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Prediction of the Boiling Point of Acrylate and Methacrylate Polymers Through Wiener Index

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Abstract

Wiener index, a topological index of a molecular graph of the molecules are widely used to study the physico-chemical properties of the molecules. We considered the molecules, acrylate and methacrylate polymers. The Wiener index of these two polymers are obtained. And using this, the boiling point of these two polymers are studied extensively. Also, the detailed comparison is described graphically.

1 Introduction

The field of graph theory known as "chemical graph theory" focuses on the non-trivial implications of problems at the molecular level. Chemical graph theory is an interdisciplinary field that applies tools from graph theory, set theory, and statistics to the study of molecular structures in order to isolate the structural features involved in structure-property-activity relationships. Classifying molecules and modelling undiscovered structures can both benefit from topological characterization of chemical structures

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with the desired properties.

Polymers, with their high strength-to-weight ratio, stiffness, toughness, ductility, and cost-effectiveness, are among the most promising candidates. Furthermore, they have a wide operating temperature range, high thermal/electrical insulation, and good corrosion and light resistance. Polymers can be synthesised using a variety of starting materials, ranging from petroleum to non-fossil. [1]-[3]

Polyacrylates and Polymethacrylates are derived from acrylic acid and methacrylic acid, respectively. The physicochemical properties of these materials are heavily influenced by the nature of the substituents in the side chain, and polymerization occurs via the vinyl group. They are appealing due to their light transparency, elasticity, good weatherability, and resilience, as well as their simple functionalization route, good biocompatibility, and low cost. All of these characteristics lead to the use of these polymers in a variety of fields ranging from biomedicine to the food industry, environmental remediation, and electronic applications.

Acrylate polymers (Figure 1) [4] are a type of polymer composed of acrylate monomers. They are strong and long-lasting, making them suitable for a wide range of applications. They can also be used to make flexible materials that are resistant to wear and tear and can withstand extreme temperatures. Different grades of acrylate polymers, each with its own optimal molecular weight and viscosity, are on the market. Methyl acrylate, ethyl acrylate, butyl acrylate, and acrylic acid esters are some of the most widely used acrylate types (acrylic esters).

Methacrylate polymers (Figure 2) [5] are a type of polymer com-

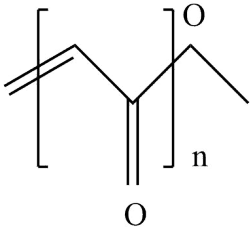


Figure 1. Poly(Acrylate)

posed of methacrylate monomers. They are utilised to create polymers and plastics for usage in things like electronics, medical or dental devices, surface coatings, acrylic sheets, and resins due to their ability to increase durability. Methacrylates strengthen polymers and plastics, making them suitable for use in dental prosthesis, bus shelters, and road marking paints, among many other places. Raw methacrylates are not likely to come into contact with the general public because of their low toxicity.

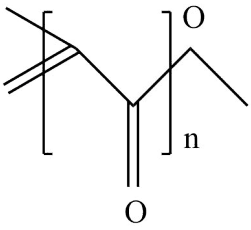


Figure 2. poly(Methacrylate)

The Wiener index is a measure that calculate the complexity of organic compound based on their molecular graph. The Wiener index of a molecule is the sum of all the shortest path between all pairs of atoms (Carbon and Oxygen) in the molecule. This index is having high impact on predicting the boiling point of various organic compounds [6].

Acrylate and Methacrylate polymers have relatively low boiling point due to their low molecular weight and weak intermolecular forces. M Firpo et.al., [7] demonstrated the possibility of resorting the new distance based topological indices as suitable molecular descriptors for a QSPR-like analysis. In order to anticipate the typical boiling points of organic compounds, Dai Yi-min et.al., [8] showed that the unique topological descriptors based on the equilibrium electro-negativity of atom and the relative bond length were helpful. Neha Kansal et.al., [9] found a strong relationship between the topological indices and the physico-chemical features of the COVID-19 medications before conducting experimental testing. A significant contribution to the knowledge concerning the Wiener index and other topological indices was accumulated in the survey papers. [10]-[18]

In this paper, we found the Wiener index of acrylate and methacrylate

polymer based on their molecular structure. Also we have used the Wiener index to predict the boiling point of acrylate and methacrylate polymers.

The framework of this paper is as follows: In section 2, the molecular graph of acrylate and methacrylate polymers are constructed in section 3 we represent some properties of Wiener index of some known graphs. The Wiener index of acrylate polymer (n-alkyl acrylates) and methacrylate polymer (n-alkyl methacrylates) are given in sections 4 and 5 respectively. Section 6 gives the prediction of boiling point of acrylate and methacrylate polymers. Finally, Section 7 concludes the paper.

2 Molecular structure of acrylate and methacrylate polymers

In this section we construct the molecular graph of acrylate and methacrylate polymers (Figure 3).

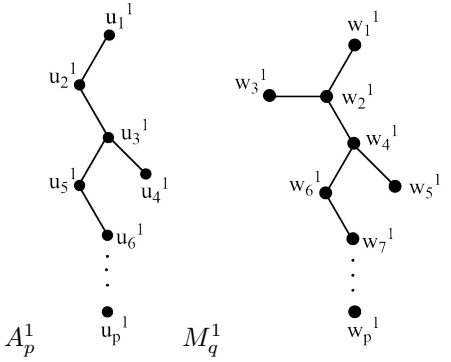


Figure 3. Acrylate and Methacrylate

2.1 Construction of Acrylate polymers

Let A_p^n denotes the n-alkyl acrylates for $n \geq 1$.
When $n = 1$, $A_p^n \cong A_p^1$, where A_p^1 is the alkyl acrylate monomer. Here, p is the number of vertices (atoms) of A_p^1, $p \geq 6$. Let $u_1^1, u_2^1, ..., u_p^1$ be the vertices of A_p^1. The graph of A_p^1 is shown in Figure-3.a.

When $n \geq 2$, consider n copies of A_p^n(monomers): $A_p^1, A_p^2, ..., A_p^n$. The vertices of A_p^i is denoted as $u_1^i, u_2^i, ..., u_p^i$, for $1 \leq i \leq n$. Then A_p^n is obtained by adding an edge between u_2^i of A_p^i and u_1^{i+1} of A_p^{i+1}, for each i, $1 \leq i \leq n-1$.

Observe that, A_p^n for $n \geq 2$, are constructed recursively, from A_p^{n-1} and A_p^1 by adding a new edge between u_1^1 of A_p^1 and the vertex u_2^{n-1} (u) of A_p^{n-1}. We also denote this by $A_p^n = A_p^{n-1} \circ A_p^1$. The general structure of A_p^n is shown in Figure 4.

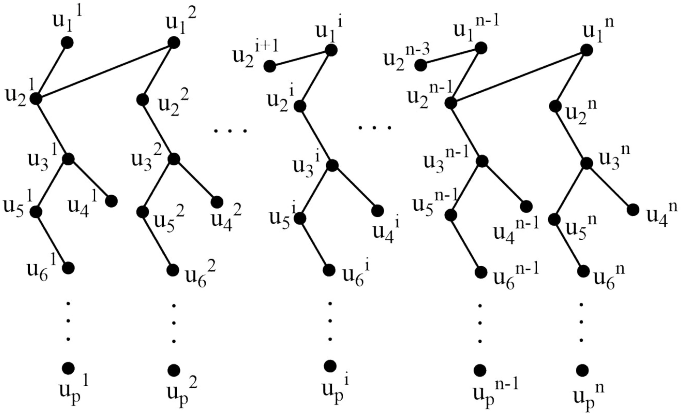


Figure 4. Poly Acrylate

2.2 Construction of Methacrylate polymers

Let M_q^n denotes the n-alkyl methacrylates for $n \geq 1$.

When $n = 1$, $M_q^n \cong M_q^1$ where M_q^1 is the alkyl methacrylate monomer. Here, q is the number of vertices (atoms) of M_q^1, $q \geq 7$. Let $w_1^1, w_2^1, ..., w_q^1$ be the vertices of M_q^1. The graph of M_q^1 is shown in Figure-3.*b*.

When $n \geq 2$, consider n copies of M_q^n(monomers): $M_q^1, M_q^2, ..., M_q^n$. The vertices of M_q^i is denoted as $w_1^i, w_2^i, ..., w_q^i$ for $1 \leq i \leq n$. Then M_q^n is obtained by adding an edge between w_2^i of M_q^i and w_1^{i+1} of M_q^{i+1}, for each i, $1 \leq i \leq n-1$.

Observe that, M_q^n for $n \geq 2$, are constructed recursively, from M_q^{n-1} and M_q^1 by adding a new edge between w_1^1 of M_q^1 and the vertex w_2^{n-1} (w) of

M_q^{n-1}. We also denote this by $M_q^n = M_q^{n-1} \circ M_q^1$. The general structure of M_q^n is shown in Figure 5.

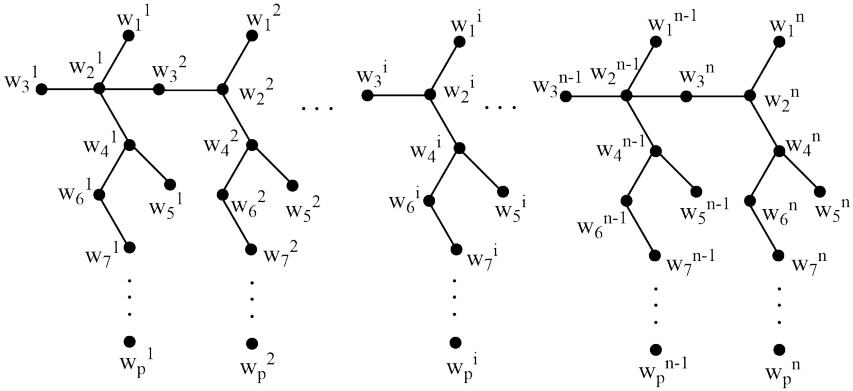


Figure 5. Poly Methacrylate

From the construction, the graph of A_p^n and M_q^n are trees. Also from the construction, the number of vertices of A_p^n is n_p and M_q^n is n_q.

3 Wiener index of graph

The Wiener index $W(G)$ of a graph G is the sum of all of the distances that exist between each pair of vertices of a connected graph G.

$$W(G) = \sum_{x,y \in V(G)} \delta_G(x, y) \tag{1}$$

where δ_G denotes the shortest distance from x and y in G. In mathematical chemistry, the Wiener index has been studied more than any other topological index due to its utility in determining average distance. The method was developed by Wiener in 1947 and bears his name since he was the first to use it to determine the boiling point of alkanes. The Wiener index has become one of the topological indices with the most widespread application in the field of chemistry because molecules are often modelled as undirected networks. This graph invariant has applications beyond just

graph theory, including crystallography, communication theory, and facility localization. It appears that in 1976 [19] the first piece of mathematical work on the Wiener index was published. Many distinguished mathematicians have devoted considerable time and energy to studying this number since then. Recently developed fields like sociometry and the idea of social networks make extensive use of this principle. [20]-[24]
It is hard to compute the Wiener index of any given tree in terms of the number of vertices or degree sequences. But there is some clever methods are obtained to compute the Wiener index of any given arbitrary tree.

Let Υ be any tree on n vertices and let u is any choosen vertex of Υ. If the vertex v is added to Υ by adding a new edge between u and v, then the Wiener index of $\Upsilon + v$ is calculated as, [25]

$$W(\Upsilon + v) = W(\Upsilon) + d_{\Upsilon}(u) + n \tag{2}$$

here $d_{\Upsilon}(u)$ is the sum of the distances of u from all other vertices of Υ. If $\delta_{\Upsilon}(u, w)$ is a shortest distance between u and w of Υ then,

$$d_{\Upsilon}(u) = \sum_{w \in \Upsilon - u} \delta_{\Upsilon}(u, w) \tag{3}$$

Let Υ_u and Υ_v be two trees with n_1 and n_2 vertices respectively. If Υ is constructed from Υ_u and Υ_v by adding an edge between the vertex u of Υ_u and a vertex v of Υ_v then the Wiener index of Υ is computed as in Theorem 1.

Theorem 1. *[19] Let Υ_u and Υ_v be two trees with n_1 and n_2 vertices and u and v be the vertices of Υ_u and Υ_v respectively. Υ arises from Υ_u and Υ_v by connecting the vertices u and v by an edge, then*

$$W(\Upsilon) = W(\Upsilon_u) + W(\Upsilon_v) + n_1 d_{\Upsilon_u}(v) + n_2 d_{\Upsilon_v}(u) + n_1 n_2 \tag{4}$$

Obtaining the Wiener index for an arbitrary tree is a difficult task, but for a number of special classes of trees (paths, stars, etc), the closed combinatorial expression for Wiener index can be found. The best known

them are:

Theorem 2. *[20] Let P_m be a path tree on m vertices, then*

$$W(P_m) = \binom{m+1}{3} \tag{5}$$

Theorem 3. *[26] Let S_m be a star tree on m vertices, then*

$$W(S_m) = (m-1)^2 \tag{6}$$

4 Wiener index of *n*-alkyl acrylates

In this section we consider the polymer structures of n-alkyl acrylates A_p^n and we found the Wiener index of A_p^n. In order to find the Wiener index of A_p^n we are using the following lemmas and observation. From the definition of $d_\Upsilon(u)$, the proof of Lemma 1 and Lemma 2 are trivial.

Lemma 1. *Let A_p^1 be 1-alkyl acrylate, then*

$$d_{A_p^1}(u_1^1) = \frac{p^2 - 3p + 8}{2} \tag{7}$$

Lemma 2. *Let A_p^1 be 1-alkyl acrylate, then*

$$d_{A_p^1}(u_2^1) = \frac{p^2 - 5p + 12}{2} \tag{8}$$

Lemma 3. *Let A_p^k be the k-alkyl acrylate $k \geq 1$, then*

$$d_{A_p^n}(u_2^k) = k\left(\frac{p^2 - 5p + 12}{2}\right) + pk(k-1) \tag{9}$$

Proof. Let A_p^k be the k-alkyl acrylate, $p \geq 6$, $k \geq 1$. By construction, the vertex u_2^k appears in the k^{th} copy of A_p^n. Therefore, the distance from the vertex u_2^k to any vertex v of A_p^k is calculated as follows,

$$d_{A_p^k}(u_2^k, v) = \begin{cases} \delta_{A_p^k}(u_2^k, v), \text{ if } v \in A_p^k \\ \delta_{A_p^i}(u_2^i, v) + 2p(k-i), \text{ if } v \in A_p^i \text{ for } 1 \leq i \leq k-1 \end{cases} \tag{10}$$

Hence,

$$d_{A_p^k}(u_2^k) = d_{A_p^k}(u_2^k) + \sum_{i=1}^{k-1} \left[d_{A_p^k}(u_2^i) + 2p(k-i) \right] \tag{11}$$

By Lemma 2,

$$d_{A_p^i}(u_2^i) = \frac{p^2 - 5p + 12}{2}, \text{for any } i, 1 \leq i \leq k \tag{12}$$

$$d_{A_p^k}(u_2^k) = \left(\frac{p^2 - 5p + 12}{2} \right) + \sum_{i=1}^{k-1} \left[\left(\frac{p^2 - 5p + 12}{2} \right) + 2p(k-i) \right] \tag{13}$$

Therefore, we get Eq. (9)

$$d_{A_p^n}(u_2^k) = k \left(\frac{p^2 - 5p + 12}{2} \right) + pk(k-1)$$ ■

Observation 1. Let A_p^1 be 1-alkyl acrylate tree, then

$$W(A_p^1) = \frac{p^3 - 13p + 48}{6} \tag{14}$$

Proof. Let A_p^1 be 1-alkyl acrylate with the vertices, $u_1^1, u_2^1, ..., u_p^1$. By the definition of Wiener index,

$$W(A_p^1) = \sum_{u,v \in V(A_p)} \delta_{A_p^1}(u, v) \tag{15}$$

Then by simple calculations, we have Eq. (14)

$$W(A_p^1) = \frac{p^3 - 13p + 48}{6} \qquad \blacksquare$$

Theorem 4. *Let A_p^n be the tree of n-alkyl acrylate, where n is the no.of monomers, $n \geq 1$, then*

$$W(A_p^n) = \frac{p^2}{3}n^3 + \left(\frac{p^3 - 5p^2 + 10p}{2}\right)n^2 - \left(\frac{2p^3 - 13p^2 + 43p - 48}{6}\right)n$$

Proof. Let A_p^n be the n-alkyl acrylate. By construction,

$$A_p^n = A_p^{n-1} \circ A_p^1 \tag{16}$$

That is, A_p^n is constructed from A_p^n by adding an edge between u_2^{n-1} of A_p^{n-1} and u_1^1 of A_p^1. Since, A_p^n is a tree, it satisfies the hypothesis of Theorem 1, then

$$\begin{aligned} W(A_p^n) =& W(A_p^{n-1}) + W(A_p^1) + d_{A_p^{n-1}}(u_2^{n-1})np + d_{A_p^1}(u_1)(n-1)q \\ &+ (np)(n-1)p \end{aligned} \tag{17}$$

By Lemma 1 , Lemma 3 and Eq. (14), we have

$$\begin{aligned} W(A_p^n) &= W(A_p^{n-1}) + \left(\frac{p^3 - 13p + 48}{6}\right) \\ &\quad + \left((n-1)\left(\frac{p^2 - 5p + 12}{2}\right) + p(n-1)(n-2)\right)p \\ &\quad + \left(\frac{p^2 - 3p + 48}{2}\right)(n-1)p + (n-1)p^2 \end{aligned} \tag{18}$$

$$\begin{aligned} W(A_p^n) - W(A_p^{n-1}) &= p^2n^2 + (p^3 - 6p^2 + 10p)n \\ &\quad - \left(\frac{5p^3 - 30p^2 + 73p - 48}{6}\right) \end{aligned} \tag{19}$$

The above Eq. (19) represent the first order linear recurrence relation on $W(A_p^n)$. By solving Eq. (19) with the help of initial condition

Eq. (14), we get the Wiener index of A_p^n as,

$$W(A_p^n) = \frac{p^2}{3}n^3 + \left(\frac{p^3 - 5p^2 + 10p}{2}\right)n^2 - \left(\frac{2p^3 - 13p^2 + 43p - 48}{6}\right)n \tag{20}$$

■

5 Wiener index of n-alkyl methacrylates

In this section we found the Wiener index of n-alkyl methacrylates M_q^n, $n \geq 1$. Before proving the main result we prove the following Lemmas and observations.

Lemma 4. *Let M_q^1 be 1-alkyl methacrylate, q is the no.of vertices, then*

$$d_{M_q^1}(w_3^1) = \frac{q^2 - 5q + 16}{2} \tag{21}$$

Lemma 5. *Let M_q^1 be 1-alkyl methacrylate, then*

$$d_{M_q^1}(w_2^1) = \frac{q^2 - 7q + 20}{2} \tag{22}$$

The proof of Lemma 4 and Lemma 5 are obvious.

Lemma 6. *Let M_q^k be the k-alkyl methacrylate $k \geq 1$, then*

$$d_{M_q^k}(w_2^k) = k\left(\frac{q^2 - 7q + 20}{2}\right) + qk(k-1) \tag{23}$$

Proof. Let M_q^k be the k-alkyl methacrylate, $q \geq 7$, $k \geq 1$. By construction, the vertex w_2^k appears in the k^{th} copy of M_q^n. Therefore, the distance from the vertex w_2^k to any vertex v of M_q^k is calculated as follows,

$$d_{M_q^k}(w_2^k, v) = \begin{cases} \delta_{M_q^k}(w_2^k, v) \text{ if } v \ \in M_q^k \\ \delta_{M_q^i}(w_2^i, v) + 2q(k-i), \text{ if } v \in M_q^i, \text{ for } 1 \leq i \leq k-1 \end{cases} \tag{24}$$

Hence,

$$d_{M_q^i}(w_2^k) = d_{M_q^k}(w_2^k) + \sum_{i=1}^{k-1}[d_{M_q^i}(w_2^i) + 2q(k-i)] \tag{25}$$

By Lemma 5,

$$d_{M_q^1}(w_2^k) = \frac{q^2-7q+20}{2}, \text{for each } i,\ 1 \le i \le k \tag{26}$$

$$d_{M_q^k}(w_2^k) = \left(\frac{q^2-7q+20}{2}\right) + \sum_{i=1}^{k-1}\left[\left(\frac{q^2-7q+20}{2}\right) + 2q(k-i)\right] \tag{27}$$

Therefore, we get Eq. (23)

$$d_{M_q^k}(w_2^k) = k\left(\frac{q^2-7q+20}{2}\right) + qk(k-1)$$ ■

Observation 2: Let M_q^1 be 1-alkyl methacrylate, then

$$W(M_q^1) = \frac{q^3-25q+108}{6} \tag{28}$$

Proof. Let M_q^1 be 1-alkyl methacrylate with vertices $w_1^1, w_2^1, ..., w_q^1$. By simple calculations, the Wiener index of M_q^1 is calculated as in Eq. (28),

$$W(M_q^1) = \frac{q^3-25q+108}{6}$$ ■

Theorem 5. *Let M_q^n be the tree of n-alkyl methacrylate polymer, where n is the no.of monomers $n \ge 1$, then*

$$W(M_q^n) = \frac{q^2}{3}n^3 + \left(\frac{q^3-7q^2+18q}{2}\right)n^2 - \left(\frac{2q^3-19q^2+79q-108}{6}\right)n$$

Proof. Let M_q^n be the n-alkyl methacrylate. By construction,

$$M_q^n = M_q^{n-1} \circ M_q^1 \tag{29}$$

That is, M_q^n is constructed from M_q^{n-1} by adding an edge between w_2^{n-1} of M_q^{n-1} and w_3^1 of M_q^1. This satisfies the hypothesis of Theorem 1,

$$W(M_q^n) = W(M_q^{n-1}) + W(M_q^1) + d_{M_q^{n-1}}(w_2^{n-1})nq + d_{M_q^1}(w_3^1)(n-1)q + (nq)(n-1)q \tag{30}$$

By Lemma 4, Lemma 6 and Eq. (5)

$$W(M_q^n) = W(M_q^{n-1}) + \left(\frac{q^3 - 25q^2 + 108}{6}\right) + \left((n-1)\left(\frac{q^2 - 7q + 20}{2}\right) + q(n-1)(n-2)\right)q + \left(\frac{q^2 - 5q + 16}{2}\right)(n-1)q + (n-1)q^2 \tag{31}$$

$$W(M_q^n) - W(M_q^{n-1}) = q^2n^2 + (q^3 - 8q^2 + 18q)n - \left(\frac{5q^3 + 42q^2 - 133q + 108}{6}\right) \tag{32}$$

The Eq. (32) represent the first order linear recurrence relation on $W(M_q^n)$. By solving Eq. (32) with the help of initial condition Eq. (28), we get the Wiener index of M_q^n as

$$W(M_q^n) = \frac{q^2}{3}n^3 + \left(\frac{q^3 - 7q^2 + 18q}{2}\right)n^2 - \left(\frac{2q^3 - 19q^2 + 79q - 108}{6}\right)n \tag{33}$$

■

6 Prediction of boiling point of acrylate and methacrylate polymers

In this section, we predicted the boiling point of acrylate and methacrylate polymers using Wiener index. Let B denote the boiling point and W denotes the Wiener index of a polymer then by QSPR analysis [27] the

relation between B and W is given by,

$$B = \alpha W^{\beta} \tag{34}$$

We use the training set of B and W for the single monomer of acrylate and methacrylate polymer which is obtained from Chemspider.

For alkyl acrylates: The Table 1 gives the Wiener index (which is obtained using Theorem 4) and the experimental boiling point of 1-alkyl acrylate. Using this Table 1 as a training data, we fit the relation between B_A and W_A as, [27]

$$B_A = 198.19\left(W_A^{0.1612}\right) \tag{35}$$

Table 1. Wiener index and experimental boiling point of Acrylate polymers

S.No	Acrylate	WI (W_A)	Experimental BP (B_A) (in K)
1	Methyl	31	344.73
2	Ethyl	50	372.35
3	Propyl	76	398.35
4	Butyl	110	422.81
5	Pentyl	153	445.91
6	Hexyl	206	467.81
7	Heptyl	270	488.67
8	Octyl	346	508.6
9	Nonyl	435	527.72

Similarly, for alkyl methacrylates: The Table 2 gives the Wiener index (which is obtained using Theorem 5) and the experimental boiling point of 1-alkyl methacrylate. Using this Table 2 as a training data, we fit the relation between B_M and W_M as,

$$B_M = 199.11\left(W_M^{0.1599}\right) \tag{36}$$

Table 2. Wiener index and experimental boiling point of Methacrylate polymers

S.No	Methacrylate	WI (W_M)	Experimental BP (B_M) (in K)
1	Methyl	46	367.25
2	Ethyl	70	392.75
3	Propyl	102	417.12
4	Butyl	143	440.28
5	Pentyl	194	462.28
6	Hexyl	256	483.24
7	Heptyl	330	503.27
8	Octyl	417	522.45
9	Nonyl	518	540.89

Using Eq. (35) and Eq. (36), we predicted the boiling point of acrylate and methacrylate polymers using Wiener index. Table 3 and Table 4 gives the predicted boiling point as well as the experimental boiling point of acrylate and methacrylate polymers. From these tables we observe that there is good correlation between our predicted boiling point and and experimental boiling point, this can be easily seen in Figure 6.
The experimental boiling point and the predicted boiling point of acrylate and methacrylate polymers are tabulated in Table 3 and Table 4 respectively and the comparison is given in Figure 7. In general for a general molecular structure of acrylate and methacrylate polymers for the various values of n, p and q using Eq. (20) and Eq. (33) the predicted boiling points are given in Table 5 and Table 6 respectively.

From these two tables we observe that the boiling point of methacrylate polymer is always higher than the boiling point of acrylate polymer.

6.1 Prediction error

The methodology assumes that error measures summarize the error characteristics into a single value. When errors are independent or uncorrelated, it's reasonable to believe that their statistical distribution captures all rel-

evant properties. Let the set of experimental values be γ_i, $\forall\ i = 1, 2, ...n$ and $\hat{\gamma_i}\ \forall\ i = 1, 2, ...n$ be the set of predicted values of the acrylate and methacrylate polymers, then $e_i = \gamma_i - \hat{\gamma_i}$, for $i = 1, 2, ...n$ is the set of errors. Here, the e_i value can be either positive or negative. For the series of given errors, the Root Mean Square Error (RMSE) is defined as, [28]

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(\hat{\gamma_i} - \gamma_i)^2}{n}}$$

For the Acrylate polymers, taking the predicted and experimental values from Table-3 and finding e_i values for each alkyl acrylate, we have the root mean square error RMSE_A as,

$$RMSE_A = 6.93 \tag{37}$$

For Methacrylate polymers, using the predicted and experimental values from Table-4, finding the values of e_i, we have the RMSE_M value as,

$$RMSE_M = 3.5 \tag{38}$$

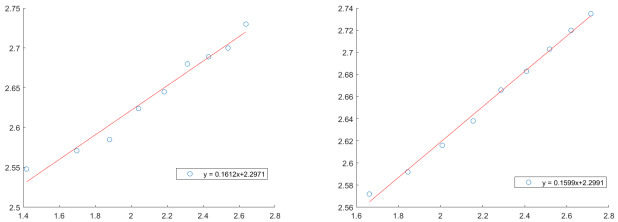
From Eq. (37) and Eq. (38) we observe that the prediction error is minimum. Hence, we can use this methodology to find the boiling point of the acrylate and methacrylate polymers accurately.

Table 3. Prediction of boiling point of Acrylate polymers

S.No	Acrylate	Predicted BP (in K)	Experimental BP (in K)
1	Methyl	353.2	344.73
2	Ethyl	373.2	372.35
3	Propyl	385.3	398.35
4	Butyl	421.2	422.81
5	Pentyl	442.5	445.91
6	Hexyl	479.17	467.81
7	Heptyl	489.05	488.67
8	Octyl	502.15	508.6
9	Nonyl	525.45	527.72

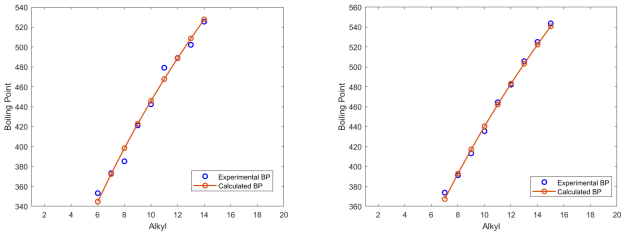
Table 4. Prediction of boiling point of Methacrylate polymers

S.No	Methacrylate	Predicted BP (in K)	Experimental BP (in K)
1	Methyl	373.7	367.25
2	Ethyl	391.2	392.75
3	Propyl	413.15	417.12
4	Butyl	435.45	440.28
5	Pentyl	464.45	462.28
6	Hexyl	482.15	483.24
7	Heptyl	505.75	503.27
8	Octyl	525.15	522.45
9	Nonyl	543.75	540.89



(a) BP of Acrylates (b) BP of Methacrylates

Figure 6. BP of Acrylates and Methacrylates



(a) Comparison of BP of Acrylates

(b) Comparison of BP of Methacrylates

Figure 7. Comparison BP of Acrylates and Methacrylates

7 Conclusion

In this investigation, the recurrence relation was used to calculate the Wiener index of the acrylate and methacrylate polymers and obtained a formula to find the boiling point of the above mentioned polymers. This opens up the possibilities for chemists to make predictions about the properties of various molecular compounds without having to conduct time-consuming and expensive experiments. For the benefit of both theoretical chemists and practicing scientists and engineers, this paper presents both a graphical representation and a numerical comparison of the computed results.

Table 5. Predicted boiling point of acrylate polymers

p	Acrylate \ n	1	2	3	4	5	6	7	8	9	10
6	Methyl $(C_4H_6O_2)_n$	344.7	476.2	565.6	633.2	688.6	860.2	917.1	969.9	1019.3	1066.1
7	Ethyl $(C_5H_8O_2)_n$	372.3	513.2	607.8	684.6	751.2	810.9	865.5	916.2	963.8	1051.6
8	Propyl $(C_6H_{10}O_2)_n$	398.3	548.3	648.0	728.5	798.0	860.2	917.1	969.9	1019.3	1066.1
9	Butyl $(C_7H_{12}O_2)_n$	422.8	464.9	686.2	765.8	831.1	887.2	936.7	981.3	1022.0	1059.6
10	Pentyl $(C_8H_{14}O_2)_n$	445.9	613.3	722.6	810.1	885.2	952.1	1013.1	1069.6	1122.5	1172.4
11	Hexyl $(C_9H_{16}O_2)_n$	467.8	643.5	757.4	848.2	925.9	995.0	1058.0	1116.2	1170.7	1222.1
12	Heptyl $(C_{10}H_{18}O_2)_n$	488.6	672.4	779.7	884.7	965.0	1036.3	1101.1	1162.0	1217.0	1269.8
13	Octyl $(C_{11}H_{20}O_2)_n$	508.6	700.1	822.7	919.8	1002.6	1076.0	1142.7	1204.2	1261.7	1315.8
14	Nonyl $(C_{12}H_{22}O_2)_n$	527.7	726.7	853.4	953.6	1038.8	1114.3	1182.7	1245.9	1304.8	1360.2

Table 6. Predicted boiling point of methacrylate polymers

q	Methacrylate \ n	1	2	3	4	5	6	7	8	9	10
7	Methyl $(C_5H_8O_2)_n$	367.2	499.7	591.6	666.9	732.4	791.3	845.3	895.5	942.6	987.1
8	Ethyl $(C_6H_{10}O_2)_n$	392.7	533.6	630.1	708.7	776.9	838.2	894.3	946.4	995.3	1041.4
9	Propyl $(C_7H_{12}O_2)_n$	417.1	566.2	667.2	749.1	820.0	883.4	941.5	995.4	1045.9	1093.6
10	Butyl $(C_8H_{14}O_2)_n$	440.2	597.5	703.1	788.0	861.4	927.0	987.0	1042.5	1094.6	1143.7
11	Pentyl $(C_9H_{16}O_2)_n$	462.2	627.5	737.3	825.5	901.3	969.0	1030.8	1088.0	1141.5	1192.0
12	Hexyl $(C_{10}H_{18}O_2)_n$	483.2	656.2	770.3	861.5	939.8	1009.5	1073.0	1131.8	1186.8	1238.6
13	Heptyl $(C_{11}H_{20}O_2)_n$	503.2	683.8	802.0	896.2	976.9	1048.5	1113.8	1174.1	1230.4	1283.6
14	Octyl $(C_{12}H_{22}O_2)_n$	522.4	710.4	832.6	929.7	1012.7	1098.7	1153.2	1215.0	1272.7	1327.0
15	Nonyl $(C_{13}H_{24}O_2)_n$	540.8	736.0	862.1	962.1	1047.3	1122.8	1191.4	1254.6	1313.5	1369.1

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