Bima Journal of Science and Technology, Vol. 9(2A) Jun, 2025 ISSN: 2536-6041

DOI: 10.64290/bimagombe.v9i2A.1090

Prediction of Boiling and Melting Points for Some Substituted Alkanes and their Isomers using Group Contribution Techniques

Charles Otobrise[1]* and Emmanuel E. Etim[2]

[1]Department of Chemistry, Delta State University, Abraka, Nigeria.
[2]Department of Chemical Sciences, Federal University Wukari

Corresponding author: otobrisec@delsu.edu.ng

ABSTRACT

The prediction of thermodynamic properties such as boiling (T_b) and melting (T_m) points is fundamental in chemical process design. This study evaluates the performance of three Group Contribution Techniques (GCTs): Constantinou – Gani (C & G), Marrero – Gani (M & G), and Joback – Reid (J & R) — in predicting two thermodynamic properties for selected substituted alkanes (SAs) and their isomers. The results indicate significant variations in predictions, with the J & R method generally estimating higher T_b, while the M & G method provides lower T_m values for most compounds. Discrepancies among the methods highlight the influence of molecular structure and functional groups on phase transition properties. The mean absolute error (MAE) across the methods was found to be 35.38 K for T_b and 39.06 K for T_m, highlighting variability in predictive accuracy. Standard deviation analysis further revealed significant fluctuations, with an average of 50.17 K for T_b and 51.21 K for T_m. Analysis of variance indicated no statistically significant difference between the three methods for T_b and T_m, suggesting that all three models perform comparably despite individual discrepancies. The findings underscore the need for further refinement of predictive models to enhance their reliability for industrial and research applications.

Keywords: Boiling Points, Melting Points, Substituted Alkanes, Isomers, Group Contribution Techniques.

INTRODUCTION

Boiling points (T_b) and melting points (T_m) are fundamental properties of organic compounds, influencing their behavior in chemical reactions, industrial processes, and environmental contexts (Joback & Reid, 1987). Substituted alkanes (SAs) also known as heteroalkanes are a class of organic compounds derived from alkanes by replacing one or more hydrogen atoms with heteroatoms like oxygen, nitrogen, sulphur or halogens (Smith & March, 2013; Carey & Giuliano, 2018). They have a wide range of applications in various fields. In the pharmaceutical industry, drugs like anesthetics, anthistamines and antibiotics are SAs (Loudon & Parise, 2016; Evers & Crowder, 2017). SAs also find use as refrigerants, pesticides, fuel additives and in the manufacture of plastics, dyes and pigments (Casida & Durkin, 2013; Mackay *et al.,* 2017; Owen & Coley, 2017; Kroschwitz & Howe-Grant, 2017; Gordon & Gregory, 2017). They present unique challenges in property prediction due to the diversity of substituents and their steric and electronic effects (Otobrise & Eferurhobo, 2024).

Experimental determination of T_b and T_m of SAs is very tasking and in some cases not feasible. Some SAs are toxic and flammable (Casida & Durkin, 2013; Evers & Crowder, 2017); maintaining temperature control can be very challenging with SAs that have high or low boiling points (Owen & Coley, 2017). SAs are thermally labile and very difficult to purify, impurities can affect laboratory

DOI: 10.64290/bimagombe.v9i2A.1090

measurements of BPs and MPs (Smith & March, 2013; Carey & Giuliano, 2018).

Computational techniques are required to predict properties of compounds when laboratory experiments are not feasible or economical (Monago & Otobrise, 2010). They predict properties of compounds with reasonable accuracy allowing researchers to quickly screen and evaluate large numbers of compounds, saving time, resources and costs (Jorgensen, 2009; Marrero & Gani, 2001; Monago & Otobrise, 2016; Lipkowitz & Boyd, 2017). A particular approach to predicting properties of organic compounds are Group Contribution Techniques (GCTs). They assign a contribution values to functional groups, atoms, groups of atoms or bonds present in a molecule (Gmehling & Kolbe, 1992; Otobrise *et al.,* 2018). GCTs assume that the properties of interest can be estimated by summing the contributions of each functional group, atom, groups of atoms or bonds present in a molecule. This approach is particularly advantageous for large datasets or compounds with complex structures where experimental data are unavailable (Constantinou & Gani, 1994). Some GCTs may require property specific parameters which are derived from experimental data or calculated using quantum mechanical methods.

The prediction of boiling and melting points for SAs using GCTs requires careful consideration of some factors. Firstly, substituents influence molecular properties through inductive, resonance, and steric effects. For example, electronegative groups like -Cl or -NO_2 typically increase boiling points due to enhanced dipole-dipole interactions. Secondly, increased branching in alkanes tends to lower boiling points by reducing surface area and intermolecular forces. Additionally, functional groups capable of hydrogen bonding, such as -OH or -NH_2, significantly elevate boiling and melting points (Constantinou & Gani, 1994; Marrero & Gani, 2001; Poling *et al.,* 2001).

GCTs offer a robust framework for predicting physical and thermodynamic properties. There are however a few challenges. Reliable parameterization requires extensive experimental data, which may be scarce for exotic substituents or rare compounds. The assumption of additivity may fail for molecules with significant intramolecular interactions. Predicting properties for compounds outside the training dataset can lead to large errors. This study compares the predictive performance of three GCTs in estimating T_b and T_m of some SAs and their isomers. It aims to identify the method that offers the most accurate and reliable estimations. This will influence the selection of computational approach in property prediction, chemical process design and similar industrial applications.

NUMERICAL METHODS

GCTs can provide reasonable estimates of T_b for SAs. Their accuracy vary depending on the specific method and compound. The T_m of SAs is frequently predicted using GCTs such as those created by Joback, Constantinou, and others (Joback & Reid, 1987; Constantinou & Gani, 1994; Marrero & Gani, 2001). These techniques entail building a structure-based model in which each group contributes a particular value to the total melting point. Three GCTs are compared for accuracy in predicting T_b and T_m of SAs and the results are juxtaposed with available experimental data.

Constantinou-Gani Method (C & G)

This method makes use of first and second order level group contributions. The second level involves groups that permit a better description of proximity effects and differentiation among isomers. For property

DOI: 10.64290/bimagombe.v9i2A.1090

estimation the C & G model takes the form of equation (1) below:

$$F(x) = \sum_i N_i C_i + W \sum_j M_j D_j \quad (1)$$

C_i in equation **(1)** is the contribution of the first order group type-*i* which occurs *Ni* times and D_j is the contribution of the second order group type-j with M_j occurrence in a compound. F(x) is a simple function of the property x. For the normal Boiling Point, F(x) = exp(T_b/t_{b0}). Since, from equation (**1**), F(x) takes the form ($\sum_i N_i t_{b1i} + \sum_j M_j t_{b2j}$)**,** then we can say;

$$\exp(T_b/t_{b0}) = (\sum_i N_i t_{b1i} + \sum_j M_j t_{b2j}) \quad (2)$$

From equation (2) above,

$$T_b = t_{b0} \ln (\sum_i N_i t_{b1i} + \sum_j M_j t_{b2j}) \quad (3)$$

T_b is the normal boiling point in Kelvin, t_{b0} is a constant (Universal adjustable parameter) with the value 204.359 K, t_{b1i} represents group contribution of the first order group of type-*i*, t_{b2j} represents group contribution of the second order group of type-*j* (Constantinou & Gani, 1994).

The correlation for T_m is expressed in equations 4 – 5.

$$\exp (T_m/t_{m0}) = (\sum_i N_i t_{m1i} + \sum_j M_j t_{m2j}) \quad (4)$$

$$T_m = t_{m0} \ln (\sum_i N_i t_{m1i} + \sum_j M_j t_{m2j}) \quad (5)$$

T_m is the melting point, t_{m0} is a constant (adjustable parameter) with value 102.425 k, t_{m1i} represents group contribution of first order of type-*i* for melting temperature, t_{m2j} represents group contribution of the second order of type-*j*. (Constantinou & Gani, 1994).

Marrero-Gani Method (M & G)

The above method considers the molecular structure of a compound to be collection of three type of groups. The property estimation method has the form of equation (6).

$$F(x) = \sum_i N_i C_i + \omega \sum_j M_j D_j + z \sum_k O_k E_k \quad (6)$$

In the above equation, *Ci* is the contribution of the first order group of type-*i* that occurs *Ni* times, *Dj* is the contribution of the second order group of type-*j* that occurs M_j times, the E_k contribution of the third order group of type-*k* that has O_k occurrence in a compound. In the first level of estimation, the constants ω and z are assigned zero values because only first order groups are employed. In the second order level, the constants ω and z are assigned unit and zero values, respectively because only the first and the second order groups are involved while the third level both ω and z are set to unity values. The left hand side of the above equation is a simple function F(x) of the target property x. For normal Boiling Point, F(x) = exp (T_b/T_{b0}) and from equation (6) above, F(x) = $\sum_i N_i C_i + \omega \sum_j M_j D_j + z \sum_k O_k E_k$. Therefore, we can infer that;

$$\exp (T_b/T_{b0}) = (\sum_i N_i T_{b1i} + \sum_j M_j T_{b2j} + \sum_k O_k T_{b3k}) \quad (7)$$

From equation 5 above, we can say that;

$$T_b = T_{b0} \ln (\sum_i N_i T_{b1i} + \sum_j M_j T_{b2j} + \sum_k O_k T_{b3k}) \quad (8)$$

T_b is normal boiling point in Kelvin, T_{b0} is a constant (adjustable parameter) with the value 222.543 K, T_{b1i} represents group contribution of first order type-i, T_{b2j} represents group contribution of second order type-j, T_{b3k} represents group contribution of third order type-k (Marrero and Gani, 2001).

The correlation for T_m is shown in equations (9 – 10).

$$\exp\left(T_m/T_{m0}\right) = \left(\textstyle\sum_i N_i T_{m1i} + \sum_j M_j T_{m2j} + \sum_k O_k T_{m3k}\right) \quad (9)$$

$$T_m = T_{m0} \ln\left(\textstyle\sum_i N_i T_{m1i} + \sum_j M_j T_{m2j} + \sum_k O_k T_{m3k}\right) \quad (10)$$

T_m is the melting point, T_{mo} is a constant (adjustable parameter) with value 147.450 k, T_{m1i} represents group contribution of first order of type-i for melting temperature, T_{m2j} represents group contribution of second order of type-j for melting temperature, T_{m3k} represents group contribution of second order of type-k (Marrero & Gani, 1994).

Joback-Reid Method (J & R)

The method assumes that the effects of individual groups are additive, neglecting potential interactions between groups. The method can produce significant deviations for complex or highly substituted compounds, as it neglects intermolecular interactions and structural effects (e.g., symmetry, branching, and crystal packing). Predictions are only as good as the database of group contributions. If a functional group is missing from the database, the method cannot be applied. Prediction of T_b takes the form of equation (11) below.

$$T_b = 198.2 + \textstyle\sum N_i \Delta T_{bi} \quad (11)$$

T_b is normal boiling point in Kelvin, N_i the number of occurrences of the ith atom, group of atoms or functional group in the molecule, ΔT_{bi} is the contribution of the ith atom, group of atoms or functional group to T_b (Joback & Reid, 1987; Reid *et al.,* 1987).

The Joback and Reid equation for predicting T_m is expressed as:

$$T_m = 122.5 + \textstyle\sum N_i \Delta T_{mi} \quad (12)$$

T_m is normal boiling point in Kelvin, N_i the number of occurrences of the ith atom, group of atoms or functional group in the molecule, ΔT_{mi} is the contribution of the ith atom, group of atoms or functional group to T_m (Joback & Reid, 1987; Reid *et al.,* 1987).

RESULTS AND DISCUSSION

The SAs and isomers chosen for the study are the most applicable to industry. They offer useful information about technique performance for frequently encountered compounds with few structural or functional variations. Table 1 presents a list of the SAs in this study, detailing their chemical formulae, structures, and molecular weights. Table 1 highlights the structural diversity within the SAs, showcasing variations in functional groups such as cyanides, aldehydes, ketones, amides, alcohols, and esters. Notably, while isomers share molecular formula, their differing structural arrangements result in unique chemical and physical properties. This comparison underscores the significance of molecular structure in predicting the T_b and T_m of the compounds, making it a valuable reference for studying chemical relationships and functional group transformations.

DOI: 10.64290/bimagombe.v9i2A.1090

Table 1: List of SAs, their formulae, structures and molecular weights.

Compound	**Formula**	**Structure**	**Molecular Weight (g/mol)**
Methyl cyanide (Acetonitrile)	C_2H_3N	CH_3-C≡N	41.05
Methyl isocyanide	C_2H_3N	CH_3N≡C	41.05
Propenal (Acrolein)	C_3H_4O	CH_2=CH-CHO	56.06
Cyclopropanone	C_3H_4O	CH_2CH_2C=O (3 membered ring)	56.06
1-Hydroxypropyne	C_3H_4O	CH≡C-CH_2OH	56.06
Acetamide	C_2H_5NO	CH_3-CO-NH_2	59.07
N-methyl formamide	C_2H_5NO	HCO-NH-CH_3	59.07
Propanone (Acetone)	C_3H_6O	CH_3-CO-CH_3	58.08
Propanal	C_3H_6O	CH_3-CH_2-CHO	58.08
Propanoic acid	$C_3H_6O_2$	CH_3-CH_2-COOH	74.08
Methyl ethanoate	$C_3H_6O_2$	CH_3-COO-CH_3	74.08
Hydroxypropanal	$C_3H_6O_2$	HO-CH_2-CH_2-CHO	74.08
1-Propanol(n-propanol)	C_3H_8O	CH_3-CH_2-CH_2-OH	60.09
2-Propanol (isopropanol or isopropyl alcohol)	C_3H_8O	CH_3-CH-OH-CH_3	60.09
Methoxyethane	C_3H_8O	CH_3-O-CH_2-CH_3	60.09

Table 2 presents the predicted T_b of the SAs using three different GCTs — C & G, M & G, and J & R—alongside available experimental data. The comparative predictions highlights the accuracy and limitations of each model in estimating T_b based on molecular structure. While some predictions closely align with experimental values, notable discrepancies emphasize the influence of structural variations and intermolecular forces on boiling behavior.

Table 2: Predictions of T_b by the three GCTs

Structure	**C & G**	**M & G**	**J & R**	**Exp. Data**
	T_b in Kelvin			
CH_3-C≡N	331.038	338.988	347.440	354.750*
CH_3N≡C	331.038	305.502	347.440	NA
CH_2=CH-CHO	313.426	302.927	318.280	325.840*
CH_2CH_2C=O (3 membered ring)	215.991	324.992	347.470	NA
CH≡C-CH_2OH	277.792	360.070	350.540	NA
CH_3-CO-NH_2	494.300	445.845	371.760	NA
HCO-NH-CH_3	347.087	348.630	344.190	NA
CH_3-CO-CH_3	305.373	306.661	322.110	NA
CH_3-CH_2-CHO	314.709	314.114	316.900	322.000*
CH_3-CH_2-COOH	415.693	422.435	413.750	414.150*
CH_3-COO-CH_3	308.522	306.941	326.460	329.900*
HO-CH_2-CH_2-CHO	340.846	417.718	409.080	NA
CH_3-CH_2-CH_2-OH	246.310	351.129	360.420	370.200*
CH_3-CH-OH-CH_3	263.021	337.557	347.440	NA
CH_3-O-CH_2-CH_3	286.621	267.947	290.660	280.400*

*Sourced from Wikipedia and C.L. Yaws, Handbook of chemical compound data for process safety (1997) NA = Not available.

Table 3 presents the predicted T_m of the SAs in the study using the GCTs of C & G, M & G, and J & R— together with available experimental data. The table provides an overview of how each predictive method performs relative to actual melting point measurements. Discrepancies between the predicted and experimental values highlight the varying accuracy of these models, emphasizing the need for careful selection of prediction methods in thermodynamic studies.

Table 3 presents the predicted T_m of the SAs in the study using the GCTs of C & G, M & G, and J & R— together with available experimental data. The table provides an

overview of how each predictive method performs relative to actual melting point measurements. Discrepancies between the predicted and experimental values highlight the varying accuracy of these models, emphasizing the need for careful selection of prediction methods in thermodynamic studies.

Table 3: Predictions of T_m by the three GCTs

Structure	C & G	M & G	J & R	Exp. Data
	T_m in Kelvin			
CH_3-C≡N	146.644	139.523	199.690	227.300*
CH_3N≡C	178.373	203.299	199.690	NA
CH_2=CH-CHO	180.491	196.255	187.730	189.000*
CH_2CH_2C=O (3 membered ring)	140.461	193.506	213.970	NA
CH≡C-CH_2OH	218.387	245.008	285.960	NA
CH_3-CO-NH_2	354.151	388.154	240.800	NA
HCO-NH-CH_3	220.028	249.259	239.200	268.000*
CH_3-CO-CH_3	171.616	191.073	193.900	178.300*
CH_3-CH_2-CHO	173.180	203.128	196.300	170.000*
CH_3-CH_2-COOH	262.333	312.945	246.300	253.000*
CH_3-COO-CH_3	155.104	154.995	210.700	174.500*
HO-CH_2-CH_2-CHO	230.398	271.632	265.500	NA
CH_3-CH_2-CH_2-OH	181.992	203.933	238.700	147.000*
CH_3-CH-OH-CH_3	162.389	197.094	243.840	184.000*
CH_3-O-CH_2-CH_3	149.717	123.522	196.800	132.000*

*Sourced from NIST Chemistry WebBook (https://webbook.nist.gov/chemistry/)

NA = Not available.

Boiling Points

J & R consistently predicts the highest T_b among the three methods. M & G tends to underestimate T_b for most compounds. C & G generally produces intermediate values. Some compounds show significant discrepancies between methods. For a few compounds, the three GCTs gave results that are closer to the experimental data.

The three GCTs underestimated T_b values for methyl cyanide. J & R provides the closest prediction of 347.44 K, which is only 7.31 K lower than the experimental data. C & G underestimates the boiling point the most. Experimental T_b was not available for methyl isocyanide in the literature. J & R predicts a higher T_b for methyl isocyanide than the other two methods. Without experimental data, it is unclear which method is most accurate.

The GCTs also underestimated T_b values for propenal. J & R gave the nearest prediction of 318.28 K, which is only 7.56 K lower than the experimental data. M & G significantly underestimated the T_b value. Experimental T_b was not available for cyclopropanone in the literature. There were large variations in predictions T_b for the latter. C & G predicts an unusually low T_b value for cyclopropanone. A similar trend is observed in the prediction of T_b for 1-hydroxypropyne and acetamide.

All methods gave close T_b predictions for n-methyl formamide. The range is small, suggesting confidence in these predictions. C & G and M & G provide nearly identical T_b values for propanone. J & R predicted a higher value. A similar trend was observed for propanal. However, J & R predicted a closer value to the experimental T_b, which was only 5.1 K lower.

J & R predicted a closely accurate T_b value for propanoic acid (only 0.4 K difference). C & G is also very accurate. M & G slightly overestimated. J & R yielded a better T_b value for methyl ethanoate with a disparity of 3.44 K. C & G and M & G significantly underestimated T_b value for the compound. This trend was also observed for 1-propanol and methoxyethane. Experimental T_b were not available for hydroxypropanal and 2-propanol in the literature. The T_b values obtained from C & G for both compounds was unusually low in comparison with the values predicted by the other two methods.

The effect of functional groups and hydrogen bonding in the accuracy of the GCTs is noteworthy. Carbonyl-containing compounds (acetamide, propanone, and propanoic acid) have relatively high T_b. Alcohols (e.g., 1-propanol, 2-propanol) tend to have significant differences in predictions, possibly due to hydrogen bonding contributions. Esters and ethers (methyl ethanoate, methoxyethane) show moderate T_b variations.

Statistical error analysis (SEA) was done for compounds with available experimental T_b. The Mean Absolute Error (MAE) and Standard Deviation of Errors (STD) for each prediction method was calculated according equations (13 – 14). The result is shown in Table 4.

$$MAE = \frac{1}{N}\sum_{i=1}^{N}(\text{Predicted}_i - \text{Experimental}_i) \tag{13}$$

$$STD = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\text{Error}_i - \text{Mean Error}_i)^2} \tag{14}$$

Table 4: Error analysis for T_b predictions.

Method	MAE	STD
C & G	28.06 K	43.02 K
M & G	15.62 K	6.36 K
J & R	6 K	3 K

J & R is the most accurate, with the lowest MAE (6.26 K) and the least variation (STD = 3.53 K). M & G has moderate accuracy, with a higher MAE (15.62 K) but low variability (STD = 6.36 K). C & G is the least accurate, with the highest MAE (28.06 K) and significant variation (STD = 43.02 K).

To ascertain whether there is a statistically significant difference between the predictions of the three models, a one-way ANOVA test was performed. With F-statistic = 1.274, p-value = 0.290 and the latter greater than the common significance level (0.05), it means that there is no statistically significant difference between the T_b predictions of the three models. In other words, while there are variations in T_b of individual compounds, the means of the three prediction models do not differ significantly. This observation is illustrated in figure 1 below.

DOI: 10.64290/bimagombe.v9i2A.1090

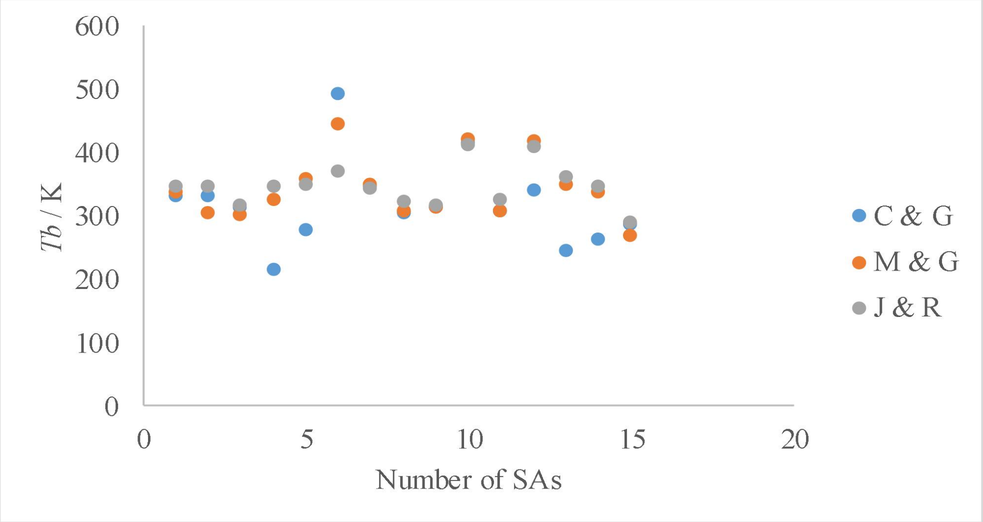

Figure 1: A scatter plot of the predictions by the GCTs.

Melting Points

The predicted T_m by the three methods vary significantly for some compounds. Some compounds show relatively close predictions among the three methods (e.g., Methyl ethanoate and Propanal). Other compounds, such as 1-Hydroxypropyne and Acetamide**,** have large variations in predictions, suggesting that the methodologies handle certain molecular structures differently.

All models underestimate T_m, for methyl cyanide; with C&G and M&G being significantly lower. J&R is closer but still off the experimental T_m of 227.3 K. Experimental T_m was not available for methyl isocyanide, but C&G yielded a lower T_m than the other two models, which have similar predictions. J&R gave the closest prediction of T_m for propenal, with only a 0.73 K error, while C&G and M&G slightly overestimated T_m.

There was a wide variation across the GCTs prediction of T_m for cyclopropanone, 1-Hydroxypropyne and acetamide with J&R giving the highest prediction for the first two and the lowest for the third. Experimental T_m was not available in the open literature for these compounds

A summary of the accuracy of each GCT vis-à-vis available experimental data is presented in Table 5. C&G is the most balanced method, often giving reasonable estimates, but it sometimes underestimates. M&G tends to overestimate melting points, especially for carboxyl and amide groups. J&R produces the most extreme values, sometimes very high (e.g., Isopropanol) or very low.

Table 5: Summary of T_m prediction accuracy by the GCTs.

Method	Closest Predictions	Overestimates	Underestimates
C&G	Acetone, Propanal, Isopropanol	Propanoic acid, 1-Propanol	Acetonitrile, n-Methyl formamide
M&G	Methoxyethane	Acetamide, Propanoic acid	Acetonitrile, Acetone
J&R	Acrolein, Propanoic acid	1-Propanol, Isopropanol	Acetamide, Acetone

SEA was done for SAs with available experimental T_m. MAE and STD for each prediction method calculated using equations (13 – 14) are shown in Table 6.

DOI: 10.64290/bimagombe.v9i2A.1090

Table 6: Error analysis for T_m predictions.

Method	MAE	STD
C & G	25.01 K	23.92 K
M & G	31.76 K	27.36 K
J & R	35.88 K	28.28 K

C&G has the lowest MAE (25.01 K), making it the most accurate method overall. M&G and J&R have higher errors, with J&R being the least accurate (35.88 K MAE). C&G also has the lowest variation in errors (SD = 31.58 K), indicating more consistent predictions. M&G and J&R show large standard deviations, meaning their predictions are more erratic.

One-way ANOVA test was performed to establish whether or not the T_m obtained from the GCTs had a statistically significant difference. With F-Statistic = 1.223, p-Value = 0.305 and the latter greater than the common significance level **(**0.05**)**, it means the variation in T_m predictions among the models is not large enough to be considered statistically significant. This suggests that the three methods are generally consistent, even though there are some individual variations for specific compounds. These observations are illustrated in figure 2 below. Further investigation with a larger dataset could provide more insights into potential biases in specific model predictions.

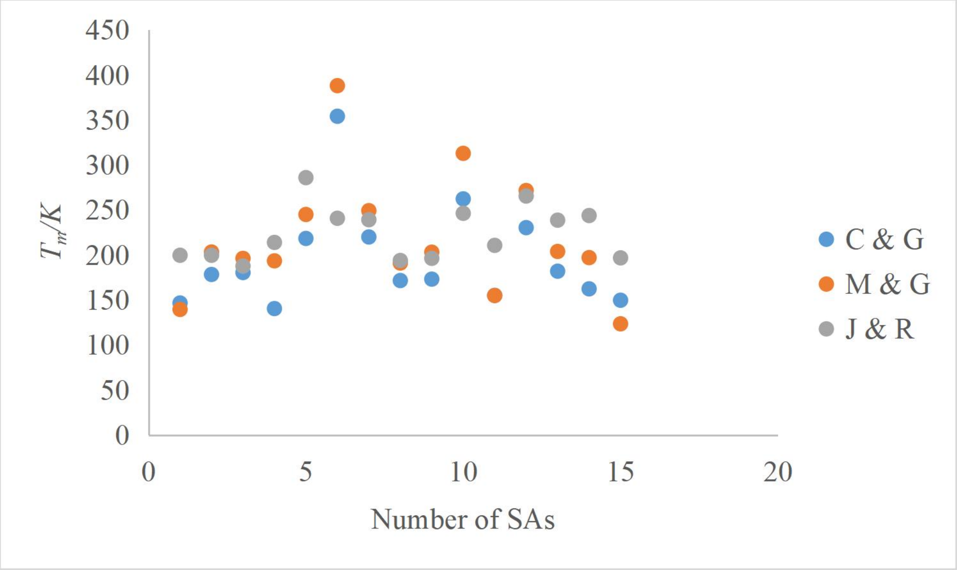

Figure 2: Scatter plot of T_m predictions by the GCTs.

CONCLUSION

This study analyzed the predictive accuracy of three GCTs—C & G, M & G, and J & R—for estimating T_b and T_m of 15 organic compounds. The results revealed notable variations among the methods, with the J & R approach generally yielding higher T_b estimates, while the M & G method exhibited significant deviations in T_m predictions. MAE and STD analyses confirmed these inconsistencies, with average deviations of 35.38 K and 39.06 K for T_b and T_m, respectively. Despite these variations, ANOVA results indicated no statistically significant difference among the methods, suggesting that while each model has distinct biases, they perform comparably overall. The observed discrepancies highlight the influence of molecular structure and functional groups on predictive accuracy, emphasizing the need for model refinement. While Group Contribution methods remain useful for estimating thermodynamic properties, their reliability depends on the specific compound class and parameterization strategies. Integrating machine learning techniques or hybrid modeling approaches as well as, expanding experimental datasets for model calibration could enhance accuracy, making these methods more applicable to industrial and research applications.

REFERENCES

Carey, F.A. & Giuliano, R.M. (2018). *Organic chemistry* (10th Edition). McGraw-Hill Education.

Casida, J.E. & Durkin, K.A. (2013). *Pesticide chemistry and bioscience: the food-environment challenge* (1st Edition). John Wiley & Sons.

Constantinou, L., & Gani, R. (1994). New group contribution method for estimating properties of pure compounds. *American Institution of Chemical Engineering journal,* 10 (40), 1697.

Evers, A.S. & Crowder, C.M. (2017). *Anesthetic pharmacology: basic principles and clinical practice* (2nd Edition). Cambridge University Press.

Gordon, P.F. & Gregory, P. (2017). Organic chemistry in colour (2nd Edition). Springer.

Joback, K.G., & Reid, R.C. (1987). Estimation of pure-component properties from group contributions. *Chemical Engineering Communications*, 57, 233-243.

Jorgensen, W.L. (2009). Efficient drug lead discovery and optimization. *Accounts of Chemical Research,* 42 (6) 724 – 733.

Kroschwitz, J.I. & Howe-Grant, M. (2017). *Kirk-Othmer encyclopedia of chemical technology* (5th Edition). John Wiley & Sons.

Lipkowitz, K.B. & Boyd, D.B. (2017). *Reviews in Computational Chemistry.* Wiley-VCH

Loudon, G.M & Praise, J. (2016). *Organic chemistry* (6th Edition). Benjamin Cummings

Mackay, D., Shiu, W.Y. & Ma, K.C. (2017). *Illustrated handbook of physical-chemical properties and environmental fate for organic chemicals* (2nd Edition). CRC Press.

Marrero, J., & Gani, R. (2001). Group-contribution based estimation of pure component properties. *Fluid Phase Equilibria, 183* (0), *183*-208.

Monago, K.O. & Otobrise, C. (2010). Estimation of pure-component properties of fatty acids and esters. *Journal of Chemical Society of Nigeria.* 35 (2), 142-148.

Monago, K.O. & Otobrise, C. (2016). Virial coefficients of nitrogen from a quadrupolar site-site potential function. *Journal of Theoretical and Computational Chemistry.* 15 (3), 1650024 (1-14).

NIST Chemistry WebBook (https://webbook.nist.gov/chemistry/)

Otobrise, C. and Eferurhobo, G. (2024). Prediction of the acentric factor of some halogenated hydrocarbons via group contribution techniques. *Journal of the Nigerian Society of Physical Sciences*. 6, 2119.

Otobrise, C., Monago, K.O. and Ibezim-Ezeani, M.U. (2018). Group contribution method for the estimation of critical properties of some linear aliphatic dimethyl esters of dicarboxylic acids. *FUW Trends in Science & Technology Journal.* 3 (2), 658-663.

DOI: 10.64290/bimagombe.v9i2A.1090

Owen, K. & Coley, T. (2017). *Automotive fuels reference book* (3rd Edition). SAE International.

Reid, R.C., Prausnitz, J.M., & Poling, B.E. (1987). *The Properties of Gases and Liquids* (4th Edition). McGraw-Hill.

Smith, M.B. & March, J. (2013). *March's advanced organic chemistry reactions, mechanisms and structure,* (7th Edition). John Wiley & Sons.

Yaws, C.L. (1997). Handbook of chemical compound data for process safety, United States of America, Gulf Publishing Company, Houston, Texas.