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QSPR Analysis of Alkanes Using Transformation Graphs

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ABSTRACT: Topological indices serves as an important tool for numerically representing chemical compounds and are widely used in QSPR/QSAR analysis to study their physicochemical and biological properties. In this study, we focus on alkanes and investigate various derived graphs obtained from their molecular graphs. While several derived structures—such as line graphs, middle graphs, subdivision graphs, and total graphs—are commonly employed in QSPR studies, our work emphasizes the use of transformation graphs as an effective tool for structural analysis. We compute and analyze topological indices for these transformation graphs and examine their correlations with some physical properties of alkanes. Linear regression models are then constructed to establish predictive relationships, and their performance is visually represented through graphical analysis. Furthermore, the root mean square error (RMSE) and correlation coefficient is used as a key metric to evaluate the predictive accuracy of the models. The results demonstrate that transformation-graph–based topological indices provide meaningful insights into the property prediction of alkanes.

Keywords: Transformation graph, topological Indices, QSPR, Alkanes.

Contents

1. Introduction

Chemical graph theory is a branch of mathematical chemistry that applies graph-theoretical concepts to model and analyze molecular structures. Using this approach, molecules are represented as graphs, where atoms correspond to vertices and chemical bonds correspond to edges. This model allows complex molecular structures to be studied using mathematical tools, enabling the assessment of structural features through topological indices and invariants. These indices such as the Wiener index, Zagreb indices, and Randić connectivity index, capture essential aspects of molecular connectivity, branching, and electronic distribution. By converting molecular structure into a mathematical form, chemical graph theory simplifies the study of molecular properties, reactivity patterns, and structure-function relationships. It is an essential theoretical foundation in cheminformatics, molecular design, and computational chemistry. The insights gained from graph-based descriptors have been widely applied in fields such as drug design, materials science, nanotechnology, and environmental chemistry.

Quantitative Structure–Property Relationship (QSPR) analysis is a computational approach used to establish mathematical correlations between the molecular structure of a compound and its physicochemical properties. Based on the fundamental principle that structurally similar molecules tend to exhibit similar properties, QSPR converts molecular structures into numerical descriptors that characterize key molecular features, including geometry, electronic distribution, and atomic connectivity. These descriptors are then used in statistical or machine-learning models to predict properties such as solubility, boiling point, reactivity, toxicity, and thermodynamic parameters. QSPR significantly reduces the amount of experimental work required by making it possible to predict molecular behaviour before conducting synthesis or tests. Due to its strong predictive capability and efficiency, QSPR has become widely employed in drug discovery, materials design, nanotechnology, environmental chemistry, and regulatory toxicology.

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Among various degree-based topological descriptors, the Zagreb indices hold particular significance. Introduced by Gutman and Trinajstić (1972) [5], the First Zagreb Index (M_1) has demonstrated strong correlations with several experimental parameters, including boiling points, molecular stability, and biological activity. To enhance the sensitivity of Zagreb-type measures, Shirdel et al. [14] proposed the Hyper Zagreb Index, which highlights degree variation and has demonstrated successful QSPR applications in nanostructure and fullerene analysis.

Further refinements have expanded the descriptive power of degree-based indices. Furtula and Gutman [3] introduced the Forgotten Index (F-index) in 2015, emphasizing the contribution of high-degree vertices and useful for studying nanomaterials and complex graph structures. Ghorbani and Hosseinzadeh [4] developed the Reduced Second Zagreb Index, which normalizes edge contributions, making it effective for modeling large or irregular molecular graphs. Additionally, Zhong and Xu [21] proposed the Harmonic Index, which complements Zagreb-type indices by assigning greater importance to edges connecting low-degree vertices. Due to their simplicity, interpretability, and broad applicability, Zagreb-type indices have become fundamental tools in both chemical graph theory and QSPR/QSAR modeling.

Recent advancements in computational chemistry and machine learning have further enhanced the scope of QSPR. Studies such as those by Rasheed et al. (2024) [11] and van den Maagdenberg et al. (2024) [19] have emphasized the continued relevance of degree-based topological indices in molecular property prediction. The development of open-source modeling platforms such as QSPRpred has facilitated the construction of reliable and reproducible QSPR models. Moreover, hybrid approaches such as quantitative read-across structure–property relationships (q-RASPR) integrate similarity-based reasoning with statistical learning to improve predictive accuracy for complex environmental and toxicological endpoints.

Throughout this paper, let the graph G be an ordered pair (V, E) where V denotes the set of vertices (atoms) and E denotes the set of edges (chemical bonds). These graphs are identified as chemical graphs which are considered to be simple, finite and undirected, representing molecular system and are used to study molecular topology, predicting physicochemical properties and calculating various topological indices which are used in QSPR analysis.

Table 1 provides an overview of the degree-based topological indices used in the present analysis.

Table 1: Degree based topological indices

Sl.No	**Name of the Topological Index**	**Notation and Definition**
1	First Zagreb Index [G. Gutman and Trinajstić, 1972]	$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$
2	Second Zagreb Index [G. Gutman and Trinajstić, 1972]	$M_2(G) = \sum_{uv \in E(G)} d_u d_v$
3	Hyper Zagreb Index [G. H. Shirdel et al., 2013]	$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2$
4	Forgotten Topological Index [Furtula and Gutman, 2015]	$F(G) = \sum_{uv \in E(G)} \left(d_u^2 + d_v^2\right)$
5	Reduced Second Zagreb Index [B. Furtula, I. Gutman, S. Ediz, 2014]	$RM_2(G) = \sum_{uv \in E(G)} (d_u - 1)(d_v - 1)$
6	Harmonic Index [Fajtlowicz, 1987]	$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$

In this study alkanes are considered to conduct QSPR analysis. All of the carbon-carbon bonds in alkanes are single covalent bonds, a class of saturated hydrocarbons made up solely of carbon (C) and hydrogen (H) atoms. Their general molecular formula is C_nH_{2n+2}. Alkanes, often referred to as paraffins, meaning "little affinity," indicating their lower reactivity under standard conditions in comparison to other organic compound classes. From a structural standpoint, alkanes can be found as straight chains (n-alkanes), branched chains, or in a cyclic form. Alkanes are crucial as industrial raw materials and fuels in the petrochemical sector due to their chemical inertness. The characteristics of low polarity, lack of conductivity, and inability to dissolve in water while being soluble in organic solvents render them beneficial for various uses, ranging from solvents to lubricants. In both theoretical and applied chemistry, the study of alkanes is crucial. Alkanes, the most basic saturated hydrocarbons, offer a basic foundation for comprehending the composition, bonding, and reactivity of organic molecules [8]. Their study not only reinforces the theoretical foundation of isomerism and free radical reaction mechanisms but also broadens its relevance to diverse industrial uses [15]. Natural gas and petroleum are composed of alkanes, which are essential fuels and feedstocks for the synthesis of alcohols and polymers [7]. Furthermore, the significance of alkanes for carbon cycling and bioremediation is highlighted by microbial degradation processes like those mediated by AlkB enzymes. Their combustion contributes to the world's energy demand while also posing problems with carbon emissions and air quality [13]. Alkane research also touches on new areas like sustainable biofuel production and alternative energy, highlighting its importance beyond traditional fuel chemistry [2].

Alkanes are frequently selected as model compounds in QSPR studies because of their simple molecular structures, well-defined bonding patterns, and availability of extensive experimental data. Their acyclic nature allows representation as tree graphs, where vertices correspond to carbon atoms and edges denote single bonds. This simplicity makes alkanes particularly suitable for validating new topological descriptors and testing theoretical relationships between molecular structure and physicochemical properties. Numerous studies have demonstrated that degree-based and distance-based topological indices effectively predict physicochemical parameters such as boiling point, molar refractivity, density, and heat of formation in alkanes. For instance, Gutman and Trinajstić (1972) [5] first introduced the Zagreb indices using alkane structures, while subsequent works by Randic (1975) [10], Kier and Hall (1976) [6], and more recent studies by Todeschini and Consonni (2009) [18] confirmed the reliability of such indices in modeling alkane properties.

As the alkane isomers are the chemical compounds with same molecular formula but different structural connectivity, hence resulting in different graph connectivity. Since the analysis is done using degree-based topological indices numerical values produced will have unique representation for isomers with same composition. Degree-based indices depend only on the vertex degree and they are sensitive to the connectivity and branching patterns in the structure hence even though the isomers have identical molecular formula they yield different topological index values.

Recent investigations continue to use alkanes as benchmark datasets to evaluate the performance of emerging topological indices and QSPR models, largely because their orderly structural progression and chemical simplicity enable clear interpretation of descriptor behavior. For instance, Sooryanarayana and Chandrakala systematically analyzed distance-2 topological models of alkanes, demonstrating how these graphs capture incremental structural variations and support reliable descriptor–property relationships [16].

Several indices have been studied on transformation graphs. Initially, Basavanagoud and Gutman [1] developed and classified many transformation graph types. Narumi Katayama [9], independently have analysied results on degree based indices on certain families of transformation graphs. Recent years have seen two complementary trends. First, systematic QSPR studies compare numerous indices (computed either on original alkane graphs, their line graphs, total graphs or other transformations) and show which descriptors best correlate with specific properties (e.g., boiling point, molar refractivity, heat of vaporization) for alkane series. Second, graph-theoretic research generalizes transformation-graph constructs (e.g., generalized total/transformation graphs, subdivision and combined graphs) and derives structural formulae for indices on these graphs, enabling scalable computation for larger molecules and facilitating direct comparison across descriptor families. These advances open practical pathways for using transformation-graph–based descriptors in predictive modeling and highlight promising indices for alkanes.

In 2001, Wu and Meng [20] introduced new graphical transformations which generalizes the concept of the total graph. The transformation graph G^{xyz} of a graph G is a simple undirected graph with x, y, z being the three variables taking +ve or −ve signs are used to derive the numerical values which are derived from molecular graphs of alkanes. Let α, β be two elements of $V(G) \cup E(G)$. Then associativity of α and β is taken as $+$ if they are adjacent or incident in G, otherwise $-$. Let xyz be a 3-permutation of the set $\{+, -\}$. The pair α and β is said to correspond to x or y or z of xyz if α and β are both in $V(G)$ or both are in $E(G)$, or one is in $V(G)$ and the other is in $E(G)$ respectively. Thus the transformation graph

G^{xyz} of G is the graph whose vertex set is $V(G) \cup E(G)$ and two of its vertices α and β are adjacent if and only if their associativity in G is consistent with the corresponding element of xyz. Based on the values of x, y, z there are eight transformation graphs namely, G^{+++}, G^{++-}, G^{+-+},G^{+--}, G^{---}, G^{--+}, G^{-+-}, G^{-++}. If the variables takes + sign connectivity between vertices and edges remain same as in case of original graph G, otherwise the two vertices or edges are not adjacent to each other but they are adjacent to the other vertices and edges.

The transformation graph G^{-++} of G is the graph with vertex set $V(G) \cup E(G)$ in which the vertices u and v are joined by an edge if one of the following holds (1) both $u, v \in V(G)$ and u and v are not adjacent in G; (1) both $u, v \in E(G)$ and u and v are adjacent in G; (3) one is in $V(G)$ and the other is in $E(G)$ and they are incident with each other in G.

The transformation graph G^{+-+} of G is the graph with vertex set $V(G) \cup E(G)$ in which the vertices u and v are joined by an edge if one of the following holds (1) both $u, v \in V(G)$ and u and v are adjacent in G; (1) both $u, v \in E(G)$ and u and v are not adjacent in G; (3) one is in $V(G)$ and the other is in $E(G)$ and they are incident with each other in G. Figure 1 represents the Chemical structure of Butane, Figure 2 represents molecular graph of Butane and Figure 3 represents all eight transformation graph of butane.

Proposition 1.1 *[12] Let G be a graph with n vertices and m edges. Let $u \in V(G)$ and $e \in E(G)$. Then the degrees of vertices in the transportation graph G^{xyz} are listed below.*

- $d_G{}^{+++}(u) = 2d_G(u)$ *and* $d_G{}^{+++}(e) = d_G(u) + d_G(v)$
- $d_G{}^{++-}(u) = m$ *and* $d_G{}^{++-}(e) = d_G(u) + d_G(v) + n - 4$
- $d_G{}^{+-+}(u) = 2d_G(u)$ *and* $d_G{}^{+-+}(e) = m - d_G(u) - d_G(v) + 3$
- $d_G{}^{-++}(u) = n - 1$ *and* $d_G{}^{-++}(e) = d_G(u) + d_G(v)$
- $d_G{}^{---}(u) = n + m - 1 - 2d_G(u)$ *and* $d_G{}^{---}(e) = n + m - d_G(u) - d_G(v) - 1$
- $d_G{}^{--+}(u) = n - 1$ *and* $d_G{}^{--+}(e) = m - d_G(u) - d_G(v) + 3$
- $d_G{}^{-+-}(u) = n + m - 1 - 2d_G(u)$ *and* $d_G{}^{-+-}(e) = n + d_G(u) + d_G(v) - 4$
- $d_G{}^{+--}(u) = m$ *and* $d_G{}^{+--}(e) = n + m - d_G(u) - d_G(v) - 1$

Lemma 1.1 *[12] Let G be a connected graph with order n and size m and let $u \in V(G)$ and $e \in E(G)$ then the size of the transformation graph G^{xyz} according to the signs associated with x, y and z are listed below.*

- *When* $x = +ve$, *size is* $m_x = m$.
- *When* $x = -ve$, *size is* $m_x = \binom{n}{2} - m$.
- *When* $y = +ve$, *size is* $m_y = \dfrac{\sum(d(u))^2}{2} - m$.
- *When* $y = -ve$, *size is* $m_y = m\binom{n}{2} - \left(\dfrac{\sum(d(u))^2}{2} - m\right)$.
- *When* $z = +ve$, *size is* $m_z = 2m$.
- *When* $z = -ve$, *size is* $m_z = m(n - 2)$.

Figure 1: Chemical structure of Butane (C_4H_{10})

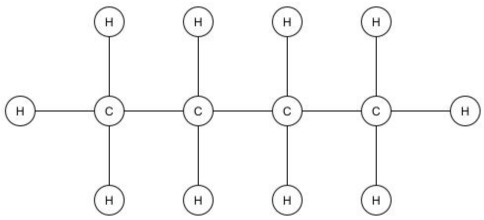


Figure 2: Molecular graph of Butane (C_4H_{10})

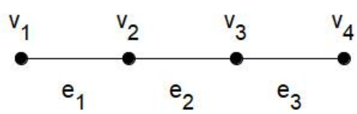
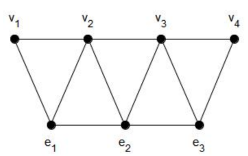
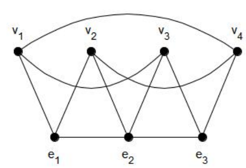


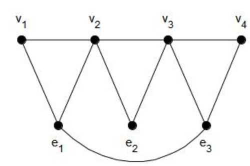
Figure 3: Transformation graphs of Butane (C_4H_{10})



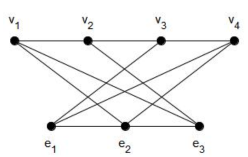
(a) Transformation graph G^{+++} of Butane (C_4H_{10})



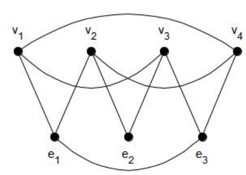
(b) Transformation graph G^{-++} of Butane (C_4H_{10})



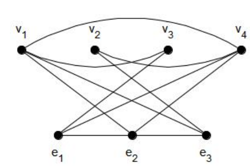
(c) Transformation graph G^{+-+} of Butane (C_4H_{10})



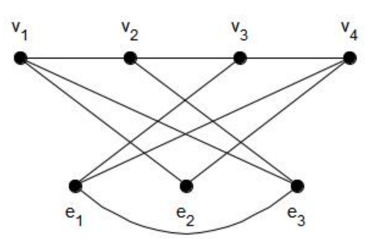
(d) Transformation graph G^{++-} of Butane (C_4H_{10})



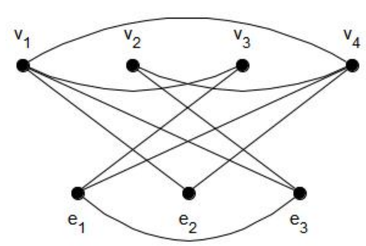
(e) Transformation graph G^{--+} of Butane (C_4H_{10})



(f) Transformation graph G^{-+-} of Butane (C_4H_{10})



(g) Transformation graph G^{+--} of Butane (C_4H_{10})



(h) Transformation graph G^{---} of Butane (C_4H_{10})

Table 2: **Alkanes Topological Indices**

Alkanes		**Topological Indices**								
		G^{+++}	G^{++-}	G^{+-+}	G^{+--}	G^{---}	G^{-++}	G^{-+-}	G^{--+}	G
Butane	M_1	74	70	62	58	62	70	74	62	10
	M_2	124	111	93	84	93	111	124	93	4
	HM	510	448	392	338	392	448	510	392	16
	F	262	226	206	170	206	226	262	206	8
	RM_2	61	52	41	36	41	52	61	41	0.5
	H	3.36	3.476	3.288	3.467	3.288	3.476	3.36	3.288	0.25
2-Methyl propane	M_1	96	84	60	48	60	84	96	48	12
	M_2	180	147	84	63	96	147	192	63	9
	HM	792	594	432	258	408	594	768	258	48
	F	432	300	264	132	216	300	384	132	30
	RM_2	96	75	33	24	45	75	108	24	1.5
	H	3.1	3.464	3.0	3.4	2.75	3.464	3.0	3.4	1.0
Pentane	M_1	106	162	106	162	202	130	202	130	14
	M_2	188	345	184	345	481	248	485	248	8
	HM	766	1388	758	1388	1964	998	1972	998	32
	F	390	698	390	698	1002	502	1002	502	16
	RM_2	97	202	93	202	300	135	304	135	1
	H	4.36	4.478	4.298	4.478	4.414	4.464	4.433	4.464	0.5
2-Methyl butane	M_1	130	182	102	146	194	146	230	118	16
	M_2	259	413	172	296	460	295	601	216	6
	HM	1102	1676	774	1192	1920	1190	2452	878	25
	F	584	850	430	600	1000	600	1250	446	13
	RM_2	145	251	84	168	286	167	393	114	0.4
	H	4.134	4.446	4.015	4.468	4.210	4.460	4.319	4.381	0.167
2,2-Dimethyl propane	M_1	180	224	96	116	180	180	244	96	5
	M_2	414	568	144	208	432	406	676	160	4
	HM	1872	2320	864	844	1836	1632	2716	672	25
	F	1044	1184	576	428	972	820	1364	352	17
	RM_2	252	366	60	108	270	246	454	78	0.4
	H	3.759	4.4	3.6	4.429	3.667	4.478	3.982	4.167	0.25
Hexane	M_1	138	308	170	353	474	215	430	293	18
	M_2	252	817	341	997	1553	481	1356	756	12
	HM	1022	3282	1396	4045	6274	1949	5498	3409	48
	F	518	1648	714	2051	3168	987	2786	1897	24
	RM_2	133	538	192	675	1115	290	960	489	1.5
	H	5.36	5.479	5.271	5.479	5.497	5.427	5.435	4.78	0.75
2-Methyl pentane	M_1	162	332	162	332	462	232	462	232	20
	M_2	324	917	315	916	1515	538	1524	537	10
	HM	1360	3700	1342	3698	6178	2170	6196	2168	41
	F	712	1866	712	1866	3148	1094	3148	1094	21
	RM_2	182	615	173	614	1088	331	1097	330	0.9
	H	5.142	5.459	5.06	5.456	5.376	5.436	5.399	5.428	0.417
3-Methyl pentane	M_1	164	334	164	334	464	234	464	234	28
	M_2	339	928	323	928	1519	545	1535	545	12
	HM	1414	3758	1382	3758	6222	2208	6254	2208	50
	F	736	1902	736	1902	3184	1118	3184	1118	26
	RM_2	195	624	179	624	1090	336	1106	336	0.8
	H	5.174	5.4445	5.0262	5.4445	5.3407	5.3889	5.3805	5.3889	0.3333
2,2-Dimethyl butane	M_1	216	386	152	290	436	270	532	242	24
	M_2	511	1160	277	750	1409	673	1915	587	8
	HM	2248	4736	1376	3032	5872	2714	7768	2702	36
	F	1226	2416	822	1532	3054	1368	3938	1528	20
	RM_2	317	806	143	488	1006	430	1420	368	0.333

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Alkanes		**Topological Indices**								
		G^{+++}	G^{++-}	G^{+-+}	G^{+--}	G^{---}	G^{-++}	G^{-+-}	G^{--+}	G
	H	4.815	5.398	4.637	5.456	5.098	5.431	5.270	4.668	0.125
2,3-Dimethyl butane	M_1	188	358	156	310	448	250	496	248	22
	M_2	412	1029	300	829	1456	598	1704	604	9
	HM	1760	4184	1328	3336	6016	2418	6960	2692	36
	F	936	2126	728	1678	3104	1222	3552	1484	18
	RM_2	245	702	163	548	1042	374	1244	380	0.333
	H	4.933	5.429	4.800	5.465	5.264	5.441	5.336	4.888	0.111
Heptane	M_1	170	478	256	670	938	334	788	435	22
	M_2	316	1500	587	2421	3993	876	3091	1168	16
	HM	1278	6022	2406	9860	16052	3574	12546	5251	64
	F	646	3022	1232	5018	8066	1822	6364	2915	32
	RM_2	169	1060	359	1797	3110	574	2353	770	2
	H	6.360	6.051	6.313	6.382	6.471	6.310	6.409	6.462	1.000
2-Methyl hexane	M_1	179	520	252	638	914	350	824	415	24
	M_2	360	1686	576	2247	3859	932	3320	1101	14
	HM	1503	6788	2394	9126	15590	3784	13492	4913	57
	F	783	3416	1242	4632	7872	1920	6852	2711	29
	RM_2	203	1206	351	1654	2999	615	2547	722	1.4
	H	5.606	6.178	5.896	6.404	6.431	6.360	6.401	6.409	0.667
3-Methyl hexane	M_1	196	550	250	641	916	352	826	390	24
	M_2	404	1798	567	2271	3866	940	3334	1004	14
	HM	1672	7250	2376	9241	15652	3824	13562	4322	57
	F	864	3654	1242	4699	7920	1944	6894	2314	29
	RM_2	232	1290	344	1675	3004	621	2559	650	1.4
	H	6.182	6.455	6.013	6.392	6.414	6.319	6.389	6.776	0.667
3-Ethyl pentane	M_1	198	550	252	642	918	354	822	360	24
	M_2	420	1800	576	2277	3876	948	3304	888	18
	HM	1728	7268	2424	9282	15720	3864	13460	3600	75
	F	888	3668	1272	4728	7968	1968	6852	1824	39
	RM_2	246	1292	351	1680	3012	627	2533	564	1.2
	H	6.219	6.470	6.000	6.391	6.398	6.274	6.435	7.200	0.500
2,2-Dimethyl pentane	M_1	248	610	230	580	872	388	902	342	28
	M_2	577	2109	486	1947	3627	1076	3841	835	12
	HM	2508	8554	2204	7892	14828	4346	15594	3478	52
	F	1354	4336	1232	3998	7574	2194	7912	1808	28
	RM_2	355	1543	281	1410	2807	723	2992	527	0.833
	H	5.828	6.419	5.701	6.430	6.296	6.390	6.353	6.819	0.375
2,3-Dimethyl pentane	M_1	222	578	240	610	894	370	864	387	26
	M_2	493	1936	534	2106	3742	1005	3578	999	15
	HM	2074	7838	2278	8548	15252	4082	14586	4407	61
	F	1088	3966	1210	4336	7768	2072	7430	2409	31
	RM_2	296	1401	320	1540	2901	669	2766	647	0.733
	H	5.977	6.452	5.809	6.415	6.357	6.345	6.368	6.505	0.278
2,4-Dimethyl pentane	M_1	218	576	236	606	890	366	860	390	26
	M_2	461	1922	516	2076	3728	989	3550	1015	12
	HM	1956	7752	2188	8398	15134	3996	14440	4468	50
	F	1034	3908	1156	4246	7678	2018	7340	2438	26
	RM_2	268	1389	306	1514	2891	657	2742	660	0.800
	H	5.930	6.450	5.859	6.429	6.398	6.416	6.390	6.447	0.333
3,3-Dimethyl pentane	M_1	252	614	234	584	459	392	904	334	28
	M_2	609	2137	504	1977	1493	1093	3852	800	16
	HM	2626	8700	2294	8042	6091	4434	15670	3286	72
	F	1408	4426	1286	4088	3105	2248	7966	1686	40
	RM_2	383	1567	295	1436	1069	736	3001	500	0.667

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Alkanes		**Topological Indices**								
		G^{+++}	G^{++-}	G^{+-+}	G^{+--}	G^{---}	G^{-++}	G^{-+-}	G^{--+}	G
	H	5.875	6.402	5.646	6.416	5.405	6.321	6.344	6.933	0.250
Octane	M_1	202	544	382	1134	1625	490	1306	596	26
	M_2	380	2048	1021	4968	8459	1481	6140	1730	20
	HM	1534	8224	4208	20342	33929	6080	24982	7172	80
	F	774	4128	2166	10406	17011	3118	12702	3712	40
	RM_2	205	1540	675	3898	6912	1032	4903	1184	2.500
	H	7.360	4.767	7.098	7.316	7.504	7.190	7.368	8.473	1.250
2-Methyl heptane	M_1	226	660	366	1096	1598	506	1346	596	28
	M_2	452	2522	951	4721	8283	1541	6440	1727	18
	HM	1872	10146	3946	19306	33322	6298	26208	7348	73
	F	968	5102	2044	9864	16756	3216	13328	3894	37
	RM_2	254	1905	620	3688	6762	1077	5164	1180	1.900
	H	7.142	5.611	6.937	7.334	7.456	7.254	7.373	8.170	0.917
3-Methyl heptane	M_1	228	578	357	1082	1600	508	1348	626	28
	M_2	468	2244	899	4598	8294	1549	6456	1848	20
	HM	1928	9050	3747	18832	33404	6338	26288	8088	82
	F	992	4562	1949	9636	16816	3240	13376	4392	42
	RM_2	268	1703	577	3579	6771	1083	5178	1271	1.800
	H	7.182	4.747	7.114	7.435	7.446	7.210	7.364	7.762	0.833
4-Methyl heptane	M_1	228	844	355	1096	1600	508	1348	626	28
	M_2	469	3176	893	4720	8293	1550	6457	1847	20
	HM	1930	12776	3709	19304	33402	6340	26290	8096	82
	F	992	6424	1923	9864	16816	3240	13376	4402	42
	RM_2	269	2388	573	3687	6770	1084	5179	1270	1.800
	H	7.190	7.463	7.160	7.333	7.446	7.218	7.365	7.771	0.833
3-Ethyl hexane	M_1	230	496	370	1098	1602	510	826	657	28
	M_2	485	1967	972	4739	8304	1558	3334	1972	22
	HM	1986	7956	4060	19402	33484	6380	13562	8871	91
	F	1016	4022	2116	9924	16876	3264	6894	4927	47
	RM_2	283	1502	637	3704	6779	1090	2559	1364	1.700
	H	7.227	3.884	6.941	7.330	7.436	7.172	6.389	7.362	0.750
2,2-Dimethyl hexane	M_1	280	730	340	1022	1540	544	1432	616	32
	M_2	641	2939	835	4244	7879	1694	7109	1814	16
	HM	2764	11902	3620	17298	31916	6878	28900	8156	68
	F	1482	6024	1950	8810	16158	3490	14682	4528	36
	RM_2	391	2254	528	3283	6414	1194	5749	1245	1.333
	H	6.828	5.574	6.666	7.356	7.377	7.316	7.361	7.250	0.625
2,3-Dimethyl hexane	M_1	252	630	354	1058	1570	526	1390	586	30
	M_2	546	2520	905	4476	8081	1619	6774	1695	19
	HM	2288	10242	3798	18268	32670	6606	27604	7248	77
	F	1196	5202	1988	9316	16508	3368	14056	3858	39
	RM_2	323	1929	585	3480	6587	1136	5455	1157	1.233
	H	7.018	4.858	6.765	7.353	7.412	7.258	7.361	7.970	0.528
2,4-Dimethyl hexane	M_1	252	724	352	1056	1564	524	1388	621	30
	M_2	541	2825	895	4458	8028	1610	6757	1828	18
	HM	2268	11436	3748	18178	32420	6558	27516	8125	75
	F	1186	5786	1958	9262	16364	3338	14002	4469	39
	RM_2	318	2147	577	3464	6540	1129	5440	1255	1.200
	H	6.970	5.865	6.787	7.357	7.442	7.280	7.369	7.510	0.500
2,5-Dimethyl hexane	M_1	250	776	350	1054	1566	522	1386	621	30
	M_2	524	2996	885	4440	8061	1601	6740	1828	16
	HM	2210	12068	3692	18082	32516	6516	27434	8125	66
	F	1162	6076	1922	9202	16394	3314	13954	4469	34
	RM_2	303	2270	569	3448	6571	1122	5425	1255	1.300

Continued on next page

(Continued from previous page)

Alkanes		**Topological Indices**								
		G^{+++}	G^{++-}	G^{+-+}	G^{+--}	G^{---}	G^{-++}	G^{-+-}	G^{--+}	G
	H	6.925	6.456	6.785	7.362	7.436	7.318	7.377	7.510	0.583
3,3-Dimethyl hexane	M_1	300	650	344	1024	1544	526	1436	606	32
	M_2	739	2679	855	4266	7899	1619	7143	1782	20
	HM	3142	10896	3726	17420	32070	6606	29070	7896	88
	F	1664	5538	2016	8888	16272	3368	14784	4332	48
	RM_2	470	2068	544	3303	6430	1136	5779	1223	1.167
	H	7.013	4.706	6.643	7.363	7.354	7.258	7.345	7.371	0.500
3,4-Dimethyl hexane	M_1	256	614	356	1060	1572	528	1392	611	30
	M_2	574	2458	916	4495	8092	1627	6790	1797	21
	HM	2388	9966	3856	18366	32752	6646	27684	7857	86
	F	1240	5050	2024	9376	16568	3392	14104	4263	44
	RM_2	347	1882	594	3497	6596	1142	5469	1234	1.133
	H	7.021	4.724	6.768	7.349	7.403	7.210	7.352	7.621	0.444
3-Ethyl-2-Methyl pentane	M_1	256	880	356	1060	1572	528	1392	616	30
	M_2	575	3390	915	4494	8091	1628	6791	1816	21
	HM	2390	13692	3854	18364	32750	6648	27686	7980	86
	F	1240	6912	2024	9376	16568	3392	14104	4348	44
	RM_2	348	2567	593	3496	6595	1143	5470	1248	1.133
	H	7.026	7.439	6.765	7.349	7.402	7.215	7.353	7.553	0.444
3-Ethyl-3-Methyl pentane	M_1	288	920	355	1028	1552	546	1440	597	32
	M_2	708	3643	909	4303	7964	1711	7176	1756	24
	HM	3006	14788	4005	17608	32402	6960	29238	7647	108
	F	1590	7502	2187	9002	16474	3538	14886	4135	60
	RM_2	450	2781	587	3336	6487	1209	5808	1206	1.000
	H	6.937	7.408	6.522	7.354	7.314	7.359	7.327	7.464	0.375
2,2,3-Trimethyl pentane	M_1	310	950	330	986	1514	550	1478	608	34
	M_2	766	3809	805	4028	7693	1703	7462	1785	18
	HM	3298	15464	3528	16390	31344	6892	30394	8120	74
	F	1766	7846	1918	8334	15958	3486	15470	4550	38
	RM_2	487	2918	507	3102	6253	1198	6057	1223	0.686
	H	6.676	7.405	6.473	7.385	7.324	7.570	7.339	7.041	0.250
2,2,4-Trimethyl pentane	M_1	302	846	324	980	1517	560	1468	602	34
	M_2	705	3415	775	3974	7744	1756	7363	1764	18
	HM	3066	13828	3378	16120	31473	7100	29954	7958	74
	F	1656	6998	1828	8172	15985	3588	15228	4430	38
	RM_2	434	2621	483	3054	6301	1241	5968	1208	0.686
	H	6.661	6.421	6.530	7.399	7.316	7.390	7.379	7.107	0.250
2,3,3-Trimethyl pentane	M_1	314	952	332	988	1515	568	1476	583	34
	M_2	799	3826	815	4046	7709	1792	7437	1691	20
	HM	3418	15552	3578	16480	31417	7292	30296	7489	85
	F	1820	7900	1948	8388	15999	3708	15422	4107	45
	RM_2	516	2933	515	3118	6268	1269	6034	1154	0.619
	H	6.671	7.400	6.448	7.380	7.327	7.274	7.342	7.364	0.208
2,3,4-Trimethyl pentane	M_1	280	912	340	1020	1540	746	1424	547	32
	M_2	648	3571	852	4235	7888	2605	7028	1551	18
	HM	2736	14446	3600	17238	31968	10658	28632	6443	72
	F	1440	7304	1896	8768	16192	5448	14576	3341	36
	RM_2	398	2717	545	3276	6423	1913	5676	1051	0.667
	H	6.783	7.428	6.600	7.374	7.388	8.147	7.406	8.176	0.222
Nonane	M_1	234	1190	542	1778	2602	690	2014	823	30
	M_2	444	4981	1658	9169	16113	2376	11049	2578	24
	HM	1790	19968	6862	37708	64572	9798	45080	10435	96
	F	902	10006	3546	19370	32346	5046	22982	5279	48
	RM_2	241	3862	1161	7476	13616	1737	9126	1820	3.000

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(Continued from previous page)

Alkanes		**Topological Indices**								
		G^{+++}	G^{++-}	G^{+-+}	G^{+--}	G^{---}	G^{-++}	G^{-+-}	G^{--+}	G
	H	8.360	8.482	7.969	8.244	8.486	8.049	8.318	10.282	1.500
2-Methyl octane	M_1	258	1226	518	1730	2564	706	2058	805	32
	M_2	516	5210	1529	8791	15795	2440	11430	2502	22
	HM	2128	20914	6364	36086	63410	10024	46618	10149	89
	F	1096	10494	3306	18504	31820	5144	23758	5145	45
	RM_2	290	4056	1055	7145	13335	1786	9464	1761	2.400
	H	8.142	8.472	7.872	8.264	8.463	8.124	8.330	10.202	1.167
3-Methyl octane	M_1	260	1228	522	1732	2564	708	2060	800	32
	M_2	532	5228	1556	8814	15786	2448	11448	2481	24
	HM	2184	21004	6480	36204	63412	10064	46708	10026	98
	F	1120	10548	3368	18576	31840	5168	23812	5064	50
	RM_2	304	4072	1078	7166	13326	1792	9480	1745	2.300
	H	8.182	8.466	7.856	8.262	8.463	8.078	8.323	10.268	0.333
4-Methyl octane	M_1	260	1228	518	1732	2564	708	2040	802	32
	M_2	533	5229	1531	8813	15785	2449	11209	2490	24
	HM	2186	21006	6390	36202	63410	10066	45770	10074	98
	F	1120	10548	3328	18576	31840	5168	23352	5094	50
	RM_2	305	4073	1057	7165	13325	1793	9261	1752	2.300
	H	8.190	8.467	7.921	8.262	8.463	8.086	8.397	10.240	1.083
3-Ethyl heptane	M_1	262	1230	526	1734	2566	718	2062	800	32
	M_2	549	5247	1582	8836	15800	2521	11467	2484	26
	HM	2242	21096	6594	36320	63512	10314	46800	10026	107
	F	1144	10602	3430	18648	31912	5272	23866	5058	55
	RM_2	319	4089	1100	7186	13338	1855	9497	1748	2.200
	H	8.227	8.462	7.838	8.259	8.457	7.943	8.315	10.268	1.000
4-Ethyl heptane	M_1	262	1230	526	1734	2566	710	2062	802	32
	M_2	550	5248	1581	8835	15799	2458	11468	2492	26
	HM	2244	21098	6592	36318	63510	10108	46802	10074	107
	F	1144	10602	3430	18648	31912	5192	23866	5090	55
	RM_2	320	4090	1099	7185	13337	1800	9498	1754	2.200
	H	8.235	8.462	7.837	8.259	8.457	8.047	8.316	10.240	1.000
2,2-Dimethyl heptane	M_1	312	1304	488	1654	2488	710	2152	784	36
	M_2	705	5731	1385	8289	15147	2458	12267	2405	20
	HM	3020	23100	5884	33812	61068	10108	49964	9994	84
	F	1610	11638	3114	17234	30774	5192	25430	5184	44
	RM_2	427	4501	939	6717	12761	1800	10209	1683	1.833
	H	7.828	8.441	7.572	8.242	8.418	8.047	8.336	9.881	0.875
2,3-Dimethyl butane	M_1	286	1266	501	1686	2528	726	2106	811	34
	M_2	622	5477	1474	8461	15485	2522	11849	2521	23
	HM	2588	22050	6117	34698	62342	10340	48346	10499	93
	F	1344	11096	3169	17776	31372	5296	24648	5457	47
	RM_2	369	4284	1016	6858	13060	1849	9836	1773	1.733
	H	7.985	8.453	7.870	8.281	8.433	8.136	8.329	9.839	0.778
2,4-Dimethyl heptane	M_1	284	1264	504	1684	2494	724	2104	782	34
	M_2	606	5459	1471	8438	15082	2514	11831	2406	22
	HM	2526	21954	6130	34586	60620	10294	48250	9742	91
	F	1314	11036	3188	17710	30456	5266	24588	4930	47
	RM_2	355	4268	1010	6837	12691	1843	9820	1687	1.700
	H	7.978	8.458	7.678	8.283	8.541	8.167	8.335	10.191	0.750
2,5-Dimethyl heptane	M_1	284	1264	504	1670	2524	716	2104	781	34
	M_2	604	5457	1473	8286	15448	2480	11829	2398	22
	HM	2522	21950	6134	34072	62158	10106	48246	9717	91
	F	1314	11036	3188	17500	31262	5146	24588	4921	47
	RM_2	353	4266	1012	6699	13027	1817	9818	1680	1.700

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(Continued from previous page)

Alkanes		Topological Indices								
		G^{+++}	G^{++-}	G^{+-+}	G^{+--}	G^{---}	G^{-++}	G^{-+-}	G^{--+}	G
	H	7.965	8.456	7.682	8.369	8.449	8.275	8.334	10.204	0.750
2,6-Dimethyl heptane	M_1	282	1244	502	1682	2522	942	2102	788	34
	M_2	588	5290	1460	8417	15433	3532	11811	2433	20
	HM	2466	21256	6066	34472	62056	14162	48156	9890	82
	F	1290	10676	3146	17638	31190	7098	24534	5024	42
	RM_2	339	4119	1001	6818	13014	2653	9802	1708	1.800
	H	7.925	8.590	7.669	8.286	8.455	8.475	8.342	10.111	0.833
3,3-Dimethyl heptane	M_1	319	1308	492	1644	2492	748	1436	810	36
	M_2	757	5769	1409	8151	15175	2619	7143	2506	24
	HM	3217	23290	6010	33422	61262	10710	29070	10688	104
	F	1703	11752	3192	17120	30912	5472	14784	5676	56
	RM_2	472	4535	959	6589	12785	1925	5779	1758	1.667
	H	7.849	8.432	7.572	8.294	8.404	8.133	7.345	9.579	0.750
3,4-Dimethyl heptane	M_1	288	1268	500	1688	2528	728	2108	806	34
	M_2	639	5496	1448	8483	15475	2531	11868	2498	25
	HM	2646	22142	6066	34814	62350	10382	48438	10388	102
	F	1368	11150	3170	17848	31400	5320	24702	5392	52
	RM_2	384	4301	991	6878	13050	1856	9853	1755	1.6333
	H	8.0289	8.4480	7.8058	8.2783	8.4345	8.0944	8.3215	9.9172	0.6944
3,5-Dimethyl heptane	M_1	286	1266	506	1686	2526	726	2106	780	34
	M_2	621	5476	1485	8462	15462	2521	11848	2399	24
	HM	2580	22042	6200	34706	62258	10332	48338	9698	100
	F	1338	11090	3230	17782	31334	5290	24642	4900	52
	RM_2	368	4283	1022	6859	13039	1848	9835	1682	1.6
	H	8.0098	8.4514	7.6925	8.2815	8.4427	8.1136	8.3271	10.2247	0.6667
4,4-Dimethyl heptane	M_1	316	1308	492	1644	2492	748	2156	812	36
	M_2	741	5771	1407	8149	15173	2621	12307	2514	24
	HM	3146	23294	6006	33418	61258	10714	50158	10744	104
	F	1664	11752	3192	17120	30912	5472	25544	5716	56
	RM_2	459	4537	957	6587	12783	1927	10245	1764	1.6667
	H	7.9016	8.4335	7.5685	8.2936	8.4031	8.1461	8.3242	9.5580	0.7500
3-Ethyl-2-Methyl hexane	M_1	288	1268	508	1688	2528	728	2108	805	34
	M_2	640	5497	1495	8482	15474	2532	11869	2493	25
	HM	2648	22144	6256	34812	62348	10384	48440	10361	102
	F	1368	11150	3266	17848	31400	5320	24702	5375	52
	RM_2	385	4302	1030	6877	13049	1857	9854	1751	1.6333
	H	8.0344	8.4486	7.6790	8.2780	8.4341	8.0999	8.3221	9.9270	0.6944
4-Ethyl-2-Methyl hexane	M_1	284	1266	506	1686	2526	278	2106	791	34
	M_2	610	5477	1484	8461	15461	730	11849	2454	24
	HM	2534	22044	6198	34704	62256	3166	48340	9959	100
	F	1314	11090	3230	17782	31334	1706	24642	5051	52
	RM_2	359	4284	1021	6858	13038	477	9836	1726	1.6
	H	8.0113	8.4520	7.6907	8.2812	8.4423	4.6192	8.3277	10.0667	0.6667
3-Ethyl-3-Methyl hexane	M_1	320	1312	496	1648	2496	752	2040	836	36
	M_2	774	5808	1432	8194	15202	2638	11384	2607	28
	HM	3266	23482	6134	33646	61454	10802	46266	11392	124
	F	1718	11866	3270	17258	31050	5526	23498	6178	68
	RM_2	488	4570	978	6628	12808	1940	9438	1833	1.5
	H	7.9509	8.4234	7.5690	8.2884	8.3890	8.0647	9.2190	9.2863	0.6250
2,2,4-Trimethyl hexane	M_1	339	1342	469	1594	2450	762	2198	764	38
	M_2	801	5980	1305	7762	14830	2675	12668	2326	20
	HM	3439	24140	5555	31712	59928	10890	51596	9670	86
	F	1837	12180	2945	16188	30268	5540	26260	5018	46
	RM_2	497	4713	877	6249	12481	1968	10565	1623	1.1333

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Alkanes		**Topological Indices**								
		G^{+++}	G^{++-}	G^{+-+}	G^{+--}	G^{---}	G^{-++}	G^{-+-}	G^{--+}	G
	H	7.6422	8.4269	7.4851	8.3214	8.4013	8.2429	8.3395	9.8454	0.4583
2,2,5-Trimethyl hexane	M_1	336	1340	468	1592	2448	760	2210	763	38
	M_2	777	5960	1296	7741	14817	2665	12832	2321	18
	HM	3358	24046	5506	31598	59830	10846	52190	9633	77
	F	1804	12126	2914	16116	30196	5516	26526	4991	41
	RM_2	476	4695	869	6230	12470	1960	10717	1619	1.2333
	H	7.6110	8.4312	7.4392	8.3242	8.4079	8.2786	8.2963	9.8446	0.5417
2,2-Dimethyl hexane	M_1	344	1348	476	1600	2456	763	2204	775	39
	M_2	849	6040	1340	7825	14869	2690	12728	2374	26
	HM	3622	24446	5738	32030	60198	10949	51902	9921	110
	F	1924	12366	3058	16380	30460	5569	26446	5173	58
	RM_2	540	4767	905	6306	12514	1982	10619	1660	1.0190
	H	7.7046	8.4165	7.4006	8.3117	8.3750	8.2902	8.3227	9.6708	0.3750
2,3,4-Trimethyl hexane	M_1	314	1304	490	1642	2490	746	2154	811	36
	M_2	729	5729	1414	8134	15154	2605	12269	2512	24
	HM	3050	23116	5930	33316	61196	10658	50076	10701	97
	F	1592	11658	3102	17048	30888	5448	25538	5677	49
	RM_2	449	4499	966	6574	12766	1913	10209	1763	1.0667
	H	7.8271	8.4466	7.5302	8.2985	8.4140	8.1468	8.3265	9.5563	0.3889
2,3,5-Trimethyl hexane	M_1	310	1302	486	1638	2150	742	2150	789	36
	M_2	695	5707	1390	8090	12231	2587	12231	2430	21
	HM	2928	22998	5804	33090	49886	10568	49886	10105	86
	F	1538	11584	3024	16910	25424	5394	25424	5245	44
	RM_2	419	4479	946	6534	10175	1899	10175	1703	1.1333
	H	7.7732	8.4433	7.5289	8.3039	8.3399	8.2163	8.3399	9.8040	0.4444
3,3,4-Trimethyl hexane	M_1	52	1350	490	1602	2458	770	2206	776	38
	M_2	72	6058	1414	7848	14884	2713	12746	2381	26
	HM	348	24536	5930	32148	60300	11086	51992	9944	110
	F	204	12420	3102	16452	30532	5660	26500	5182	58
	RM_2	28	4783	966	6327	12527	1998	10635	1666	1.0190
	H	2.5381	8.4107	7.5302	8.3094	8.3689	8.1298	8.3149	9.6584	0.3750
3,3-Diethyl pentane	M_1	324	1324	500	1652	2500	756	2164	866	24
	M_2	808	5913	1456	8238	15230	2656	12382	2724	18
	HM	3388	23942	6260	33872	61648	10892	50536	12218	75
	F	1772	12116	3348	17396	31188	5580	25772	6770	39
	RM_2	518	4663	998	6668	12832	1954	10312	1920	1.2
	H	8.0032	8.3571	7.5671	8.2828	8.3744	7.9863	8.2962	8.9615	0.5000
3-Ethyl-2,2-Dimethyl pentane	M_1	341	1348	476	1600	2457	768	2204	753	38
	M_2	834	6040	1340	7825	14883	2705	12728	2294	24
	HM	3553	24440	5744	32036	60259	11040	51896	9345	99
	F	1885	12360	3064	16386	30493	5630	26440	4757	51
	RM_2	528	4767	905	6306	12527	1992	10619	1602	1.0857
	H	7.7838	8.4157	7.4226	8.3119	8.3738	8.1657	8.3219	9.9436	0.4167
3-Ethyl-2,3-Dimethyl pentane	M_1	342	1352	480	1604	2460	480	2198	799	38
	M_2	859	6078	1364	7869	14897	1364	12626	2466	28
	HM	3636	24636	5864	32256	60392	5864	51542	10559	121
	F	1918	12480	3136	16518	30598	3136	26290	5627	65
	RM_2	552	4801	925	6346	12538	925	10523	1728	0.9524
	H	7.9228	8.4068	7.3994	8.3061	8.3606	7.3994	8.3355	9.3906	0.3333
3-Ethyl-2,4-Dimethyl pentane	M_1	314	1306	490	1642	2490	746	2154	810	36
	M_2	731	5747	1412	8132	15152	2607	12271	2506	24
	HM	3054	23192	5926	33312	61192	10662	50080	10682	97
	F	1592	11698	3102	17048	30888	5448	25538	5670	49
	RM_2	451	4515	964	6572	12764	1915	10211	1758	1.0667

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Alkanes		Topological Indices								
		G^{+++}	G^{++-}	G^{+-+}	G^{+--}	G^{---}	G^{-++}	G^{-+-}	G^{--+}	G
	H	7.8367	8.4353	7.5261	8.2978	8.4133	8.1564	8.3276	9.5747	0.3889
2,2,3,3-Tetramethyl pentane	M_1	372	1427	446	1514	2386	810	2302	737	42
	M_2	958	6575	1210	7203	14291	2890	13609	2223	24
	HM	4100	26729	5300	29378	58162	11768	55474	9293	100
	F	2184	13579	2880	14972	29580	5988	28256	4847	52
	RM_2	622	5225	803	5768	12004	2137	11404	1545	0.5833
	H	7.5093	8.3943	7.1372	8.3467	8.3140	8.2358	8.3140	9.5394	0.1875
2,2,3,4-Tetramethyl pentane	M_1	368	1384	458	1552	2416	784	2248	753	40
	M_2	922	6270	1266	7462	14542	2770	13110	2288	21
	HM	3962	25394	5418	30438	58966	11274	53442	9517	85
	F	2118	12854	2886	15514	29882	5734	27222	4941	43
	RM_2	590	4962	848	5990	12226	2042	10958	1595	0.6190
	H	7.4844	8.4068	7.2522	8.3373	8.3668	8.2611	8.3321	9.6273	0.1944
2,2,4,4-Tetramethyl pentane	M_1	390	1418	434	1502	2374	798	2290	746	42
	M_2	970	6485	1144	7077	14213	2830	13489	2253	16
	HM	4258	26240	4970	28748	57628	11450	54856	9560	72
	F	2318	13270	2682	14594	29202	5790	27878	5054	40
	RM_2	617	5144	749	5654	11938	2089	11296	1566	0.6667
	H	7.3140	8.4027	7.2335	8.3662	8.3686	8.3752	8.3484	9.4648	0.2500
2,3,3,4-Tetramethyl pentane	M_1	372	1388	460	1548	2420	788	2256	740	40
	M_2	958	6310	1276	7408	14568	2790	13207	2244	24
	HM	4100	25600	5476	30288	59144	11380	53876	9164	98
	F	2184	12980	2924	15472	30008	5800	27462	4676	50
	RM_2	622	4998	856	5940	12248	2058	11047	1564	0.5714
	H	7.5093	8.3998	7.2385	8.3623	8.3487	8.2188	8.3154	9.7716	0.1667

2. Results and Discussion

The data corresponding to molecular structure and experimental properties of alkanes are collected from reliable online databases such as PubChem and from article [16]. Construction of transformation graph of alkanes and the corresponding topological indices are determined by the definition as well as, the results in Proposition 1.1 and Lemma 1.1, which is listed in Table 2. Further QSPR analysis is conducted for Correlation Coefficient (r) values between the physical properties such as boiling point (Bp) ^oC, molar refraction (Mr) cm^3mol^{-1}, molar volume (Mv) m^3mol^{-1}, heat of vaporization (Hv) $kJmol$, critical temperature (Ct) ^oC, surface tension (St) $dyn\ cm^{-1}$ and topological indices.

2.1. Correlation Coefficient

Correlation coefficient values are compared between different transformation graphs (TG) of alkanes and the values showing the highest correlation are listed in the following tables.

Table 3 presents the correlation coefficients and RMSE values obtained between the boiling points of various alkane groups and a set of commonly used topological indices (TIs). This comparison allows for a comprehensive assessment of each index's predictive performance and sensitivity toward structural variations within the alkane series.

Table 3: Correlation coefficient of Bp with different TIs for each TG of alkanes

	Parameter	G^{+++}	G^{++-}	G^{+-+}	G^{+--}	G^{---}	G^{-++}	G^{-+-}	G^{--+}	G
M_1	r	0.701	0.863	0.949	0.932	0.876	0.896	0.963	0.924	0.850
	RMSE	26.6	18.8	11.7	13.5	18.0	16.5	10.0	14.3	19.6
M_2	r	0.620	0.846	0.923	0.898	0.846	0.860	0.951	0.890	0.926
	RMSE	29.3	19.9	14.4	16.4	19.9	19.0	11.5	17.0	14.1
HM	r	0.589	0.845	0.922	0.897	0.852	0.860	0.949	0.890	0.897
	RMSE	30.1	19.9	14.4	16.5	19.5	19.0	11.7	17.0	16.5
F	r	0.561	0.845	0.921	0.897	0.857	0.860	0.941	0.891	0.858
	RMSE	30.9	20.0	14.6	16.5	19.2	19.0	12.6	17.0	19.2
RM_2	r	0.582	0.842	0.911	0.890	0.837	0.853	0.946	0.884	0.816
	RMSE	30.3	20.1	15.3	17.0	20.4	19.4	12.1	17.4	21.5
H	r	0.868	0.773	0.985	0.977	0.911	0.963	0.936	0.981	0.486
	RMSE	18.5	23.6	6.53	8.00	15.4	10.0	13.1	7.26	32.6

The correlations presented in Table 3 show that for every alkane type, the topological indices for derived graphs provide stronger predictive performance for boiling point (Bp) than the for graph G of alkanes. For M_1, r value for G (0.85) is exceeded by derived graph such as G^{+-+} (0.949) and G^{+--} (0.932), which show notably stronger correlations and lower RMSE values, indicating better predictive reliability. A similar trend is observed for M_2, where r value for G (0.926) is still outperformed by G^{+-+} (0.923) and G^{+--} (0.898), which maintain high accuracy with smaller errors. For HM, r value for G shows a moderate correlation (0.897), whereas derived graph such as G^{+-+} (0.922) and G^{+--} (0.897) show equal or stronger performance with reduced RMSE. In the F, the r value for G (0.858) is surpassed by G^{+-+} (0.921) and G^{+--}(0.897), demonstrating better structural sensitivity. The largest improvement occurs for index H, where the r value for G drops to 0.486, while indices such as G^{+-+}(0.985), G^{+--}(0.977), and G^{-+-}(0.963) show extremely strong correlations with substantially lower RMSE values. This indicates that the indices for modified graphs capture branching effects far more effectively than G.

Overall, compared to the r value for G across all alkane types, the extended Zagreb-type indices consistently show higher correlations and lower prediction errors, confirming their superior ability to encode structural differences relevant to boiling point prediction.

Table 4 summarizes the correlation coefficients and RMSE values between the molar refractivity (Mr) of different alkane groups and a set of topological indices, enabling an evaluation of each index's predictive capability and consistency across structural variations.

Table 4: Correlation Coefficient (r) and RMSE of Mr with Different TIs for Each TG of alkanes

	Parameter	G^{+++}	G^{++-}	G^{+-+}	G^{+--}	G^{---}	G^{-++}	G^{-+-}	G^{+-+}	G
M_1	r	0.763	0.909	0.973	0.969	0.905	0.941	0.985	0.966	0.857
	RMSE	3.69	2.20	1.23	1.03	2.25	1.80	0.91	1.37	2.73
M_2	r	0.691	0.905	0.951	0.946	0.888	0.918	0.979	0.945	0.895
	RMSE	4.13	2.25	1.63	1.71	2.43	2.09	1.08	1.74	2.36
HM	r	0.668	0.904	0.954	0.945	0.894	0.918	0.973	0.945	0.884
	RMSE	4.25	2.26	1.58	1.72	2.37	2.10	1.23	1.73	2.47
F	r	0.647	0.903	0.955	0.944	0.898	0.918	0.958	0.945	0.862
	RMSE	4.36	2.27	1.57	1.74	2.32	2.10	1.51	1.72	2.68
RM_2	r	0.652	0.903	0.947	0.941	0.882	0.914	0.976	0.941	0.760
	RMSE	4.33	2.27	1.77	1.79	2.49	2.15	1.14	1.80	3.44
H	r	0.729	0.767	0.977	0.993	0.901	0.966	0.914	0.987	0.464
	RMSE	3.91	3.39	1.14	0.64	2.24	1.38	1.55	0.84	4.68

Table 4 demonstrates that for all alkane classes, the topological indices for derived graphs consistently outperform for the graph G of alkanes in predicting molar refraction (Mr). For the M_1 group, the r value for G is 0.857, whereas for G^{+-+}(0.97), G^{+--} (0.97), and G^{--+} (0.985) show markedly higher correlations and lower RMSE values, confirming their superior predictive accuracy. The M_2 class shows a similar pattern: r value for G (0.895) is outperformed by G^{+-+}(0.95), G^{+--}(0.95), and G^{--+}(0.979), all achieving stronger correlations and substantially reduced RMSE. For HM, the predictive improvement remains evident. The r value for G (0.884) is lower than G^{+-+} (0.95), G^{+--}(0.95), and G^{--+}(0.973), with these indices offering better alignment between structural variation and Mr. A comparable trend appears in the F group, where r value for G is 0.862, while G^{+-+}(0.96), G^{+--} (0.94), and G^{--+}(0.958) and in RM_2 where r value for G is 0.76, while G^{+-+}(0.95), G^{+--} (0.94), and G^{--+}(0.976) each exhibit superior correlation strength and improved RMSE performance. The distinction becomes most pronounced for the H index. Here, r value for G (0.464) provides only weak correlation, whereas enhanced for derived graphs such as G^{+--} (0.99), G^{+-+}(0.98), and G^{---}(0.987) capture the molecular branching effects far more effectively. These higher r values combined with lower RMSE clearly establish the superiority of these descriptors for modeling Mr in highly branched alkanes.

Overall, the modified Zagreb-type indices demonstrate a consistent and significant improvement. Their enhanced correlation and reduced prediction error confirm their robustness and sensitivity for QSPR modeling of molar refraction in alkane systems.

Table 5 presents the correlation coefficients and RMSE values obtained between the heat of vaporization (Hv) of different alkane groups and a range of topological indices, enabling a comparative evaluation of their predictive performance and structural sensitivity within QSPR modeling.

Table 5: Correlation coefficient of Hv with different TIs for each TG of alkanes

	Parameter	G^{+++}	G^{++-}	G^{+-+}	G^{+--}	G^{---}	G^{-++}	G^{-+-}	G^{--+}	G
M_1	r	0.641	0.825	0.959	0.943	0.828	0.868	0.958	0.931	0.745
	RMSE	4.46	3.08	1.55	1.80	3.05	2.70	1.56	1.98	3.63
M_2	r	0.550	0.816	0.948	0.925	0.811	0.839	0.953	0.911	0.930
	RMSE	4.85	3.15	1.74	2.07	3.19	2.96	1.64	2.25	2.00
HM	r	0.517	0.814	0.942	0.925	0.818	0.840	0.944	0.910	0.903
	RMSE	4.97	3.16	1.83	2.07	3.13	2.96	1.80	2.26	2.33
F	r	0.488	0.812	0.935	0.925	0.825	0.840	0.927	0.908	0.867
	RMSE	5.07	3.18	1.94	2.06	3.07	2.95	2.05	2.27	2.71
RM_2	r	0.505	0.813	0.942	0.921	0.805	0.834	0.951	0.907	0.717
	RMSE	5.01	3.17	1.82	2.13	3.23	3.00	1.68	2.03	3.80
H	r	0.752	0.707	0.982	0.944	0.844	0.927	0.931	0.959	0.637
	RMSE	3.83	3.85	1.04	1.79	2.92	2.05	1.99	1.55	4.20

The correlation results for Hv indicate that the topological indices for derived graphs consistently outperform than the graph G of alkanes across all alkane groups, demonstrating their stronger structural sensitivity in QSPR modeling. For the M_1 class, the r value (0.745) is noticeably lower than several enhanced indices, particularly G^{+-+} (0.96), G^{++-}(0.83), and G^{--+} (0.958). These indices also exhibit reduced RMSE values (1.55–1.56), confirming superior predictive accuracy relative to the higher RMSE for G (3.63). A similar improvement is observed for M_2, where the r value (0.93) is surpassed by G^{+-+}(0.95), G^{+--}(0.93), and especially G^{--+}(0.953), each providing stronger correlations and lower RMSE. In the HM group, although the r value for G is relatively high (0.903), indices for derived graphs including G^{+-+}(0.94), G^{+--}(0.93), and G^{--+}(0.944) achieve comparable or slightly superior correlations with substantially lower RMSE values, reinforcing their stability across moderately branched structures. For the F group, the correlation (0.867) is again exceeded by G^{+-+}(0.94), G^{--+} (0.927), and G^{++-}(0.81), each showing better predictive strength and reduced error. The RM_2 class exhibits a similar trend: while $r = 0.717$, higher correlations are achieved by G^{+--}(0.92), G^{+-+}(0.94), and G^{--+}(0.907), indicating markedly improved modeling capability for isomer-rich sets. The largest discrepancy appears in the H group, where the r value (0.637) provides weak predictive power. In contrast, the enhanced indices demonstrate excellent performance, especially G^{+-+}(0.98), G^{++-}(0.71), G^{+--}(0.94), and G^{--+}(0.931), all accompanied by significantly lower RMSE values. This clearly demonstrates their superior ability to account for extensive branching effects. Overall, across linear, moderately branched, and highly branched alkane categories, the modified Zagreb-type indices achieve higher correlation coefficients and lower RMSE than the for G. These findings highlight their robustness, structural responsiveness, and enhanced suitability for accurate QSPR prediction of heat of vaporization in alkane systems.

Table 6 summarizes the correlation coefficients and RMSE values relating molar volume (Mv) to a set of topological indices across different alkane groups. This comparison enables assessment of each index's predictive capability relative to the baseline G index within QSPR modeling.

Table 6: Correlation coefficient of Mv with different TIs for each TG of alkanes

	Parameter	G^{+++}	G^{++-}	G^{+-+}	G^{+--}	G^{---}	G^{-++}	G^{-+-}	G^{--+}	G
M_1	r	0.782	0.886	0.963	0.959	0.890	0.922	0.974	0.953	0.844
	RMSE	18.1	8.25	1.79	5.03	8.10	6.86	4.02	5.37	9.53
M_2	r	0.683	0.879	0.942	0.936	0.873	0.898	0.967	0.931	0.860
	RMSE	21.3	8.46	5.98	6.23	8.66	7.83	4.50	6.47	9.08
HM	r	0.665	0.878	0.942	0.935	0.878	0.897	0.959	0.931	0.846
	RMSE	21.7	8.51	5.96	6.28	8.51	7.84	5.03	6.47	9.48
F	r	0.645	0.876	0.941	0.935	0.882	0.897	0.943	0.931	0.822
	RMSE	22.2	8.57	6.03	6.33	8.36	7.84	5.89	6.47	10.1
RM_2	r	0.630	0.877	0.933	0.931	0.867	0.893	0.965	0.937	0.695
	RMSE	22.6	8.53	6.41	6.47	8.84	8.00	4.68	6.65	12.8
H	r	0.450	0.749	0.976	0.981	0.891	0.955	0.949	0.981	0.507
	RMSE	26.0	11.8	3.90	3.46	8.07	5.03	5.58	3.49	15.3

The results in Table 6 clearly demonstrate that the topological indices for derived graphs provide stronger predictive performance for molar volume (Mv) than the r value for G across all alkane groups. For M1 alkanes, where r value for G is 0.844, higher correlations are achieved by G^{++-}(0.89), G^{+-+}(0.96), G^{+--}(0.96), and especially G^{--+}(0.974), each also showing substantially lower RMSE values than the high RMSE of G (9.53). This improvement reflects greater structural sensitivity in the modified indices. In the M_2 class, the r value for G (0.868) is outperformed by G^{+-+}(0.94), G^{+--}(0.94), and G^{--+}(0.967), which achieve both stronger correlations and reduced prediction errors. The same trend holds in the HM group, where the r value for G (0.801) is surpassed by G^{+-+}(0.94), G^{+--}(0.94), and G^{--+}(0.959), highlighting the reliability of these indices for moderately branched structures. For the F indices, r value for G is 0.822, whereas G^{+-+}(0.94), G^{+--}(0.94), and G^{--+}(0.943) exhibit clearly superior correlations along with lower RMSE values, confirming their enhanced modeling capability. A similar enhancement appears in the RM_2 group, where r value for G (0.695) is significantly weaker than the correlations of G^{+-+}(0.93), G^{+--}(0.93), and G^{--+}(0.965). The most notable improvement occurs in the H group, where the r value for G (0.507) shows poor predictive strength for Mv. In contrast, indices of derived graphs such as G^{+--}(0.98), G^{-++}(0.89), and G^{-+-}(0.955) provide substantially stronger correlations and markedly lower RMSE values, indicating that these descriptors effectively capture the complex branching effects characteristic of highly branched alkanes.

Overall, across linear, lightly branched, and heavily branched alkane groups, the extended Zagreb-type indices consistently demonstrate higher correlation coefficients and lower RMSE than the for G. Their superior performance highlights their suitability for accurate QSPR modeling of molar volume.

Table 7 summarizes the correlation performance of various topological index (TI) groups in predicting the physicochemical property ct across different alkane groups. For each group, both the correlation coefficient (r) and RMSE are reported. The final column lists the r and RMSE value of alkanes, representing the reference or benchmark structural parameter for each alkane group. This allows a direct comparison between TI-based predictive strength and the structural characteristics quantified by G.

Table 7: Correlation coefficient of Ct with different TIs for each TG of alkanes

	Parameter	G^{+++}	G^{++-}	G^{+-+}	G^{+--}	G^{---}	G^{-++}	G^{-+-}	G^{--+}	G
M_1	r	0.727	0.871	0.930	0.914	0.859	0.899	0.950	0.909	0.869
	RMSE	31.2	22.3	16.7	18.4	23.2	20.0	14.2	18.9	22.5
M_2	r	0.665	0.857	0.901	0.878	0.829	0.865	0.937	0.876	0.928
	RMSE	34.0	23.4	19.7	21.7	25.4	22.8	15.8	21.9	16.9
HM	r	0.636	0.857	0.904	0.878	0.835	0.865	0.940	0.877	0.903
	RMSE	35.1	23.4	19.4	21.8	25.0	22.8	15.6	21.9	19.6
F	r	0.609	0.857	0.905	0.877	0.841	0.865	0.935	0.878	0.867
	RMSE	36.0	23.4	19.3	21.9	24.6	22.8	16.1	21.8	22.7
RM_2	r	0.634	0.853	0.888	0.870	0.820	0.859	0.932	0.870	0.869
	RMSE	35.1	23.7	20.9	22.4	26.0	23.3	16.5	22.4	22.5
H	r	0.840	0.780	0.961	0.970	0.888	0.958	0.916	0.969	0.388
	RMSE	24.6	28.5	12.6	11.1	20.9	13.0	18.2	11.3	41.9

The results in Table 7 clearly demonstrates the topological indices for derived graphs for the property (Ct), and r value for G across all alkane groups. For M_1 alkanes, where r value for G is 0.869. M_1 exhibits moderately high, and the strongest correlations occur for G^{+-+}(0.93) and G^{-+-}(0.899), which align well with its relatively high value. In the M_2 class, the r value for G is 0.928. M_2 shows maximum correlation for G^{+-+} (0.90) and G^{-+-}(0.865). RMSE values follow the same trend, where G^{--+}(15.8) and G^{+-+}(19.7) give lowest prediction errors. These results demonstrate that TI groups sensitive to mixed-degree interactions match well with the elevated G value of M_2. HM ($r = 0.903$) is comparable to M_1 and M_2, and correspondingly the highest r values are seen in G^{+-+}(0.91) and G^{-+-}(0.865). RMSE is lowest for G^{--+}(15.6) and G^{---}(21.9), indicating that the TI groups capturing both branching and distance effects best approximate the structural information encoded by G. With a moderate r value for G (0.867), F shows strong correlations for G^{+-+}(0.91) and G^{-+-}(0.865). The lowest RMSE occurs for G^{--+}(16.1) and G^{---}(21.8). These patterns are consistent with its G value, suggesting that the same TI groups that perform well for similarly sized or branched alkanes (M_1, HM) apply to F as well. RM_2, with a G ($r = 0.887$) slightly higher than F, achieves maximum correlation with G^{+-+}($r = 0.89$) and $G{-}{+}{-}$($r = 0.859$). RMSE values for these groups are also the lowest G^{--+}(16.5) and G^{---}(22.4). H has the lowest r value (0.388) among all groups, indicating minimal structural complexity. Correspondingly, TI groups show exceptionally high correlations with G^{+-+} (0.96) and G^{+--}(0.97). The lowest RMSE occurs for G^{+--}(11.1) and G^{---}(11.3). Across all alkane groups, TI for G^{+-+}, G^{++-}, and G^{-++} consistently show the strongest correlations and lowest RMSE values.

Table 8 presents a comparative analysis of how different TI's (M_1, M_2, HM, F, RM_2, and H) relate to the property (St) across various alkane groups for (G^{+++} to G^{---}). Each TI's correlation and RMSE are benchmarked against the alkanes G, offering insight into which TI's for derived graphs provides the most reliable and consistent predictive relationship.

Table 8: Correlation coefficient of St with different TIs for each TG of alkanes

	Parameter	G^{+++}	G^{++-}	G^{+-+}	G^{+--}	G^{---}	G^{-++}	G^{-+-}	G^{--+}	G
M_1	r	0.543	0.779	0.868	0.852	0.760	0.807	0.876	0.845	0.688
	RMSE	1.65	0.606	0.973	1.03	1.27	1.16	0.946	1.05	1.44
M_2	r	0.494	0.775	0.854	0.830	0.740	0.783	0.870	0.824	0.938
	RMSE	1.71	1.24	1.02	1.09	1.32	1.22	0.969	1.11	0.681
HM	r	0.462	0.775	0.856	0.830	0.749	0.783	0.868	0.825	0.920
	RMSE	1.74	1.24	1.01	1.09	1.30	1.22	0.973	1.11	0.768
F	r	0.435	0.775	0.857	0.831	0.757	0.784	0.859	0.825	0.894
	RMSE	1.77	1.24	1.01	1.09	1.28	1.22	1.00	1.11	0.879
RM_2	r	0.470	0.774	0.847	0.825	0.627	0.779	0.867	0.820	0.813
	RMSE	1.73	1.24	1.04	1.11	1.53	1.23	0.978	1.12	1.14
H	r	0.712	0.651	0.880	0.873	0.773	0.855	0.833	0.873	0.426
	RMSE	1.38	1.49	0.931	0.958	1.24	1.02	1.09	0.955	1.78

In Table 8 across all alkane groups, the correlation coefficients (r) reveal that r for indices of derived graphs consistently outperform for the unmodified G, indicating improved linear relationships with (St). For instance, in M_1, the correlations of 0.85–0.876 (G^{+--} and G^{--+}) notably exceed that of G (0.688), with lower or comparable RMSE values (0.97– 1.44), suggesting enhanced predictive accuracy. In M_2 and HM, where r values for G (0.938, 0.92) respectively is better than that for derived graphs. The F and RM_2 groups follow the same pattern, showing the correlations of G (0.894 and 0.81) better than derived graphs. Notably, group H exhibits the weakest correlations overall (r = 0.65–0.85), yet even here, the alternative TIs for derived graphs provide improved performance over G (r = 0.426), highlighting the robustness of the modified indices. In summary, the table demonstrates that the TIs for derived graphs consistently enhance correlation strength and reduce error relative to that of G across all alkane groups, confirming their superior predictive reliability in representing St–TI relationships.

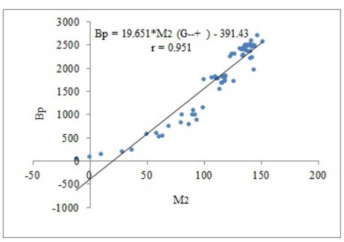
2.2. Regression Models

Linear regression will be of the form $y = mx + c$ where y is physical property, x stands for topological Index, m is the intercept and predicts where the regression line cuts the y-axis, c predicts the change in y for every unit change in x. Regression equations in Table 9 are equations corresponding to the highest correlation coefficient values listed. Among all the indices highest correlation is observed for G^{+--},G^{+-+},G^{--+}which indicates structural information captured by these contribute more significantly to predict physical properties.Also it can be concluded that the models listed effectively describe molecular topology of alkanes hence considered as predictive models for estimation properties of untested isomers with in same homologous series. Scatter plot of regression between properties and TI's are represented in Figure 4.

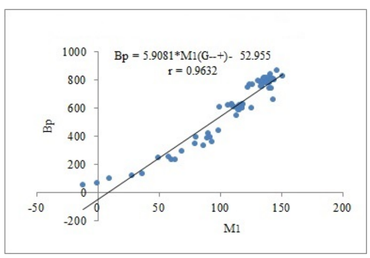
Table 9: Linear regression equation between physical properties and TIs

$B_p = 0.0317 * H(G^{+-+}) + 3.1723$	$C_t = 4.7792 * M_1(G^{--+}) - 767.42$
$B_p = 5.9081 * M_1(G^{--+}) - 52.955$	$C_t = 66.028 * HM(G^{--+}) - 11362$
$B_p = 19.651 * M_2(G^{--+}) - 391.43$	$C_t = 0.0272 * H(G^{+--}) - 0.5044$
$M_r = 39.251 * M_1(G^{--+}) - 929.16$	$C_p = -65.24 * M_1(G^{--+}) + 2338.8$
$M_r = 133.35 * M_2(G^{--+}) - 3419.4$	$C_p = -216.86 * M_2(G^{--+}) + 7560.3$
$M_r = 0.2062 * H(G^{+--}) - 0.7102$	$C_p = -0.359 * H(G^{+-+}) + 16.244$
$H_v = 22.567 * M_1(G^{+-+}) - 495.24$	$S_t = 90.135 * M_1(G^{--+}) - 1262.1$
$H_v = 91.626 * RM_2(G^{--+}) - 2287.4$	$S_t = 223.7 * RM_2(G^{--+}) - 3398.9$
$H_v = 0.188 * H(G^{+-+}) - 0.5044$	$S_t = 0.4352 * H(G^{+-+}) - 2.2746$
$M_v = 11.552 * M_1(G^{--+}) - 1256.8$	
$M_v = 39.224 * M_2(G^{--+}) - 4529$	
$M_v = 0.0606 * H(G^{+--}) - 2.4261$	

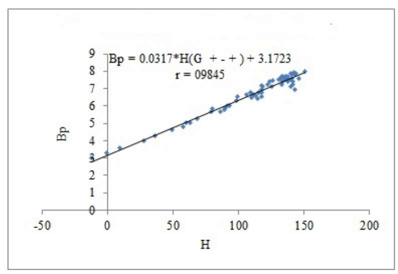
Figure 4: Regression between properties and TIs of transformation graphs



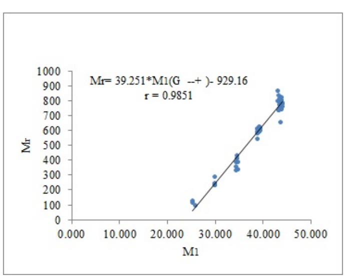
(a) Regression between Bp and M_2 for G^{--+}



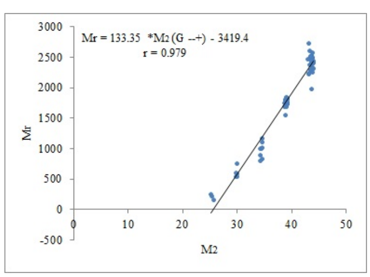
(b) Regression between Bp and M_1 for G^{--+}



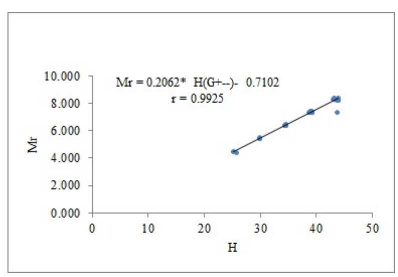
(c) Regression between Bp and H for G^{+-+}



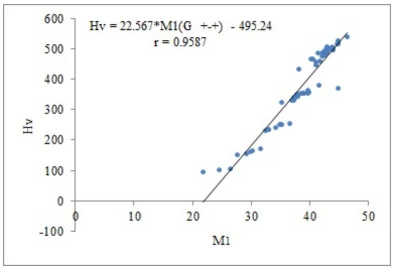
(a) Regression between Mr and M_1 for G^{--+}



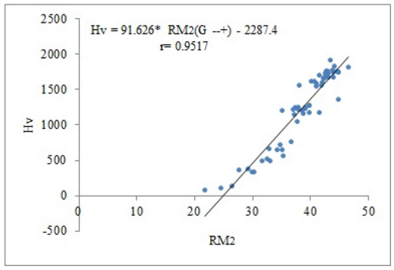
(b) Regression between Mr and M_2 for G^{--+}



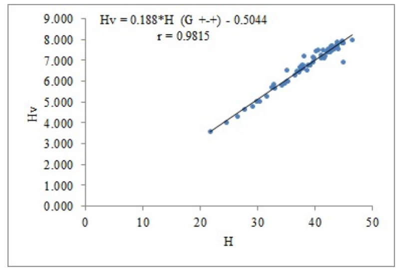
(c) Regression between Mr and H for G^{+--}



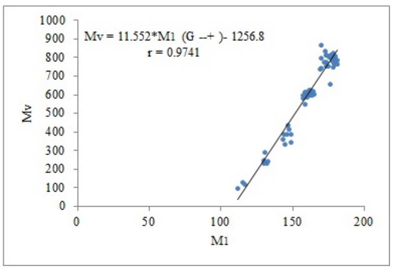
(a) Regression between Hv and M_1 for G^{+-+}



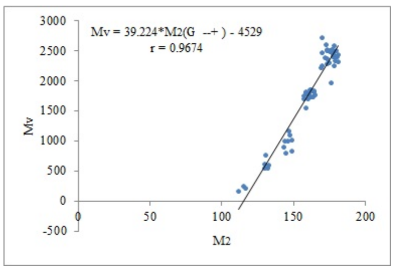
(b) Regression between Hv and RM_2 for G^{--+}



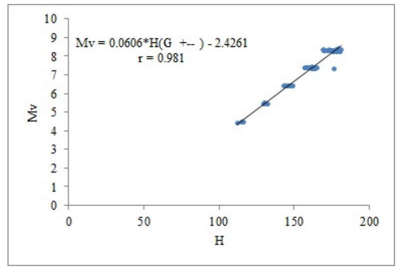
(c) Regression between Hv and H for G^{+-+}



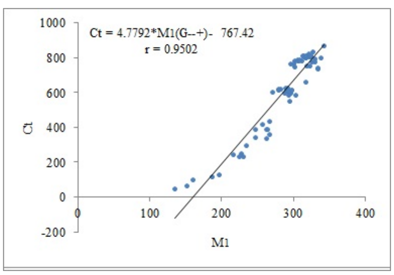
(a) Regression between Mv and M_1 for G^{--+}



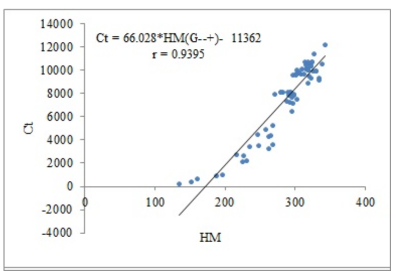
(b) Regression between Mv and M_2 for G^{--+}



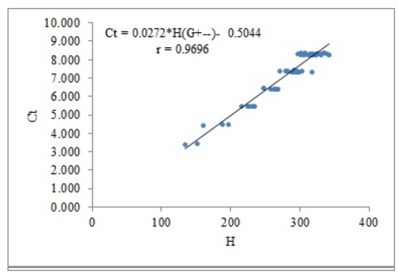
(c) Regression between Mv and H for G^{+--}



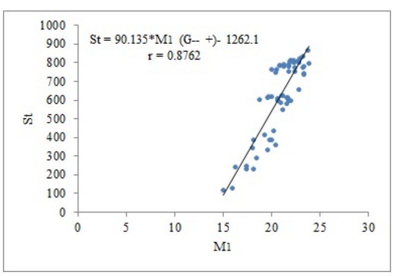
(a) Regression between Ct and M_1 for G^{--+}



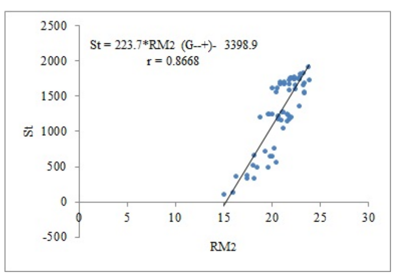
(b) Regression between Ct and HM for G^{--+}



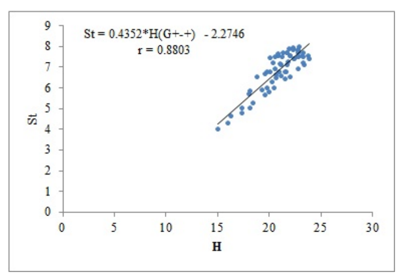
(c) Regression between Ct and H for G^{+--}



(a) Regression between St and M_1 for G^{--+}



(b) Regression between St and RM_2 for G^{--+}



(c) Regression between St and H for G^{+-+}

3. Conclusion

In this study, eight transformation graphs of 67 alkanes were systematically constructed and analyzed to evaluate the effectiveness of degree-based topological indices in QSPR modeling. The computed indices for all transformation graphs demonstrated strong and consistent correlations with physicochemical properties such as boiling point, molar refraction, molar volume, heat of vaporization, critical temperature, and surface tension. Comparing r values, it is observed that transformation graphs derived from molecular graphs give better results than the correlation coefficient values obtained from molecular graphs. Hence, transformation graphs can be considered a better choice in predicting the properties of alkanes. Among the models examined, several transformation-graph–based descriptors provided significantly enhanced structural sensitivity, enabling improved discrimination of alkane isomers and more reliable property prediction. Transformation graphs G^{--+},G^{+-+} and G^{+--} are found to be effective in predicting all the physical properties considered in this study. Linear regression analyses, supported by high correlation coefficients and low RMSE values, further validated the predictive capacity of these indices. Overall, the results highlight that transformation graphs offer a best mathematical framework for enriching structural information and strengthening QSPR models. This work strengthens the role of graph-theoretical approaches in chemical informatics and enables further development for extending transformation-graph–based descriptors to more complex molecular systems in future studies.

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