdots + \beta_z \log X_z + \varepsilon$$

where Y is the dependent variable, β_0 is the Y-intercept, β_i is the coefficient of the independent variable, log is the logarithmic function, and ε is the error term.
Relationships in which the independent variables have multiplicative rather than additive effects on the dependent variable can be modeled using the logarithmic transformation. It is commonly used in situations where there is a curvilinear relationship between the variables, meaning that rates of change or declining returns are both present.
Economic, financial, biological, and environmental sciences are just a few of the fields in which logarithmic regression can be used to analyze data. Researchers can use the logarithmic scale to make predictions or derive insights, as well as to document and assess non-linear correlations between variables.

Table 3: Statistical Analysis of Tosha Index in QSPR Modeling

Y	r	r^2	S_E	F	Sig
bp	0.973	0.946	7.307	964.919	0.000
mv	0.982	0.965	3.142	1816.401	0.000
mr	0.975	0.952	1.112	1295.003	0.000
hv	0.972	0.945	1.178	1129.849	0.000
ct	0.913	0.833	14.295	329.337	0.000
cp	0.943	0.890	0.854	533.364	0.000
st	0.843	0.711	1.045	162.311	0.000

For the physical properties - bp, mv, mr, hv, ct, cp and st of low alkanes, the logarithmic regression models are displayed below:

$$bp = 39.674 \cdot ln(T(G)) - 149.498 \tag{3.1}$$

$$mv = 23.103 \cdot ln(T(G)) + 8.589 \tag{3.2}$$

$$mr = 6.903 \cdot ln(T(G)) - 6.522 \tag{3.3}$$

$$hv = 6.831 \cdot ln(T(G)) - 6.681 \tag{3.4}$$
$$ct = 44.763 \cdot ln(T(G)) - 6.445 \tag{3.5}$$
$$cp = -3.404 \cdot ln(T(G)) + 49.003 \tag{3.6}$$
$$st = 2.297 \cdot ln(T(G)) + 5.563 \tag{3.7}$$

Figure 1: Graphical representation of the scattered points and its logarithmic fit using $T(G)$ for boiling points.

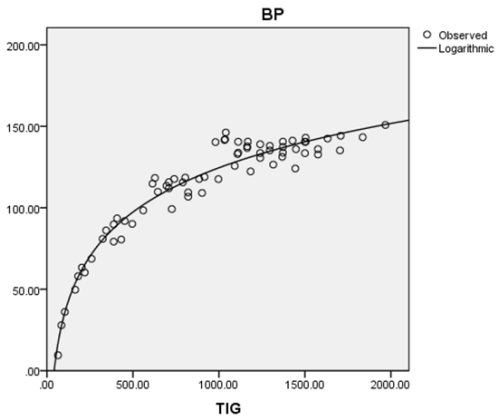

Figure 2: Graphical representation of the scattered points and its logarithmic fit using $T(G)$ for molar volumes.

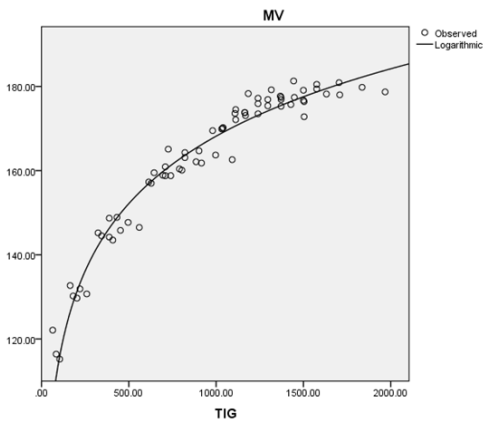

Figure 3: Graphical representation of the scattered points and its logarithmic fit using $T(G)$ for molar refractions.

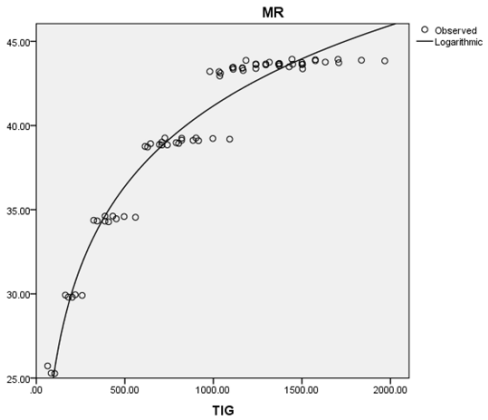

Figure 4: Graphical representation of the scattered points and its logarithmic fit using $T(G)$ for heats of vaporisation.

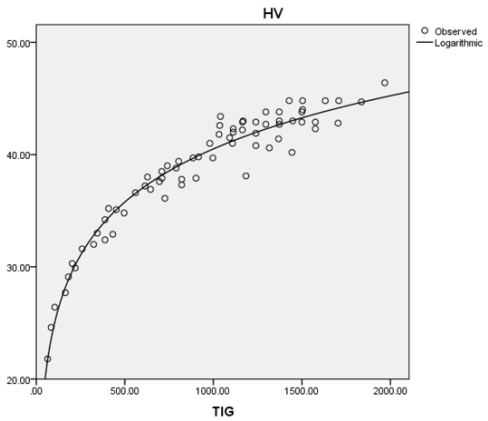

Figure 5: Graphical representation of the scattered points and its logarithmic fit using $T(G)$ for critical temperatures.

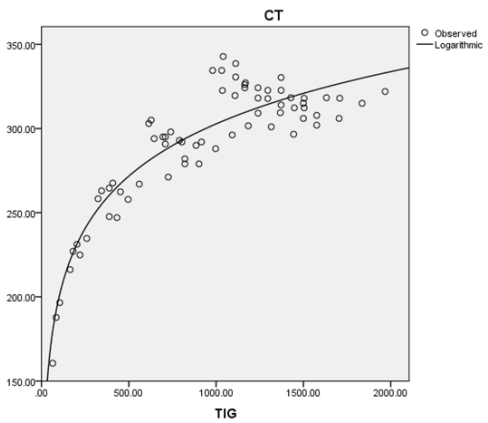

Figure 6: Graphical representation of the scattered points and its logarithmic fit using $T(G)$ for critical pressures.

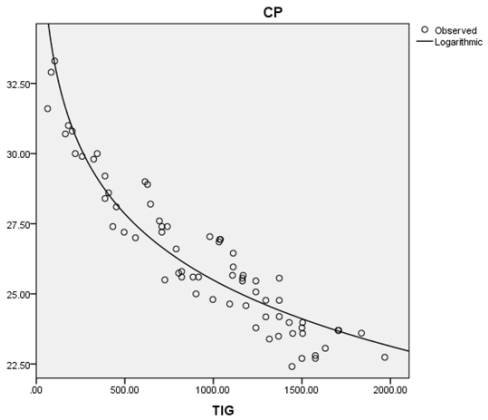

Figure 7: Graphical representation of the scattered points and its logarithmic fit using $T(G)$ for surface tensions.

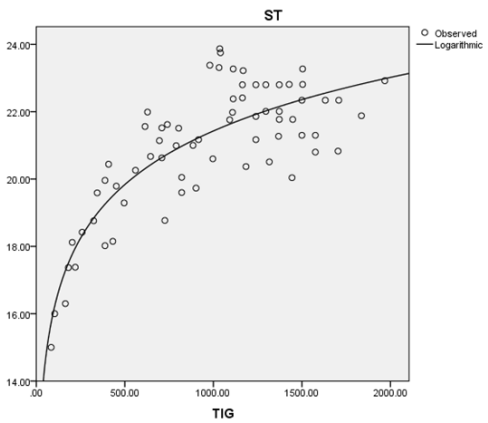

Table 4: Comparison of boiling point (BP) between experimental and predicted values

Alkane	**BP from experiments**	**BP computed using regression model**
Pentane	36.1	34.8
2-Methylbutane	27.9	26.3
2,2-Dimethylpropane	9.5	15.6
Hexane	68.7	71
2-Methylpentane	60.3	64.5
3-Methylpentane	63.3	61.3
2,2-Dimethylbutane	49.7	52.9
2,3-Dimethylbutane	58	56.8
Heptane	98.4	101.6
2-Methylhexane	90.1	96.8
3-Methylhexane	91.9	93.1
3-Ethylhexane	93.5	89
2,2-Dimethylpentane	79.2	87
2,3-Dimethylpentane	89.8	87
2,4-Dimethylpentane	80.5	91.3
3,3-Dimethylpentane	86.1	82.3
2,3,3-Trimethylbutane	80.9	79.9

Alkane	BP from experiments	BP computed using regression model
Octane	125.7	128.1
2-Methylheptane	117.6	124.5
3-Methylheptane	118.9	121.1
4-Methylheptane	117.7	119.8
3-Ethylhexane	118.5	116
2,2-Dimethylhexane	106.8	116.8
2,3-Dimethylhexane	115.6	115.3
2,4-Dimethylhexane	109.4	116.8
2,5-Dimethylhexane	109.1	120.5
3,3-Dimethylhexane	112	111
3,4-Dimethylhexane	117.7	112.7
3-Ethyl-2-methylpentane	115.7	111
3-Ethyl-3-methylpentane	118.3	106.2
2,2,3-Trimethylpentane	109.8	107.2
2,2,4-Trimethylpentane	99.2	111.9
2,3,3-Trimethylpentane	114.8	105.3
2,3,4-Trimethylpentane	113.5	110.2
Nonane	150.8	151.5
2-Methyloctane	143.3	148.7
3-Methyloctane	144.2	145.8
4-Methyloctane	142.5	144
3-Ethylheptane	143	140.8
4-Ethylheptane	141.2	138.7
2,2-Dimethylheptane	132.7	142.7
2,3-Dimethylheptane	140.5	140.7
2,4-Dimethylheptane	133.5	140.7
2,5-Dimethylheptane	136	142.7
2,6-Dimethylheptane	135.2	145.8
3,3-Dimethylheptane	137.3	137.2
3,4-Dimethylheptane	140.6	137.2
3,5-Dimethylheptane	136	139.3
4,4-Dimethylheptane	135.2	134.9
3-Ethyl-2-methylhexane	138	134.9
4-Ethyl-2-methylhexane	133.8	137.2
3-Ethyl-3-methylhexane	140.6	130.8
3-Ethyl-4-methylhexane	140.46	140.8
2,2,3-Trimethylhexane	133.6	133.1
2,2,4-Trimethylhexane	126.5	135.5
2,2,5-Trimethylhexane	124.1	139.2
2,3,3-Trimethylhexane	137.7	130.6
2,3,4-Trimethylhexane	139	133.1
2,3,5-Trimethylpentane	131.3	137
2,4,4-Trimethylhexane	130.6	133.1
3,3,4-Trimethylhexane	140.5	128.8
3,3-Diethylpentane	146.2	126.2
2,2-Dimethyl-3-ethylpentane	133.8	128.8
2,3-Dimethyl-3-ethylpentane	142	126
2,4-Dimethyl-3-ethylpentane	136.7	130.6
2,2,3,3-Tetramethylpentane	140.3	123.8
2,2,3,4-Tetramethylpentane	133	128.7
2,2,4,4-Tetramethylpentane	122.3	131.3
2,3,3,4-Tetramethylpentane	141.6	125.9

Table 5: Comparison of molar volume (MV) between experimental and predicted values

Alkane	**MV from experiments**	**MV computed using regression model**
Pentane	115.2	115.9
2-Methylbutane	116.4	111
2,2-Dimethylpropane	122.1	104.7
Hexane	130.7	137
2-Methylpentane	131.9	133.2
3-Methylpentane	129.7	131.4
2,2-Dimethylbutane	132.7	126.5
2,3-Dimethylbutane	130.2	128.7
Heptane	146.5	154.8
2-Methylhexane	147.7	152
3-Methylhexane	145.8	149.9
3-Ethylhexane	143.5	147.5
2,2-Dimethylpentane	148.7	146.4
2,3-Dimethylpentane	144.2	146.4
2,4-Dimethylpentane	148.9	148.8
3,3-Dimethylpentane	144.5	143.6
2,3,3-Trimethylbutane	145.2	142.2
Octane	162.6	170.3
2-Methylheptane	163.7	168.2
3-Methylheptane	161.8	166.2
4-Methylheptane	162.1	165.4
3-Ethylhexane	160.1	163.2
2,2-Dimethylhexane	164.3	163.7
2,3-Dimethylhexane	160.4	162.8
2,4-Dimethylhexane	163.1	163.7
2,5-Dimethylhexane	164.7	165.8
3,3-Dimethylhexane	160.9	160.3
3,4-Dimethylhexane	158.8	161.3
3-Ethyl-2-methylpentane	158.8	160.3
3-Ethyl-3-methylpentane	157	157.5
2,2,3-Trimethylpentane	159.5	158.1
2,2,4-Trimethylpentane	165.1	160.8
2,3,3-Trimethylpentane	157.3	157
2,3,4-Trimethylpentane	158.9	159.8
Nonane	178.7	183.9
2-Methyloctane	179.8	182.3
3-Methyloctane	178	180.6
4-Methyloctane	178.2	179.5
3-Ethylheptane	176.4	177.7
4-Ethylheptane	175.7	176.5
2,2-Dimethylheptane	180.5	178.7
2,3-Dimethylheptane	176.7	177.6
2,4-Dimethylheptane	179.1	177.6
2,5-Dimethylheptane	179.4	178.7
2,6-Dimethylheptane	180.9	180.5
3,3-Dimethylheptane	176.9	175.5
3,4-Dimethylheptane	175.3	175.5
3,5-Dimethylheptane	177.4	176.8
4,4-Dimethylheptane	176.9	174.2
3-Ethyl-2-methylhexane	175.4	174.2
4-Ethyl-2-methylhexane	177.4	175.5
3-Ethyl-3-methylhexane	173.1	171.8
3-Ethyl-4-methylhexane	172.8	177.7
2,2,3-Trimethylhexane	175.9	173.2

Alkane	MV from experiments	MV computed using regression model
2,2,4-Trimethylhexane	179.2	174.6
2,2,5-Trimethylhexane	181.3	176.7
2,3,3-Trimethylhexane	173.8	171.7
2,3,4-Trimethylhexane	173.5	173.2
2,3,5-Trimethylpentane	177.7	175.5
2,4,4-Trimethylhexane	177.2	173.2
3,3,4-Trimethylhexane	172.1	170.7
3,3-Diethylpentane	170.2	169.1
2,2-Dimethyl-3-ethylpentane	174.5	170.7
2,3-Dimethyl-3-ethylpentane	170.1	169
2,4-Dimethyl-3-ethylpentane	173.8	171.7
2,2,3,3-Tetramethylpentane	169.5	167.8
2,2,3,4-Tetramethylpentane	173.6	170.6
2,2,4,4-Tetramethylpentane	178.3	172.1
2,3,3,4-Tetramethylpentane	169.9	169

Table 6: Comparison of molar refractivity (MR) between experimental and predicted values

Alkane	MR from experiments	MR computed using regression model
Pentane	25.27	25.6
2-Methylbutane	25.29	24.1
2,2-Dimethylpropane	25.72	22.2
Hexane	29.91	31.9
2-Methylpentane	29.95	30.8
3-Methylpentane	29.8	30.2
2,2-Dimethylbutane	29.93	28.7
2,3-Dimethylbutane	29.81	29.4
Heptane	34.55	37.2
2-Methylhexane	34.59	36.4
3-Methylhexane	34.46	35.7
3-Ethylhexane	34.28	35
2,2-Dimethylpentane	34.62	34.7
2,3-Dimethylpentane	34.32	34.7
2,4-Dimethylpentane	34.62	35.4
3,3-Dimethylpentane	34.33	33.8
2,3,3-Trimethylbutane	34.37	33.4
Octane	39.19	41.8
2-Methylheptane	39.23	41.2
3-Methylheptane	39.1	40.6
4-Methylheptane	39.12	40.4
3-Ethylhexane	38.94	39.7
2,2-Dimethylhexane	39.25	39.9
2,3-Dimethylhexane	38.98	39.6
2,4-Dimethylhexane	39.13	39.9
2,5-Dimethylhexane	39.26	40.5
3,3-Dimethylhexane	39.01	38.8
3,4-Dimethylhexane	38.85	39.1
3-Ethyl-2-methylpentane	38.84	38.8
3-Ethyl-3-methylpentane	38.72	38
2,2,3-Trimethylpentane	38.92	38.2
2,2,4-Trimethylpentane	39.26	39
2,3,3-Trimethylpentane	38.76	37.8
2,3,4-Trimethylpentane	38.87	38.7
Nonane	43.84	45.9
2-Methyloctane	43.88	45.4

Alkane	MR from experiments	MR computed using regression model
3-Methyloctane	43.73	44.9
4-Methyloctane	43.77	44.6
3-Ethylheptane	43.64	44
4-Ethylheptane	43.49	43.7
2,2-Dimethylheptane	43.91	44.4
2,3-Dimethylheptane	43.63	44
2,4-Dimethylheptane	43.74	44
2,5-Dimethylheptane	43.85	44.4
2,6-Dimethylheptane	43.93	44.9
3,3-Dimethylheptane	43.69	43.4
3,4-Dimethylheptane	43.55	43.4
3,5-Dimethylheptane	43.64	43.8
4,4-Dimethylheptane	43.6	43
3-Ethyl-2-methylhexane	43.66	43
4-Ethyl-2-methylhexane	43.65	43.4
3-Ethyl-3-methylhexane	43.27	42.3
3-Ethyl-4-methylhexane	43.37	44
2,2,3-Trimethylhexane	43.62	42.7
2,2,4-Trimethylhexane	43.76	43.1
2,2,5-Trimethylhexane	43.94	43.7
2,3,3-Trimethylhexane	43.43	42.3
2,3,4-Trimethylhexane	43.39	42.7
2,3,5-Trimethylpentane	43.65	43.4
2,4,4-Trimethylhexane	43.66	42.7
3,3,4-Trimethylhexane	43.34	41.9
3,3-Diethylpentane	43.11	41.5
2,2-Dimethyl-3-ethylpentane	43.46	41.9
2,3-Dimethyl-3-ethylpentane	42.95	41.5
2,4-Dimethyl-3-ethylpentane	43.4	42.3
2,2,3,3-Tetramethylpentane	43.21	41.1
2,2,3,4-Tetramethylpentane	43.44	41.9
2,2,4,4-Tetramethylpentane	43.87	42.4
2,3,3,4-Tetramethylpentane	43.2	41.4

Table 7: Comparison of heats of vaporisation (HV) between experimental and predicted values

Alkane	HV from experiments	HV computed using regression model
Pentane	26.4	25.1
2-Methylbutane	24.6	23.6
2,2-Dimethylpropane	21.8	21.8
Hexane	31.6	31.3
2-Methylpentane	29.9	30.2
3-Methylpentane	30.3	29.7
2,2-Dimethylbutane	27.7	28.2
2,3-Dimethylbutane	29.1	28.9
Heptane	36.6	36.6
2-Methylhexane	34.8	35.8
3-Methylhexane	35.1	35.1
3-Ethylhexane	35.2	34.4
2,2-Dimethylpentane	32.4	34.1
2,3-Dimethylpentane	34.2	34.1
2,4-Dimethylpentane	32.9	34.8
3,3-Dimethylpentane	33	33.3
2,3,3-Trimethylbutane	32	32.9
Octane	41.5	41.2

Alkane	HV from experiments	HV computed using regression model
2-Methylheptane	39.7	40.5
3-Methylheptane	39.8	40
4-Methylheptane	39.7	39.7
3-Ethylhexane	39.4	39.1
2,2-Dimethylhexane	37.3	39.2
2,3-Dimethylhexane	38.8	38.9
2,4-Dimethylhexane	37.8	39.2
2,5-Dimethylhexane	37.9	39.9
3,3-Dimethylhexane	37.9	38.2
3,4-Dimethylhexane	39	38.5
3-Ethyl-2-methylpentane	38.5	38.2
3-Ethyl-3-methylpentane	38	37.4
2,2,3-Trimethylpentane	36.9	37.6
2,2,4-Trimethylpentane	36.1	38.4
2,3,3-Trimethylpentane	37.2	37.2
2,3,4-Trimethylpentane	37.6	38.1
Nonane	46.4	45.2
2-Methyloctane	44.7	44.7
3-Methyloctane	44.8	44.2
4-Methyloctane	44.8	43.9
3-Ethylheptane	44.8	43.3
4-Ethylheptane	44.8	43
2,2-Dimethylheptane	42.3	43.7
2,3-Dimethylheptane	43.8	43.3
2,4-Dimethylheptane	42.9	43.3
2,5-Dimethylheptane	42.9	43.7
2,6-Dimethylheptane	42.8	44.2
3,3-Dimethylheptane	42.7	42.7
3,4-Dimethylheptane	43.8	42.7
3,5-Dimethylheptane	43	43.1
4,4-Dimethylheptane	42.7	42.3
3-Ethyl-2-methylhexane	43.8	42.3
4-Ethyl-2-methylhexane	43	42.7
3-Ethyl-3-methylhexane	43	41.6
3-Ethyl-4-methylhexane	44	43.3
2,2,3-Trimethylhexane	41.9	42
2,2,4-Trimethylhexane	40.6	42.4
2,2,5-Trimethylhexane	40.2	43.1
2,3,3-Trimethylhexane	42.2	41.6
2,3,4-Trimethylhexane	42.9	42
2,3,5-Trimethylpentane	41.4	42.7
2,4,4-Trimethylhexane	40.8	42
3,3,4-Trimethylhexane	42.3	41.3
3,3-Diethylpentane	43.4	40.8
2,2-Dimethyl-3-ethylpentane	42	41.3
2,3-Dimethyl-3-ethylpentane	42.6	40.8
2,4-Dimethyl-3-ethylpentane	42.9	41.6
2,2,3,3-Tetramethylpentane	41	40.4
2,2,3,4-Tetramethylpentane	41	41.3
2,2,4,4-Tetramethylpentane	38.1	41.7
2,3,3,4-Tetramethylpentane	41.8	40.8

Table 8: Comparison of critical temperatures (CT) between experimental and predicted values

Alkane	**CT from experiments**	**CT computed using regression model**
Pentane	196.6	201.5
2-Methylbutane	187.8	191.9
2,2-Dimethylpropane	160.6	179.8
Hexane	234.7	242.3
2-Methylpentane	224.9	235.0
3-Methylpentane	231.2	231.4
2,2-Dimethylbutane	216.2	221.9
2,3-Dimethylbutane	227.1	226.3
Heptane	267.0	276.9
2-Methylhexane	257.9	271.4
3-Methylhexane	262.4	267.3
3-Ethylhexane	267.6	262.7
2,2-Dimethylpentane	247.7	260.4
2,3-Dimethylpentane	264.6	260.4
2,4-Dimethylpentane	247.1	265.2
3,3-Dimethylpentane	263.0	255.0
2,3,3-Trimethylbutane	258.3	252.4
Octane	296.2	306.8
2-Methylheptane	288.0	302.7
3-Methylheptane	292.0	298.9
4-Methylheptane	290.0	297.3
3-Ethylhexane	292.0	293.1
2,2-Dimethylhexane	279.0	294.0
2,3-Dimethylhexane	293.0	292.3
2,4-Dimethylhexane	282.0	294.0
2,5-Dimethylhexane	279.0	298.2
3,3-Dimethylhexane	290.8	287.4
3,4-Dimethylhexane	298.0	289.3
3-Ethyl-2-methylpentane	295.0	287.4
3-Ethyl-3-methylpentane	305.0	282.0
2,2,3-Trimethylpentane	294.0	283.2
2,2,4-Trimethylpentane	271.2	288.5
2,3,3-Trimethylpentane	303.0	281.0
2,3,4-Trimethylpentane	295.0	286.5
Nonane	322.0	333.1
2-Methyloctane	315.0	330.0
3-Methyloctane	318.0	326.8
4-Methyloctane	318.3	324.7
3-Ethylheptane	318.0	321.1
4-Ethylheptane	318.3	318.8
2,2-Dimethylheptane	302.0	323.2
2,3-Dimethylheptane	315.0	321.0
2,4-Dimethylheptane	306.0	321.0
2,5-Dimethylheptane	307.8	323.2
2,6-Dimethylheptane	306.0	326.7
3,3-Dimethylheptane	314.0	317.0
3,4-Dimethylheptane	322.7	317.0
3,5-Dimethylheptane	312.3	319.4
4,4-Dimethylheptane	317.8	314.4
3-Ethyl-2-methylhexane	322.7	314.4
4-Ethyl-2-methylhexane	330.3	317.0
3-Ethyl-3-methylhexane	327.2	309.8
3-Ethyl-4-methylhexane	312.3	321.1
2,2,3-Trimethylhexane	318.1	312.4

Alkane	CT from experiments	CT computed using regression model
2,2,4-Trimethylhexane	301.0	315.1
2,2,5-Trimethylhexane	296.6	319.3
2,3,3-Trimethylhexane	326.1	309.6
2,3,4-Trimethylhexane	324.2	312.4
2,3,5-Trimethylpentane	309.4	316.8
2,4,4-Trimethylhexane	309.1	312.4
3,3,4-Trimethylhexane	330.6	307.6
3,3-Diethylpentane	342.8	304.6
2,2-Dimethyl-3-ethylpentane	338.6	307.6
2,3-Dimethyl-3-ethylpentane	322.6	304.4
2,4-Dimethyl-3-ethylpentane	324.2	309.6
2,2,3,3-Tetramethylpentane	334.5	301.9
2,2,3,4-Tetramethylpentane	319.6	307.4
2,2,4,4-Tetramethylpentane	301.6	310.4
2,3,3,4-Tetramethylpentane	334.5	304.2

Table 9: Comparison of critical pressures (CP) between experimental and predicted values

Alkane	CP from experiments	CP computed using regression model
Pentane	33.3	33.2
2-Methylbutane	32.9	34
2,2-Dimethylpropane	31.6	34.9
Hexane	29.9	30.1
2-Methylpentane	30	30.7
3-Methylpentane	30.8	31
2,2-Dimethylbutane	30.7	31.7
2,3-Dimethylbutane	31	31.4
Heptane	27	27.5
2-Methylhexane	27.2	27.9
3-Methylhexane	28.1	28.2
3-Ethylhexane	28.6	28.6
2,2-Dimethylpentane	28.4	28.8
2,3-Dimethylpentane	29.2	28.8
2,4-Dimethylpentane	27.4	28.4
3,3-Dimethylpentane	30	29.2
2,3,3-Trimethylbutane	29.8	29.4
Octane	24.64	25.2
2-Methylheptane	24.8	25.5
3-Methylheptane	25.6	25.8
4-Methylheptane	25.6	26
3-Ethylhexane	25.74	26.3
2,2-Dimethylhexane	25.6	26.2
2,3-Dimethylhexane	26.6	26.3
2,4-Dimethylhexane	25.8	26.2
2,5-Dimethylhexane	25	25.9
3,3-Dimethylhexane	27.2	26.7
3,4-Dimethylhexane	27.4	26.6
3-Ethyl-2-methylpentane	27.4	26.7
3-Ethyl-3-methylpentane	28.9	27.1
2,2,3-Trimethylpentane	28.2	27
2,2,4-Trimethylpentane	25.5	26.6
2,3,3-Trimethylpentane	29	27.2
2,3,4-Trimethylpentane	27.6	26.8
Nonane	22.74	23.2
2-Methyloctane	23.6	23.5

Alkane	CP from experiments	CP computed using regression model
3-Methyloctane	23.7	23.7
4-Methyloctane	23.06	23.9
3-Ethylheptane	23.98	24.1
4-Ethylheptane	23.98	24.3
2,2-Dimethylheptane	22.8	24
2,3-Dimethylheptane	23.79	24.2
2,4-Dimethylheptane	22.7	24.2
2,5-Dimethylheptane	22.7	24
2,6-Dimethylheptane	23.7	23.7
3,3-Dimethylheptane	24.19	24.5
3,4-Dimethylheptane	24.77	24.5
3,5-Dimethylheptane	23.59	24.3
4,4-Dimethylheptane	24.18	24.7
3-Ethyl-2-methylhexane	24.77	24.7
4-Ethyl-2-methylhexane	25.56	24.5
3-Ethyl-3-methylhexane	25.66	25
3-Ethyl-4-methylhexane	23.59	24.1
2,2,3-Trimethylhexane	25.07	24.8
2,2,4-Trimethylhexane	23.39	24.6
2,2,5-Trimethylhexane	22.41	24.3
2,3,3-Trimethylhexane	25.56	25
2,3,4-Trimethylhexane	25.46	24.8
2,3,5-Trimethylpentane	23.49	24.5
2,4,4-Trimethylhexane	23.79	24.8
3,3,4-Trimethylhexane	26.45	25.2
3,3-Diethylpentane	26.94	25.4
2,2-Dimethyl-3-ethylpentane	25.96	25.2
2,3-Dimethyl-3-ethylpentane	26.94	25.4
2,4-Dimethyl-3-ethylpentane	25.46	25
2,2,3,3-Tetramethylpentane	27.04	25.6
2,2,3,4-Tetramethylpentane	25.66	25.2
2,2,4,4-Tetramethylpentane	24.58	25
2,3,3,4-Tetramethylpentane	26.85	25.4

Table 10: Comparison of surface tension (ST) between experimental and predicted values

Alkane	ST from experiments	ST computed using regression model
Pentane	16	16.3
2-Methylbutane	15	15.8
2,2-Dimethylpropane		
Hexane	18.42	18.4
2-Methylpentane	17.38	18
3-Methylpentane	18.12	17.8
2,2-Dimethylbutane	16.3	17.3
2,3-Dimethylbutane	17.37	17.6
Heptane	20.26	20.1
2-Methylhexane	19.29	19.9
3-Methylhexane	19.79	19.7
3-Ethylhexane	20.44	19.4
2,2-Dimethylpentane	18.02	19.3
2,3-Dimethylpentane	19.96	19.3
2,4-Dimethylpentane	18.15	19.6
3,3-Dimethylpentane	19.59	19
2,3,3-Trimethylbutane	18.76	18.9
Octane	21.76	21.7

Alkane	ST from experiments	ST computed using regression model
2-Methylheptane	20.6	21.5
3-Methylheptane	21.17	21.3
4-Methylheptane	21	21.2
3-Ethylhexane	21.51	21
2,2-Dimethylhexane	19.6	21
2,3-Dimethylhexane	20.99	20.9
2,4-Dimethylhexane	20.05	21
2,5-Dimethylhexane	19.73	21.2
3,3-Dimethylhexane	20.63	20.7
3,4-Dimethylhexane	21.62	20.8
3-Ethyl-2-methylpentane	21.52	20.7
3-Ethyl-3-methylpentane	21.99	20.4
2,2,3-Trimethylpentane	20.67	20.5
2,2,4-Trimethylpentane	18.77	20.7
2,3,3-Trimethylpentane	21.56	20.4
2,3,4-Trimethylpentane	21.14	20.6
Nonane	22.92	23
2-Methyloctane	21.88	22.9
3-Methyloctane	22.34	22.7
4-Methyloctane	22.34	22.6
3-Ethylheptane	22.81	22.4
4-Ethylheptane	22.81	22.3
2,2-Dimethylheptane	20.8	22.5
2,3-Dimethylheptane	22.34	22.4
2,4-Dimethylheptane	21.3	22.4
2,5-Dimethylheptane	21.3	22.5
2,6-Dimethylheptane	20.83	22.7
3,3-Dimethylheptane	22.01	22.2
3,4-Dimethylheptane	22.8	22.2
3,5-Dimethylheptane	21.77	22.3
4,4-Dimethylheptane	22.01	22.1
3-Ethyl-2-methylhexane	22.8	22.1
4-Ethyl-2-methylhexane	21.77	22.2
3-Ethyl-3-methylhexane	23.22	21.8
3-Ethyl-4-methylhexane	23.27	22.4
2,2,3-Trimethylhexane	21.86	22
2,2,4-Trimethylhexane	20.51	22.1
2,2,5-Trimethylhexane	20.04	22.3
2,3,3-Trimethylhexane	22.41	21.8
2,3,4-Trimethylhexane	22.8	22
2,3,5-Trimethylpentane	21.27	22.2
2,4,4-Trimethylhexane	21.17	22
3,3,4-Trimethylhexane	23.27	21.7
3,3-Diethylpentane	23.75	21.6
2,2-Dimethyl-3-ethylpentane	22.38	21.7
2,3-Dimethyl-3-ethylpentane	23.87	21.6
2,4-Dimethyl-3-ethylpentane	22.8	21.8
2,2,3,3-Tetramethylpentane	23.38	21.4
2,2,3,4-Tetramethylpentane	21.98	21.7
2,2,4,4-Tetramethylpentane	20.37	21.9
2,3,3,4-Tetramethylpentane	23.31	21.6

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