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Similarity Transfer Mechanisms of Transition Metals Revealed by Chemical Network Topology

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Abstract

In this work, we investigate similarity transfer in transition metal networks from a graph-theoretical perspective. Using binary compound data, we construct large-scale chemical element networks comprising more than 2000 edges. Within this framework, we define similarity transfer ratio (ST) as a new graph-theoretical descriptor that quantifies how similarity between elements can be propagated through mediating neighbors. Three fundamental transfer mechanisms—horizontal, vertical, and diagonal—are formally characterized, and their mathematical properties, including symmetry and topological inequalities, are rigorously proven.

Analysis of 29 transition metals shows that more than 79% of ST values exceed 90%, demonstrating the robustness of similarity transfer as a structural feature of chemical networks. Beyond its chemical interpretation, the ST framework complements classical graph-theoretical indices such as Wiener and Randić descriptors by capturing the *transferability* of similarity rather than measuring only

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static adjacency or distance. This study bridges network topology and chemical graph theory, establishing a transferable and quantifiable descriptor that offers new insights into periodic trends. In addition, the framework suggests potential for guiding compound prediction, although its primary contribution lies in extending the mathematical foundations of chemical similarity.

1 Introduction

Similarity among chemical elements is a fundamental concept in chemistry. The Periodic Table, as the systematic classification of chemical elements into groups with similar properties [1,2], serves as a cornerstone for understanding elemental relationships. Typically, it is believed that adjacent elements exhibit similarities in their properties; for instance, elements within the same group of the PT share comparable characteristics. Over the past several decades, researchers have focused on identifying similarities among elements by analyzing their chemical, physical, and physicochemical properties [3–5]. This approach has laid a foundation for exploring elemental relationships and understanding their behavior in various chemical systems.

At the beginning of this century, with the advancement of network theory, researchers began constructing networks based on compounds and investigating similarities using relational properties of chemical elements [6]. The topological properties of chemical networks have emerged as a powerful tool for analyzing elemental relationships [7–12]. Building on our previous work, where we established large-scale chemical element networks with more than 2000 edges [8], this research further explores similarity transfer among transition metals. The network-topological perspective enables quantitative characterization of similarity propagation paths, the identification of bridge elements that facilitate inter-group transfer, and the derivation of topological constraints governing compound formation.

While most classical studies emphasize similarity as a static reflection of shared physicochemical properties, the present work focuses on how similarity propagates across the network. The concept of similarity transfer therefore represents a dynamic process rather than a redundant restatement of similarity itself. In chemical terms, this transfer indicates the preservation and transmission of comparable bonding environments through mediating elements. Conversely, dissimilarity plays an equally important role: it often underlies chemical reactivity and bond formation, since dissimilar elements tend to complement one another in valence or electronic configuration. Hence, analyzing both similarity and dissimilarity provides a more complete view of how chemical relationships emerge and evolve within the periodic system.

Chemical graph theory has long provided powerful tools for characterizing chemical structures through graph-theoretical descriptors such as the Wiener index [13], the Randić index [14], and Zagreb indices [15]. These classical measures capture distances, degrees, and connectivity, and have been successfully applied to correlate molecular graphs with chemical and physical properties. However, these indices are essentially static; they do not capture how similarity can be transferred across a network through mediating neighbors.

It is worth noting that in mathematical terms, a *network* is equivalent to a graph; the term "network" is commonly used when dealing with large-scale systems, while "graph" is typically adopted in chemical graph theory. In this paper, we use both terms interchangeably, with "network" referring to the scale of the data and "graph" emphasizing the theoretical framework. In this study, we extend chemical graph theory by introducing the *similarity transfer ratio* (ST) as a new graph-theoretical descriptor embedded in transition metal networks. ST formalizes how similarity between two vertices can be propagated via intermediate nodes, thereby providing a propagation-based perspective that complements existing indices. We characterize three fundamental transfer mechanisms—horizontal, vertical, and diagonal—prove their mathematical properties, and validate them with large-scale element network data. In doing so, we aim to bridge the perspectives of network topology and chemical graph theory, enriching the ethodological foundations of mathematical chemistry.

2 Graph-theoretical framework for similarity transfer

2.1 Chemical element network

We represent chemical elements and their binary compounds as a chemical element network. Each vertex corresponds to a chemical element, and an edge is established between two vertices if the corresponding elements co-occur in at least one binary compound. The stoichiometries of elements are disregarded. Following our previous work, the dataset comprises 97 elements and results in a large-scale network containing 2198 edges [8], reflecting the extensive connectivity among elements in the compound space.

From a mathematical perspective, this network is equivalent to a simple undirected graph $G = (V, E)$, where V denotes the set of vertices (elements) and E denotes the set of edges representing co-occurrence relations. For the purpose of this paper, we restrict our attention to the 29 transition metals contained in this larger network. This restriction is motivated by the fact that rows such as Ga, Ge, and As, and columns such as B, Al, and Ga exhibit substantial variations in elemental properties, which complicate the definition of consistent similarity transfer. By contrast, the transition metals constitute a more homogeneous subset, allowing for meaningful comparison and reliable validation of the proposed descriptor.

2.2 Neighbor sets and degrees

For a vertex $v \in V$, the neighbor set is defined as

$$N(v) = \{u \in V \,:\, (u, v) \in E\},$$

which represents the set of elements that directly co-occur with v in binary compounds. The degree of vertex v is defined as

$$\deg(v) = |N(v)|,$$

which indicates the number of distinct elements connected to v. These quantities are fundamental in graph theory and serve as the basis for defining similarity transfer descriptors, as they capture the relational environment of each element within the network.

2.3 Similarity transfer ratio

We introduce ST as a novel graph-theoretical descriptor that quantifies how similarity between two elements can be transmitted through one or more mediating elements.

Definition 1 (Horizontal/Vertical ST). For three distinct vertices $A, B, C \in V$ aligned horizontally or vertically in the Periodic Table, the similarity transfer ratio is defined as

$$\mathrm{ST}(A,B,C) = \frac{|N(A) \cap N(C)| - |(N(A) \cap N(C)) \setminus (N(A) \cap N(B))|}{|N(A) \cap N(C)|}.$$

The above definition quantifies the portion of shared chemical information that remains transferable through an intermediate vertex. In topological terms, the intersection operation identifies common bonding environments between two elements, while the subtraction term isolates the part that fails to propagate via the mediator. Consequently, the ratio expresses the efficiency of information transmission through the network, bridging the abstract graph representation with chemical interpretability. A high ST value indicates that most of the structural neighborhood around the two elements can be reconstructed through their shared mediator, reflecting a strong propagation of similarity.

Definition 2 (Diagonal ST). For four distinct vertices $A, B, C, D \in V$, where A and D are diagonally positioned in the Periodic Table and B, C serve as mediating vertices, the diagonal similarity transfer ratio is defined as

$$E_{AD} := N(A) \cap N(D), \qquad E_{BC} := N(B) \cup N(C).$$

$$\mathrm{ST}(A,B,C,D) = \frac{|E_{AD}| - |E_{AD} \setminus (N(A) \cap E_{BC})|}{|E_{AD}|}.$$

Although the diagonal ST employs intersection with one mediator (B) and union with the other (C), this asymmetry reflects their distinct topological roles along two diagonal orientations of the Periodic Table. Specifically, B and C occupy adjacent but non-equivalent environments in electronic configuration, so the union operation accounts for their complementary influence on A and D. Despite this asymmetric formulation, the overall descriptor remains symmetric under permutation of A and D, ensuring mathematical consistency of the definition.

2.4 Transfer mechanisms (horizontal, vertical, and diagonal)

From a topological viewpoint, horizontal, vertical, and diagonal transfers correspond respectively to propagation within a period, within a group, and across both directions of the Periodic Table. The asymmetric form of the diagonal case (intersection with one mediator and union with another) reflects their complementary roles along two distinct diagonal orientations, while the overall definition preserves symmetry between the terminal elements.

Based on these definitions, three fundamental transfer mechanisms can be distinguished:

1. **Horizontal transfer**: Similarity propagates between adjacent elements within the same period, mediated by an intermediate element.
2. **Vertical transfer**: Similarity propagates between adjacent elements within the same group, mediated by an intermediate element.
3. **Diagonal transfer**: Similarity propagates between diagonally related elements, mediated by two intermediate elements that jointly facilitate the transfer.

To illustrate these mechanisms, we consider a concrete case of horizontal transfer from our dataset. As shown in Figure 1, the similarity between Y and Nb is mediated through the intermediate element Zr. Specifically, 97% (= (35-1)/35) of the common neighbors between Y and Nb are preserved when the transfer is mediated by Zr, reinforcing the similarity relation between Y and Nb.

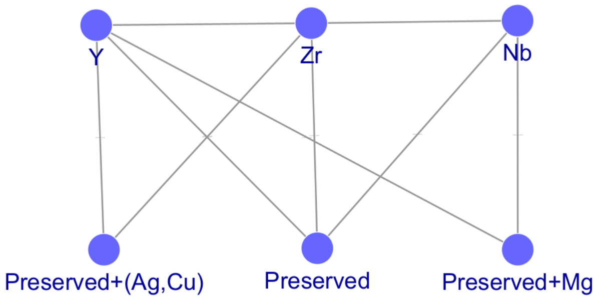

Figure 1. Horizontal similarity transfer: $Y \rightarrow Nb$ mediated by Zr

3 Mathematical analysis and results

3.1 Horizontal ST

Horizontal ST values were calculated for all adjacent triplets of transition metals in the same row, and the results are summarized in Table 1. Values are generally high, with only two combinations containing Tc having values less than 80%.

To further explore robustness, we extended the calculation by replacing the third element C with another element X positioned further to the right in the same row. This "extended horizontal ST" consistently yielded values close to or above 90%, as presented in Table 2.

It is also important to note that

$$\mathrm{ST}(A, B, C) = \mathrm{ST}(C, B, A).$$

Table 1. Horizontal ST (%).

Combination	ST	Combination	ST	Combination	ST
Sc, Ti, V	97	Y, Zr, Nb	97	Hf, Ta, W	96
Ti, V, Cr	91	Zr, Nb, Mo	94	Ta, W, Re	82
V, Cr, Mn	95	Nb, Mo, Tc	76	W, Re, Os	90
Cr, Mn, Fe	86	Mo, Tc, Ru	75	Re, Os, Ir	93
Mn, Fe, Co	93	Tc, Ru, Rh	94	Os, Ir, Pt	96
Fe, Co, Ni	88	Ru, Rh, Pd	90	Ir, Pt, Au	94
Co, Ni, Cu	96	Rh, Pd, Ag	87	Pt, Au, Hg	86
Ni, Cu, Zn	82	Pd, Ag, Cd	88		

Table 2. Extended horizontal ST (%).

Combination	ST	Combination	ST	Combination	ST
Sc, Ti, Cr	97	Y, Zr, Mo	100	Hf, Ta, Re	88
Sc, Ti, Mn	97	Y, Zr, Tc	100	Hf, Ta, Os	88
Sc, Ti, Fe	97	Y, Zr, Ru	96	Hf, Ta, Ir	88
Sc, Ti, Co	96	Y, Zr, Rh	93	Hf, Ta, Pt	84
Sc, Ti, Ni	97	Y, Zr, Pd	97	Hf, Ta, Au	84
Sc, Ti, Cu	97	Y, Zr, Ag	93	Hf, Ta, Hg	92
Sc, Ti, Zn	97	Y, Zr, Cd	91		

Proof. Let $E := N(A) \cap N(C)$. By the definition of horizontal ST,

$$\begin{aligned}\mathrm{ST}(A, B, C) &= \frac{|E| - |(N(A) \cap N(C)) \setminus (N(A) \cap N(B))|}{|E|} \\ &= 1 - \frac{|E \setminus (N(A) \cap N(B))|}{|E|}.\end{aligned}$$

Since $E \subseteq N(A)$, we have the set identity

$$E \setminus (N(A) \cap N(B)) \;=\; E \setminus N(B).$$

(Generally, if $E \subseteq F$, then $E \setminus (F \cap G) = E \setminus G$.) Similarly, because $E \subseteq N(C)$, we also have

$$E \setminus (N(C) \cap N(B)) \;=\; E \setminus N(B).$$

Hence

$$|E \setminus (N(A) \cap N(B))| = |E \setminus N(B)| = |E \setminus (N(C) \cap N(B))|.$$

The numerators of $\mathrm{ST}(A, B, C)$ and $\mathrm{ST}(C, B, A)$ are therefore equal, and their denominators are both $|E|$. It follows that $\mathrm{ST}(A, B, C) = \mathrm{ST}(C, B, A)$.

This symmetry also applies to vertical and diagonal ST.

3.2 Vertical ST

Vertical similarity transfer is investigated by considering triplets of transition metals located in the same column of the periodic table (Table 3). Values are generally high, with several combinations reaching or approaching 100%. (The column containing Sc and Y is excluded because no lanthanoid element is specified to complete a triplet.)

Table 3. Vertical ST (%).

Combination	ST	Combination	ST
Ti, Zr, Hf	100	Co, Rh, Ir	90
V, Nb, Ta	95	Ni, Pd, Pt	92
Cr, Mo, W	90	Cu, Ag, Au	91
Mn, Tc, Re	74	Zn, Cd, Hg	73
Fe, Ru, Os	96		

3.3 Diagonal ST

Diagonal ST takes two patterns: positive diagonal ST (transfer from upper-left to lower-right) and negative diagonal ST (upper-right to lower-left). Results are shown in Tables 4 and 5, respectively.

These findings suggest that similarity transfer among transition metals is not confined to a single orientation but can occur robustly along horizontal, vertical, and diagonal directions of the periodic table. The consistently high transfer ratios underscore the universality of preserved neighbors as the foundation of similarity propagation.

Table 4. Positive diagonal ST (%).

Combination	ST	Combination	ST	Combination	ST
Sc, Ti, Y, Zr	97	Co, Ni, Rh, Pd	96	Tc, Ru, Re, Os	100
Ti, V, Zr, Nb	98	Ni, Cu, Pd, Ag	94	Ru, Rh, Os, Ir	98
V, Cr, Nb, Mo	100	Cu, Zn, Ag, Cd	100	Rh, Pd, Ir, Pt	96
Cr, Mn, Mo, Tc	88	Zr, Nb, Hf, Ta	100	Pd, Ag, Pt, Au	100
Mn, Fe, Tc, Ru	96	Nb, Mo, Ta, W	93	Ag, Cd, Au, Hg	89
Fe, Co, Ru, Rh	91	Mo, Tc, W, Re	91		

Table 5. Negative diagonal ST (%).

Combination	ST	Combination	ST	Combination	ST
Ti, Sc, Zr, Y	97	Ni, Co, Pd, Rh	96	Ru, Tc, Os, Re	96
V, Ti, Nb, Zr	100	Cu, Ni, Ag, Pd	100	Rh, Ru, Ir, Os	98
Cr, V, Mo, Nb	100	Zn, Cu, Cd, Ag	98	Pd, Rh, Pt, Ir	96
Mn, Cr, Tc, Mo	97	Nb, Zr, Ta, Hf	97	Ag, Pd, Au, Pt	96
Fe, Mn, Ru, Tc	95	Mo, Nb, W, Ta	97	Cd, Ag, Hg, Au	97
Co, Fe, Rh, Ru	100	Tc, Mo, Re, W	100		

4 Validation and theoretical implications

This section validates the ST framework against classical graph-theoretical indices and chemical databases, and discusses both theoretical implications and practical predictive applications.

4.1 Comparison with classical graph descriptors

Traditional graph-theoretical descriptors, such as the Wiener index and the Randić index, typically measure global or pairwise structural features of chemical graphs. In contrast, ST captures higher-order relations by quantifying how similarity propagates across triplets or quadruplets of elements. This makes ST a complementary descriptor: while classical indices emphasize aggregate connectivity or branching, ST emphasizes the preservation of common neighbors through mediators, reflecting local propagation mechanisms that are not visible from pairwise descriptors alone.

4.2 Topological inequalities and constraints

The formulation of ST naturally gives rise to topological inequalities that constrain how neighbor sets can overlap in the chemical element network. In particular, two inclusion relations hold:

$$N(A) \cap N(C) \subseteq N(A) \cap N(B), \tag{1}$$
$$N(A) \cap N(D) \subseteq N(A) \cap (N(B) \cup N(C)). \tag{2}$$

which further lead to the cardinality inequalities:

$$|N(A) \cap N(C)| \leq |N(A) \cap N(B)|, \tag{3}$$
$$|N(A) \cap N(D)| \leq |N(A) \cap (N(B) \cup N(C)). \tag{4}$$

Detailed numerical values in (3) and (4) are provided in the supplementary file. Of the 86 value pairs examined, 78 pairs meet either (3) or (4), representing a 90.7% satisfaction rate. Therefore, we can regard the above inequalities as generally valid and use them as a guide to identify potential compounds. For example, for ST(Fe,Co,Ni) in row 1 of Table 1, $|N(Fe) \cap N(Ni)|$=57 and $|N(Fe) \cap N(Co)|$=52, while from (3) we know $|N(Fe) \cap N(Co)|$ should be greater than or equal to $|N(Fe) \cap N(Ni)|$. Therefore, Fe and Co are expected to have more common neighbors.

It is worth noting that the present formulation of ST is not the only conceivable one. If the logical operations of intersection and union were inverted, alternative multi-valued descriptors could be obtained, possibly distinguishing "fundamental" and "excited" transfer states. However, such variants generally lack monotonicity and complicate numerical comparison. The definition adopted in this paper was therefore chosen for its uniqueness and stability, ensuring a single-valued and comparable measure of transferability across all element pairs.

4.3 Compounds prediction

Among all 86 ST values in the five tables listed above, the minimum ST observed is 73, with only four STs being smaller than 80; 68 STs are greater than or equal to 90, accounting for over 79% of all STs. The average value for all STs is 93, which is a high value that supports our belief in the existence of a pattern for ST among elements, i.e., $N(A) \cap N(B)$ can be regarded as the source of $N(A) \cap N(X)$, and $N(A) \cap (N(B) \cup \ N(C))$ can be regarded as the source of $N(A) \cap N(D)$.

The ST pattern provides a systematic basis for predicting potential binary compounds. For instance, in the case of $\mathrm{ST}(\mathrm{Ni}, \mathrm{Cu}, \mathrm{Pd}, \mathrm{Ag})$ in Table 4, $|N(\mathrm{Ni}) \cap N(\mathrm{Ag})| = 51$, Three elements— K,C and W—appear in $N(Ni) \cap N(Ag)$ but are absent from $N(Ni) \cap (N(Cu) \cup (N(Pd)$, resulting in an ST value of 94% (= (51-3)/51). To increase this value, at least one of Cu or Pd must form binary compounds with K, C or W. Verification through Chemspider [16], a website that provides search engines to get various kinds of compounds, confirms the existence of PdC, CuC, and CuW, reducing the discrepancy to a single element (K) and effectively increasing the ST value to 98%.

5 Conclusions

This study introduced ST as a novel graph-theoretical descriptor for analyzing the propagation of similarity among transition metals. By formalizing three transfer mechanisms—horizontal, vertical, and diagonal—and proving their mathematical properties such as symmetry and topological inequalities, we established a rigorous framework that enriches the methodological toolbox of chemical graph theory. The analysis of 29 transition metals demonstrated that similarity transfer is highly robust, thereby offering a new perspective on periodic trends from a network-topological viewpoint.

The present analysis focuses on 29 transition metals, which constitute a compact and chemically homogeneous subset suitable for initial validation. Nevertheless, the framework is not limited to these elements. In future work, we plan to extend the model to include s-, p-, and f-block elements and to analyze inter-block transfer mechanisms. Such expansion will test the generality of the ST descriptor and may further enhance its applicability to predicting new compounds and uncovering broader periodic trends.

Future research will also extend this approach to non-transition elements, incorporate stoichiometric weights into the network model, and explore connections with other topological indices, thereby strengthening the link between mathematical chemistry and real compound formation.

Beyond its theoretical contribution, the ST framework thus enriches the mathematical foundations of chemical similarity while offering a unified basis for both structural interpretation and predictive analysis across the Periodic Table.

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Availability of data and materials: The data used in this paper are attached as supplementary files in [10] and [11]; data for this paper are also uploaded as supplementary material.

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