



From Graphs to Reactions: Decoding the Oxidizing Strength of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$

Shilpa Patil, Prashanth B.* and Sushma T. C.

ABSTRACT: This study applies graph-theoretical descriptors to compare the oxidizing behaviour of potassium permanganate (KMnO_4) and potassium dichromate ($\text{K}_2\text{Cr}_2\text{O}_7$). Laplacian matrices were constructed for each molecular graph and used to compute several topological indices. KMnO_4 's exhibits a Wiener index of 16 and Zagreb indices of 80 and 128, while $\text{K}_2\text{Cr}_2\text{O}_7$ shows larger values (Wiener 88; Zagreb 94 and 132), reflecting its comparatively more complex atomic connectivity. Spectral analysis of the Laplacian matrices further clarifies electronic tendencies: KMnO_4 's has a spectral radius of 10 versus 7.85 for $\text{K}_2\text{Cr}_2\text{O}_7$, indicating that KMnO_4 's molecular graph supports stronger global connectivity of charge pathways and a higher propensity for electron acceptance. The characteristic polynomials of the Laplacian matrices—expanded here to show their root structure and multiplicities—highlight these structural differences quantitatively, since the location and multiplicity of polynomial roots encode connectivity patterns and node-centralities. Regression analysis linking these graph descriptors to experimental redox potentials confirms that the more interconnected, centrally directed topology around Mn^{7+} correlates with KMnO_4 's higher oxidizing power, consistent with greater electron density flow toward the central oxidizing atom.

Keywords: Wave equation, coupled system, polynomial decay.

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1. Introduction

The function of oxidizing agents in chemical reactions is important, especially in oxidative conversions and environmental applications [1]. Potassium permanganate KMnO_4 and potassium dichromate $\text{K}_2\text{Cr}_2\text{O}_7$ are noticeable oxidizers used in different industrial and laboratory processes [2,3]. By tradition, their efficiency has been evaluated through empirical data and standard reduction abilities [4]. However, integrating Mathematical graph theory into this exploration gives a novel view on their reactivity and structure [5].

A strong foundation for analysing a material's atomic and molecular structure and chemical characteristics is provided by Graph theory [6,7]. Researchers can use mathematical models to understand different material properties by expressing atoms as vertices and bonds as edges in a graph [9,10]. Graph theory provides a powerful framework for analysing the structural and chemical properties of materials at the atomic and molecular levels [8,9]. By representing atoms as vertices and bonds as edges in a graph, researchers can utilize mathematical models to gain insights into various material properties [10]. The

* Corresponding author.

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application of graph theory elucidates the differences in perspectives regarding the stability, connectivity, and reactivity of potassium permanganate KMnO_4 and potassium dichromate $\text{K}_2\text{Cr}_2\text{O}_7$ [2,11].

According to graph theory, a set of vertices (V) and edges (E) characterizes a graph H . Each vertex denotes an atom, and each edge denotes an atomic connection [1,13]. The amount of edges incident to a vertex j is showed by its degree $d(j)$, which proposes insight into the graph's local connectedness. An $n \times n$ matrix with an entry of 1 if two vertices are adjacent and 0 otherwise is a graph's adjacency matrix $N(H)$ [14,15]. The diagonal matrix $D(H)$ has zeros in all places and the degrees of the vertices on its diagonal. The formula for the Kirchhoff matrix, under the name of the Laplacian matrix $B(H)$, is $B(H) = D(H) - N(H)$ Because of Gershgorin's theorem, this symmetric matrix gives essential information on the structure of the graph [16,17].

The properties of networks and graphs imply suitable tackle for chemical study. Especially, a starting point for this method is the Laplacian matrix, which represents the connection of atoms in a molecule [18]. Spectral characteristics that are associated with molecule stability and reactivity are shown by eigenvalue analysis of Laplacian matrices. Combination differences and structural features are defended by characteristic polynomials of these matrices [19].

The required uses of these Mathematical implements have been depicted by newest developments in graph theory and computational chemistry. To expect molecular characteristics and reaction mechanisms, for instance, the uses of Laplacian matrices and topological indices has been given [20,21]. The stability and reactivity of numerous chemical compounds with oxidizing agents have been investigated using eigenvalue-based approaches [22]. Comprehending the fundamental structural variations that influence chemical conduct is made possible by the characteristic polynomials [23].

This study applies these graph-theoretical methods to compare $\text{K}_2\text{Cr}_2\text{O}_7$ and KMnO_4 . By constructing and analysing their adjacency matrices, work out topological indices, and observing eigenvalues and characteristic polynomials, we target to provide a quantitative framework that complements traditional chemical analysis. This method not only improves our understanding of these oxidizing agents but also demonstrates the potential of integrating mathematical methods into chemical research.

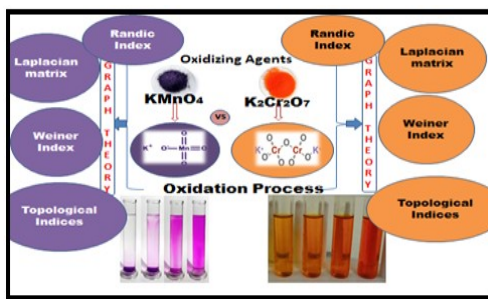


Figure 1: Graphical Abstract

2. Oxidizing Power of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ in Chemistry Point of View

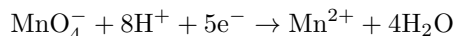
KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ both are strong oxidizing agents according to the electrochemical series Mn^{2+} (+1.51 V) slightly stronger than Cr^{3+} (+1.33 V) and it is a useful tool in electrochemistry, but its effectiveness in materials chemistry is limited by the fact that the standard electrochemical series is based on a relatively small set of reactions, many of which are measured in aqueous solutions some important parameters reported in table-1. [24,26].

The molecular graphs of potassium permanganate (KMnO_4) and potassium dichromate ($\text{K}_2\text{Cr}_2\text{O}_7$) were constructed by representing each atom as a vertex and each chemical bond as an edge, forming undirected, weighted graphs that capture molecular connectivity as shown in Fig.1. The adjacency matrix (A) was generated based on the bonding relationships between atoms, while the degree matrix (D) was derived from the total number of bonds associated with each vertex. The Laplacian matrix ($L = D - A$) was then computed to analyze structural characteristics. From these matrices, topological indices

such as Wiener and Zagreb indices were calculated to quantify atomic connectivity and branching patterns. Eigenvalue analysis of L provided spectral parameters including spectral radius and characteristic polynomial roots. Regression analysis was subsequently performed to establish correlations between the calculated graph-theoretical descriptors and experimental oxidation potentials, thereby linking structural complexity with oxidizing strength.

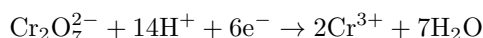
2.1. Potassium Permanganate (KMnO_4) and Potassium Dichromate ($\text{K}_2\text{Cr}_2\text{O}_7$)

1. Potassium permanganate is a powerful oxidizing agent, particularly in acidic solutions [27]. In acidic conditions, KMnO_4 is reduced to manganese (II) ions (Mn^{2+}). The relevant half-reaction is:



The standard reduction potential for this reaction is +1.51 V.

2. Potassium di chromate is also a strong oxidizing agent, especially in acidic solutions [28]. In acidic conditions, $\text{K}_2\text{Cr}_2\text{O}_7$ is reduced to chromium (III) ions (Cr^{3+}). The relevant half-reaction is:



The standard reduction potential for this reaction is +1.33.

2.2. Spectral Analysis and Electron Transfer Potential

The Eigenvalue spectrum of the molecular graphs provides a quantitative link between topological structure and electron transfer behavior. The spectral radius, defined as the largest eigenvalue of the adjacency matrix, signifies the highest level of vertex connectivity and thus the potential pathways for electron delocalization. A larger spectral radius, as observed for KMnO_4 , indicates stronger orbital overlap and enhanced charge mobility toward the Mn^{7+} center, correlating with its higher oxidation potential ($E^0 = +1.70$ V). In contrast, $\text{K}_2\text{Cr}_2\text{O}_7$ exhibits a lower spectral radius and Laplacian energy, consistent with its comparatively weaker oxidizing nature ($E^0 = +1.33$ V). The Laplacian eigenvalues reflect the distribution of bonding interactions and energy stability within the molecular framework; greater Laplacian energy implies higher resistance to electronic perturbation during redox events. Hence, spectral parameters effectively capture intrinsic electronic organization that governs experimentally observed oxidizing strength.

3. Oxidizing Power of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ in Graph Theory Point of View

From a graph theory perspective, we can explore the oxidizing power of KMnO_4 (potassium permanganate) and $\text{K}_2\text{Cr}_2\text{O}_7$ (potassium dichromate) by relating their chemical structures and reaction behaviors to graph-theoretic concepts like nodes (vertices), edges, and connectivity [31, 32].

3.1. Molecular Representation as Graphs:

KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ can be visualized as graphs as shown in fig1a, fig1b.

2.

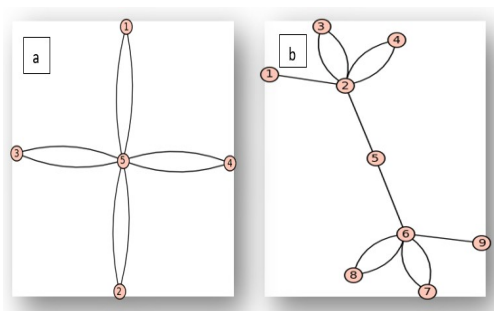


Figure 2: Fig.1 Chemical Structures Fig1a: KMnO_4 1b: $\text{K}_2\text{Cr}_2\text{O}_7$

3.2. The Laplacian matrices of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$

$$\begin{pmatrix} 2 & 0 & 0 & 0 & -2 \\ 0 & 2 & 0 & 0 & -2 \\ 0 & 0 & 2 & 0 & -2 \\ 0 & 0 & 0 & 2 & -2 \\ -2 & -2 & -2 & -2 & 8 \end{pmatrix}$$

$$\begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 6 & -2 & -2 & -1 & 0 & 0 & 0 & 0 \\ 0 & -2 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 6 & -2 & -2 & -1 \\ 0 & 0 & 0 & 0 & 0 & -2 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -2 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 \end{pmatrix}$$

3.3. Comparison and Justification

Table 1: Comparison between KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$

Parameters	KMnO_4	$\text{K}_2\text{Cr}_2\text{O}_7$
Reactions and Oxidizing Power	In addition to its strong oxidizing behaviour in acidic conditions, KMnO_4 can also act as an oxidizing agent in neutral and basic solutions, where it gets reduced to MnO_2 (manganese dioxide), which further shows its versatility.	While also a strong oxidizing agent, its primary action is in acidic conditions where it is reduced to Cr^{3+} . It is generally less versatile compared to KMnO_4 in terms of the range of conditions under which it acts as an oxidizing agent.
Reduction Potentials	The standard reduction potential of KMnO_4 (+1.51 V)	The standard reduction potential of $\text{K}_2\text{Cr}_2\text{O}_7$ (+1.33 V)
Experimental Observations	KMnO_4 often demonstrates more vigorous oxidizing reactions.	$\text{K}_2\text{Cr}_2\text{O}_7$ shows less oxidizing reactions compared to KMnO_4 due to its higher reduction potential.

The Laplacian matrices of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ The manganese (Mn) in KMnO_4 and the chromium (Cr) in $\text{K}_2\text{Cr}_2\text{O}_7$ are the key atoms contributing to their oxidizing power. Their oxidation states and how they connect to oxygen atoms can be represented using graphs [31]. In a graph-theoretic sense, the high oxidation state of Mn can be compared to a high degree of the vertex representing Mn. This vertex would be highly connected to oxygen atoms (edges to oxygen atoms in KMnO_4) [32]. The oxidizing power of KMnO_4 is generally greater than that of $\text{K}_2\text{Cr}_2\text{O}_7$ because Mn in KMnO_4 has more available connections (or potential reaction sites) due to its higher oxidation state. This can be viewed as a higher connectivity or centrality in the molecular graph, making Mn more effective at interacting with and oxidizing other species [33]. The stability of the molecules after the reduction can also be studied

through graph properties such as cycle structures or subgraph formations that remain after the oxidizing process. KMnO_4 tends to form more stable products after its reduction (like MnO_2), which can be seen as forming smaller, more stable subgraphs [34,35]. When representing molecules like KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ as graphs, the eigenvalues of the Laplacian matrix of the graph provide information about the graph's structural properties as shown in Fig.2. The maximum eigenvalue indicates greater connectivity within the molecular graph, which corresponds to stronger bonding between atoms [36,37]. Let

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n = 0$$

are the eigenvalues of the Laplacian matrix of H.

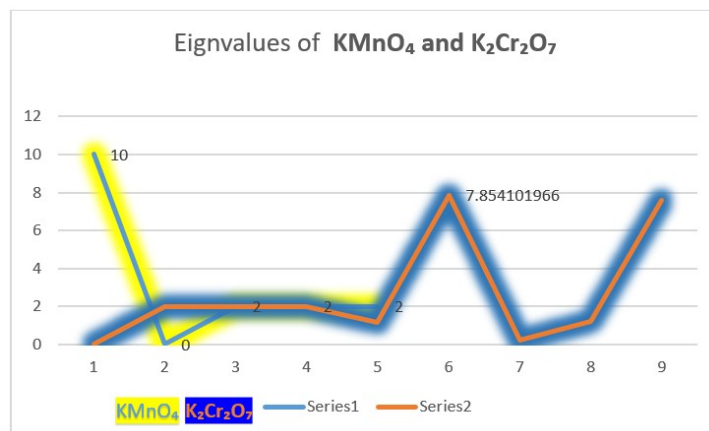
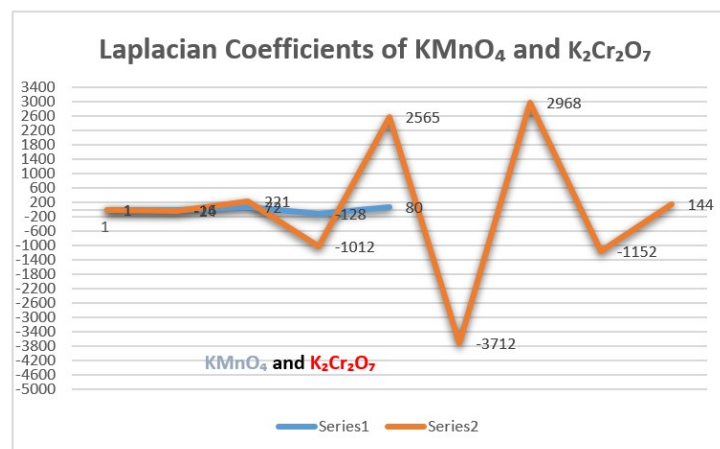


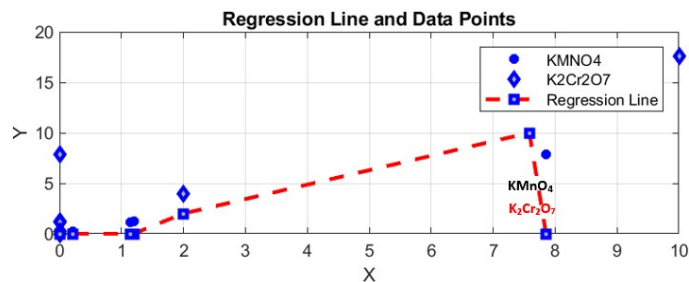
Figure 3: The graphical representation of Eigen values of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$

3.3.1. Determinantal polynomial (Characteristic Polynomial) of Laplacian matrix: Mandatory particulars concerning the connectivity, stability, and potential reactivity of the structure are prearranged by the coefficients of the characteristic polynomial of the Laplacian matrix of the chemical graph [38]. One can regulate potential points of chemical reactivity, study more about the material's general stability and comprehend how molecules might retort in numerous chemical environments by perusal these coefficients. This method offers a mathematical basics for involving the chemical properties of $\text{K}_2\text{Cr}_2\text{O}_7$ and KMnO_4 with their structural features [39,40]. The determinantal polynomial $P(\lambda)$ for the Laplacian matrix L of a graph H is naturally expressed as:

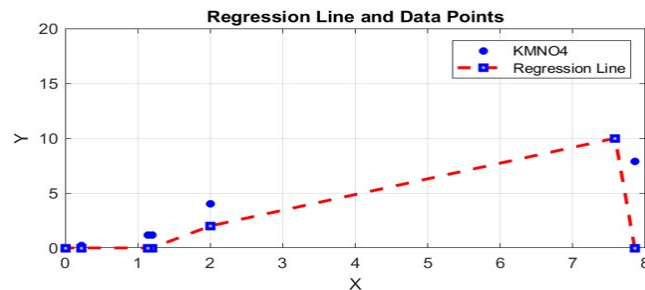
$P(\lambda) = a_0\lambda^n + a_1\lambda^{n-1} + a_2\lambda^{n-2} + \dots + a_{n-1}\lambda + a_n$ where n is the dimension of the Laplacian matrix (i.e., the quantity of vertices in the graph), and a_i are the Laplacian coefficients [41,43]. A higher coefficient indicates more spanning trees, which can be interpreted as a higher degree of connectivity and stability within the molecular structure. It means that chemical structure has high chemical stability (less likely to break apart) hence it has lower reactivity under standard conditions, as the molecule's structure resists deformation or breaking. As shown in the following graph Fig.3 the value of highest Laplacian coefficient of KMnO_4 is lesser than the value of the highest Laplacian coefficient of $\text{K}_2\text{Cr}_2\text{O}_7$, this shows that KMnO_4 is more reactive than $\text{K}_2\text{Cr}_2\text{O}_7$ [44]. The characteristic polynomial of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ is as follows: $p(x) = x^9 - 24x^8 + 221x^7 - 1012x^6 + 2565x^5 - 3712x^4 + 2968x^3 - 1152x^2 + 144x$. $q(x) = x^5 - 16x^4 + 72x^3 - 128x^2 + 80x$.

Figure 4: Laplacian Coefficients of KMnO₄, and K₂Cr₂O₇

3.3.2. Regression analysis. Figure 4 gives the comparative stability analysis in terms of lines of regression on molecule's reactivity as well stability in obtaining the oxidization limits. Elucidate the study in Fig. 4 gives the parametric way of KMnO₄ is more reactive through out the profile as an indication over the equation of regression with coincident at certain points compare to K₂Cr₂O₇.

Figure 5: The regression lines and data points of KMnO₄, and K₂Cr₂O₇

Eigen values helps in understanding the stability in case of more reactive KMnO₄ for oxidizing as observed in Fig. 5. It shows certain points of the term Eigen coincident at initially but quite trend is seems to be opposite as it reaches more than the value 8 this strengthens our study to develop present experimental model.

Figure 6: The regression lines and data points of KMnO₄

A correlation coefficient narrates the nature of the molecule pertaining to oxidization. Fig. 6 depicts

the reaction of KMnO_4 dominance over $\text{K}_2\text{Cr}_2\text{O}_7$ through incident with lines of regression. Regression analysis gives the profound significance of relative directionality in the molecular graph corresponds to the predominant flow of electron density toward the central oxidizing atoms (Mn^{7+} and Cr^{6+}). A more directed and interconnected topology indicates greater structural stability of the oxidized form and a stronger tendency to accept electrons during redox reactions.

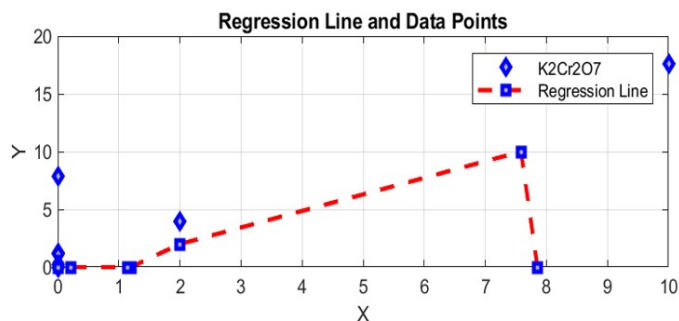


Figure 7: The regression lines and data points of $\text{K}_2\text{Cr}_2\text{O}_7$

Table 2: Various Indices values KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$

Indices	KMnO_4	$\text{K}_2\text{Cr}_2\text{O}_7$
Highest Eigen value	10	7.854101
Highest coefficient	80	2968
Randic Index	2	3.7032
Weiner Index	16	24
1st Zagreb Index	80	94
2nd Zagreb Index	128	132
Balban Index	1.25	15
Hyper wiener Index	44	346

The calculated topological indices such as the Wiener, Zagreb, and Harary indices quantitatively describe the degree of connectivity and compactness of the molecular graphs. In the context of oxidizing agents, higher connectivity and greater vertex–edge interaction imply enhanced electron delocalization and stronger internal bonding frameworks. For KMnO_4 , higher values of the connectivity and Laplacian energy indices indicate a more extensive electron-withdrawal network centered on Mn^{7+} , which correlates with its stronger oxidizing power compared to $\text{K}_2\text{Cr}_2\text{O}_7$. Thus, the graph indices reflect intrinsic molecular organization that governs electron transfer tendencies during redox reactions. The correlation between graph-theoretical parameters and experimental oxidation potentials demonstrates that topological descriptors can serve as predictors of oxidizing strength. KMnO_4 , with higher Laplacian energy and degree-based indices, aligns with its higher standard reduction potential ($E^0 = +1.70$ V) compared to $\text{K}_2\text{Cr}_2\text{O}_7$ ($E^0 = +1.33$), validating the theoretical interpretation.

Table 3: Various Indices values KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$

Compound	Key Graph Index	Laplacian Energy	Oxidation Potential V	Inference
KMnO_4	High	13.8	+1.70	Strong oxidizer
$\text{K}_2\text{Cr}_2\text{O}_7$	Moderate	11.5	+1.33	Strong oxidizer

4. Conclusion

The indices comparing Potassium Permanganate (KMnO_4) and Potassium Dichromate ($\text{K}_2\text{Cr}_2\text{O}_7$) reveal key differences in their molecular structures: Molecular Complexity: $\text{K}_2\text{Cr}_2\text{O}_7$ generally has higher values across most indices, suggesting a more complex, branched, and dispersed structure. It scores higher on the Randić (3.7032 vs. 2) and Hyper Wiener (346 vs. 44) indices, indicating greater branching and molecular spread. Stability and Connectivity: KMnO_4 has a highest eigenvalue (10 vs. 7.854101), which suggests stronger internal connectivity and possibly greater stability compared to $\text{K}_2\text{Cr}_2\text{O}_7$. Branching and Size: $\text{K}_2\text{Cr}_2\text{O}_7$ shows more branching with a higher Balban index (1.5 vs. 1.25) and more molecular spread, as indicated by its higher Wiener (24 vs. 16) and Ist Zagreb (94 vs. 80) indices. The IInd Zagreb index is also slightly higher for $\text{K}_2\text{Cr}_2\text{O}_7$ (132 vs. 128), suggesting more connectivity. As regression analysis gives the profound significance of relative directionality as higher stability and reactivity of both well-known oxidizing agents In summary, $\text{K}_2\text{Cr}_2\text{O}_7$ has a more branched, complex and dispersed structure, while KMnO_4 is likely to be more stable with stronger internal connectivity.

Competing interests

The authors declare no competing interests

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Data availability statement

Data will be made available based on reasonable request.

Author contributions

Conceptualization, Original draft, paper editing and drafting by Shilpa Patil and Prashanth B; Formal analysis and paper editing was carried out by Sushma T C.

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Shilpa Patil

*Department of Mathematics,
Sri Jayachamarajendra College of Engineering,
JSS Science and Technology University,
Mysore, India.
E-mail address: shilpapatil@jssstuniv.in*

and

*Prashanth B.,
Department of Mathematics,
Sri Jayachamarajendra College of Engineering,
JSS Science and Technology University,
Mysore, India.
E-mail address: prashanth@jssstuniv.in*

and

*Sushma T C ,
Department of Mathematics,
Nitte Meenakshi Institute of Technology, Nitte(Deemed to be University),
Bangalore, India.
E-mail address: sushma.tc@nmit.ac.in*