SUMMARY Computing an invariant of a graph such as treewidth and pathwidth is one of the fundamental problems in graph algorithms. In general, determining the pathwidth of a graph is NP-hard. In this paper, we propose several reduction methods for decreasing the instance size without changing the pathwidth, and implemented the methods together with an exact algorithm for computing pathwidth of graphs. Our experimental results show that the number of vertices in all chemical graphs in NCI database decreases by our reduction methods by 53.81% in average.

key words: pathwidth, exact algorithms, graphs, chemical graphs

1. Introduction

Treewidth of undirected graphs has been extensively studied. The notion of undirected treewidth is defined by Robertson and Seymour [12], which has been used as an important measure for the graph minor theory [13] and for designing efficient algorithms for NP-hard problems by Arnborg and Proskurowski [1]. Furthermore, the notion is extended into the case of digraphs by Johnson et al. [7]. Yamaguchi et al. [15] designed a fast algorithm for computing the treewidth of undirected graphs and computed the distribution of treewidth of chemical graphs in the LIGAND database [6].

As well as treewidth, pathwidth of graphs has been studied as another important feature of graph structure. While the pathwidth of an undirected graph was defined by Robertson and Seymour [11], the pathwidth of a digraph was generalized by Reed et al. according to Barát [2]. Kashiwabara and Fujisawa [8] proved that given an integer \( k \) and an undirected graph \( G \), it is NP-complete to decide whether the pathwidth of \( G \) is at most \( k \). Bodlaender et al. [4, 3] showed that when the treewidth is fixed the problem can be solved in linear time. On the other hand, nontrivial exponential algorithms are proposed. Suchan et al. [14] designed an algorithm that runs in \( 1.9657^n n^{O(1)} \) time and space, and afterwards Kitsunai et al. [9] gave an algorithm that runs in \( 1.89^n n^{O(1)} \) time and space.

Robertson and Seymour [13] led to a consequence of the graph minor theorem that for a fixed \( k \) there is a polynomial time algorithm that decides whether the pathwidth of a given graph is at most \( k \). Nagamochi [10] proposed a branching algorithm for finding a linear layout with a bounded width that minimizes a given cost function, based on which it takes \( O(k m n^{2k}) \) time and \( O(m + n) \) space to test whether the pathwidth of a given digraph with \( n \) vertices and \( m \) edges is at most \( k \).

In this paper, to reduce the running time of the computation in the undirected graph case, we show sufficient conditions such that the pathwidth remains unchanged after removing or contracting some vertices.

The rest of this paper is organized as follows. Section 2 introduces some notations and terminologies. Section 3 gives sufficient conditions for vertices in an undirected graph so that the pathwidth remains unchanged after removing or contracting the vertices. Section 4 reports some experimental results on our reduction methods and finally Sect. 5 makes some concluding remarks.

2. Preliminaries

Sequences For two positive integers \( i \leq j \), we denote by \([i, j]\) the set of all integers \( h \) satisfying \( i \leq h \leq j \).

Let \( V \) be a finite set with \( n \geq 1 \) elements. We call a sequence \( \sigma \) consisting of some elements of \( V \) non-duplicating if each element of \( V \) occurs at most once in \( \sigma \). Let \( \Sigma(V) \) denote the set of non-duplicating sequences of all elements in \( V \). For each sequence \( \sigma \in \Sigma(V) \), we denote by \( V(\sigma) \) the set of elements constituting \( \sigma \) and by \( |\sigma| = |V(\sigma)| \) the length of \( \sigma \). A sequence \( \tau \) is called a \textit{prefix} of a sequence \( \sigma \) if it is a subsequence of \( \sigma \) that consists of the first \( |\tau| \) elements in \( \sigma \). For a sequence \( \sigma \in \Sigma \) and an integer \( i \in [1, |\sigma|] \), we denote by \( \sigma(i) \) the \( i \)-th element in \( \sigma \) and by \( \sigma_i \) the prefix of \( \sigma \) with length \( i \).

Pathwidth Let \( G \) be an undirected graph. Let \( V(G) \) and \( E(G) \) denote the sets of vertices and edges, respectively. We denote by \([u, v]\) an undirected edge between \( u \) and \( v \). For each subset \( X \subseteq V(G) \), we define the set \( N_G(X) \) of neighbors of \( X \) in \( G \) to be

\[
N_G(X) = \{ v \in V(G) - X \mid u \in X, [u, v] \in E(G) \},
\]

and let \( dg(X) = |N_G(X)| \). When \( X \) is a singleton set \([v]\), we may denote \( N_G(X) \) and \( dg(X) \) as \( N_G(v) \) and \( dg(v) \), respectively. We call a vertex \( v \) a \textit{degree-} \( k \) \textit{vertex} if \( dg(v) = k \).

Let \( X \) be a subset of \( V(G) \). We denote by \( G - X \) the subgraph obtained from \( G \) by removing all vertices \( X \) together with edges incident to vertices in \( X \). Contracting \( X \) is to identify the vertices in \( X \) as a single vertex \( x \) removing any resulting
self-loops and multiple edges incident to $x$. We denote by $G/X$ the graph obtained from $G$ by contracting $X$.

For a sequence $\sigma$ consisting of some elements in $V(G)$. We denote $N_G(V(\sigma))$ and $d_G(V(\sigma))$ by $N_\sigma(\sigma)$ and $d_\sigma(\sigma)$. The “pathwidth” of a graph $G$ is defined based on a path-like representation of $G$. In this paper, we use the following definition for convenience.

**Definition 1:** Let $G$ be an undirected graph. The pathwidth $pw(\sigma)$ of a sequence $\sigma \in \Sigma(V(G))$ is defined to be the maximum $d_G(\sigma')$ over all prefixes $\sigma'$ of $\sigma$ with $1 \leq |\sigma'| < |V(G)|$. The pathwidth $pw(G)$ of $G$ is defined to be the minimum $pw(\sigma)$ over all sequences $\sigma \in \Sigma(V(G))$.

Let $PW(G)$ denote the set of the sequences $\sigma \in \Sigma(V(G))$ such that $pw(\sigma) = pw(G)$. The input and output of the problem of computing the pathwidth of undirected graphs are described as follows:

**Pathwidth of Undirected Graphs:**

**Input:** an undirected graph $G$ and a positive integer $k$;

**Output:** a sequence $\sigma \in PW(G)$ if $pw(G) \leq k$, or a message of “$pw(G) > k$” otherwise.

### 3. Reducing Instance Size in Undirected Graphs

In this section, we propose four reduction rules based on sufficient conditions for a degree-1 vertex and a pair of two degree-1 vertices so that the pathwidth remains unchanged after removing the vertices, and for a pair of a degree-3 vertex and a degree-1 vertex so that the pathwidth remains unchanged after contracting the vertices. The sufficient conditions will be shown in Theorems 3, 4, 6, and 9. Theorems 3, 4, and 6 are sufficient conditions for degree-1 vertices to be removed while Theorem 9 is a sufficient condition for a pair of a degree-3 vertex and a degree-1 vertex to be contracted without changing the pathwidth.

To prove Theorem 3, the following lemma is used.

**Lemma 2:** Let $G$ be an undirected graph and $v$ be a vertex such that there is a sequence $\sigma' \in PW(G)$ in which a vertex $v$ appears after all neighbors of $v$. Let $\sigma \in \Sigma(V(G))$ be the sequence constructed from $\sigma'$ by moving $v$ at the position immediately before the last neighbor of $v$ in $\sigma'$ (see Fig. 1). Then $pw(\sigma) = pw(\sigma')$.

**Proof.** Since clearly $pw(\sigma) \geq pw(G) = pw(\sigma')$ holds, we prove $pw(\sigma) \leq pw(\sigma')$. Let $n = |V(G)|$ and let $v_i$ and $v_b$ be the last two neighbors of $v$ which appear in $\sigma'$ in this order. Let $i_a$, $i_b$, and $i_c$ denote the positions of the vertices $v_a$, $v_b$, and $v$ in $\sigma'$, respectively; i.e., $\sigma'(i_a) = v_a$, $\sigma'(i_b) = v_b$, and $\sigma'(i_c) = v$. By assumption, $i_a < i_b < i_c$. The sequence $\sigma \in \Sigma(V(G))$ from $\sigma'$ by moving $v$ immediately before $v_b$ is given by

$$\sigma(i) = \begin{cases} \sigma'(i) & (1 \leq i \leq i_b - 1) \\ v & (i = i_b) \\ \sigma'(i - 1) & (i_b + 1 \leq i \leq i_c) \\ \sigma'(i) & (i_c + 1 \leq i \leq n). \end{cases}$$

To prove $pw(\sigma) \leq pw(\sigma')$, it suffices to show that for each $i \in [1, n]$ there is a $j \in [1, n]$ such that $d_G(\sigma_i) \leq d_G(\sigma'_j)$ or $|N_G(\sigma_i) \setminus N_G(\sigma'_j)| \leq |N_G(\sigma'_j) \setminus N_G(\sigma_i)|$.

For each $i \in [1, i_b - 1] \cup [i_c, n]$, it holds that $N_G(\sigma_i) = N_G(\sigma'_j)$ and $d_G(\sigma_i) = d_G(\sigma'_j)$. For $i \in [i_b, i_c - 1]$, we have $N_G(\sigma_i) \setminus N_G(\sigma'_j) \subseteq \{v_b\}$ since $v$ is not adjacent to any other vertex than $v_b$ in $G \setminus V(\sigma_{i_b+1})$, while we have $N_G(\sigma'_j) \setminus N_G(\sigma_i) \supseteq \{v\}$ since $v \in N_G(\sigma'_j) \setminus N_G(\sigma_{i_c - 1})$ and $v \notin N_G(\sigma_i)$, indicating that $d_G(\sigma_i) \leq d_G(\sigma'_j)$. $\square$

Now we prove Theorem 3 using Lemma 2. We remark that the reduction rule implied by Theorem 3 includes a reduction rule proposed by Bodlaender et al. [5] that removes all but one of two or more degree-1 vertices adjacent to the same vertex.

**Theorem 3:** Let $G$ be an undirected graph with a degree-1 vertex $u$ whose unique neighbor $v_0$ is adjacent to a vertex $u'$ (≠ $u$) of degree at most 2 (see Fig. 2 (a)). Then the pathwidth remains unchanged after removing $u$.

**Proof.** Let $n = |V(G)|$, and let $G'$ be the subgraph obtained from $G$ by removing $u$ (see Fig. 2 (b)). Since clearly $pw(G) \geq pw(G')$ holds, we show that $pw(G) \leq pw(G')$. We here claim that there is a sequence $\sigma' \in PW(G')$ such that $u'$ appears before at least one of its two neighbors (if $u'$ is a degree-2 vertex in $G'$). If there exists a sequence in $PW(G')$ in which $u'$ appears after its two neighbors, then by applying Lemma 2 with $v := u'$, we can obtain a sequence in $PW(G')$ such that $u'$ appears between its two neighbors, proving the claim.

To prove that $pw(G) \leq pw(G')$, it suffices to show that $pw(\sigma) \leq pw(\sigma')$ holds for the sequence $\sigma \in \Sigma(V(G))$ obtained from $\sigma'$ by inserting the vertex $u$ immediately before $v_0$ in $\sigma'$. Let $i'$ denote the position of the vertex $v_0$ in sequence $\sigma'$, i.e., $\sigma'(i') = v_0$. Then $\sigma$ is given by

![Fig. 1 Illustrations for Lemma 2.](image1)

![Fig. 2 Illustrations for (a) a given graph $G$ and (b) the subgraph $G'$ reduced from $G$ by Theorem 3.](image2)
To prove \( \text{pw}(\sigma) \leq \text{pw}(\sigma') \), we show that for each \( i \in [1, n] \) there is a \( j \in [1, n] \) such that \( d_G(\sigma_i) \leq d_G(\sigma'_j) \) or \( |N_G(\sigma_i) \setminus N_G(\sigma'_j)| \leq |N_G(\sigma'_j) \setminus N_G(\sigma_i)| \).

For each \( i \in \{1, i^* - 1\} \), it holds that \( N_G(\sigma_i) = N_G(\sigma'_j) \) and \( d_G(\sigma_i) = d_G(\sigma'_j) \). For each \( i \in \{i^* + 1, n\} \), we have that \( N_G(\sigma_i) = N_G(\sigma'_j) \) and \( d_G(\sigma_i) = d_G(\sigma'_j) \). For \( i = i^* \), we distinguish two cases.

Case 1. At least one neighbor of \( v_0 \) appears before \( v_0 \) in \( \sigma' \) (see Fig. 3(a)): Since \( v_0 \in N_G(\sigma'_{i^*-1}) \) and \( u \) is not incident to any other edge than \( v_0, u \) in \( G \), we have \( N_G(\sigma_i) = N_G(\sigma'_j) \) and \( d_G(\sigma_i) = d_G(\sigma'_j) \).

Case 2. No neighbor of \( v_0 \) appears before \( v_0 \) in \( \sigma' \) (see Fig. 3(b)): In this case, by the choice of \( \sigma', u' \) appears before the other neighbor than \( v_0 \) in \( \sigma' \) (if \( u' \) is a degree-2 vertex in \( G' \)). Hence it holds that \( u' \notin N_G(\sigma'_{i^*-1}) \) since \( u' \) has no neighbor before \( v_0 \) in \( \sigma' \) since \( d_G(\sigma') \leq 2 \). Next we have \( u' \notin N_G(\sigma'_j) \) since there is an edge \( v_0, u' \) in \( G' \). Finally any vertex in \( N_G(\sigma'_{i^*-1}) \) also belongs to \( N_G(\sigma'_j) \) since \( v_0 \) has no neighbor in \( V(\sigma'_{i^*-1}) \). As a consequence of these, the numbers \( d_G(\sigma'_{i^*-1}) \) and \( d_G(\sigma'_j) \) of neighbors of the sequences \( \sigma'_{i^*-1} \) and \( \sigma'_j \) satisfy that \( d_G(\sigma'_{i^*-1}) \leq d_G(\sigma'_j) \). Since there is an edge \( v_0, u \) in \( G \), the number of neighbors of the sequence \( \sigma_j \) satisfies that

\[
d_G(\sigma_j) = d_G(\sigma'_j) + 1 \leq d_G(\sigma'_j) \quad \square
\]

Next we show a reduction rule based on Theorem 4.

**Theorem 4:** Let \( G \) be an undirected graph and \( v_1 \) be a degree-3 vertex adjacent to a degree-1 vertex \( u_1 \), a degree-3 vertex \( v_2 \), and a vertex \( v_3 \) such that \( v_2 \) is adjacent to the vertex \( v_3 \) and a degree-1 vertex \( u_2 \) (see Fig. 4(a)). Then the pathwidth remains unchanged after removing \( u_1 \) and \( u_2 \).

**Proof.** Let \( n = |V(G)| \). Let \( G' \) be the subgraph obtained from \( G \) by removing \( u_1 \) and \( u_2 \) (see Fig. 4(b)). Since clearly \( \text{pw}(G) \geq \text{pw}(G') \), we prove that \( \text{pw}(G) \leq \text{pw}(G') \). If there exists a sequence in \( \text{pw}(G') \) in which \( v_3 \) appears between the two degree-2 neighbors \( v_1 \) and \( v_2 \), then by applying Lemma 2 with \( v \vdash v_1 \) or \( v \vdash v_2 \) we can obtain a sequence in \( \text{pw}(G') \) such that \( v_3 \) appears after \( v_1 \) and \( v_2 \). Hence there is a sequence \( \sigma' \in \text{pw}(G') \) where \( v_3 \) does not appear between \( v_1 \) and \( v_2 \). Let \( i_1, i_2, \) and \( i_3 \) denote the positions of the vertices \( v_1, v_2, \) and \( v_3 \) in \( \sigma' \), respectively; i.e., \( \sigma'(i_1) = v_1, \sigma'(i_2) = v_2, \) and \( \sigma'(i_3) = v_3 \), where \( i_1 < i_2 \) is assumed without loss of generality.

To prove that \( \text{pw}(G) \leq \text{pw}(G') \), it suffices to show that \( \text{pw}(\sigma) \leq \text{pw}(\sigma') \) holds for the sequence \( \sigma \in \Sigma(V(G)) \) obtained from \( \sigma' \) by inserting the vertex \( u_1 \) (resp., \( u_2 \)) immediately before \( v_1 \) (resp., \( v_2 \)). Then \( \sigma \) is given by

\[
\sigma(j) = \begin{cases} 
\sigma'(i) & (1 \leq i \leq i_1 - 1) \\
u_1 & (i = i_1) \\
\sigma'(i - 1) & (i_1 + 1 \leq i \leq i_2) \\
u_2 & (i = i_2 + 1) \\
\sigma'(i - 2) & (i_2 + 2 \leq i \leq n) 
\end{cases}
\]

See Fig. 5. To prove \( \text{pw}(\sigma) \leq \text{pw}(\sigma') \), we show that for each \( i \in [1, n] \) there is a \( j \in [1, n] \) such that \( d_G(\sigma_i) \leq d_G(\sigma'_j) \) or \( |N_G(\sigma_i) \setminus N_G(\sigma'_j)| \leq |N_G(\sigma'_j) \setminus N_G(\sigma_i)| \).

For each \( i \in [1, i_1 - 1] \), it holds that \( N_G(\sigma_i) = N_G(\sigma'_j) \) and \( d_G(\sigma_i) = d_G(\sigma'_j) \). For each \( i \in [i_1 + 1, i_2] \), it holds that

![Fig. 3](image-url) Illustrations for the proof of (a) Case 1 and (b) Case 2 of Theorem 3.

![Fig. 4](image-url) Illustrations for (a) a given graph \( G \) and (b) the subgraph \( G' \) reduced from \( G \) by Theorem 4.

![Fig. 5](image-url) Illustrations for the proof of (a) Case 1 and (b) Case 2 of Theorem 4.
There is an edge $\sigma$ in $G$ and we have $v_2 \in N_G(\sigma'_{i-1})$ since $v_2$ has a neighbor $v_1$ in $V(\sigma'_{i-1})$, and hence it holds that $N_G(\sigma_{i+1}) = N_G(\sigma'_{i-1})$ and $d_G(\sigma_{i+1}) = d_G(\sigma'_{i-1})$. For each $i \in [i_2 + 2, n]$, we have that $N_G(\sigma_i) = N_G(\sigma'_{i-2})$ and $d_G(\sigma_i) = d_G(\sigma'_{i-2})$.

Finally for $i = i_1$ we distinguish two cases.

Case 1. $i_3 < i_1$ (see Fig. 5(a)): The vertex $u_1$ is not incident to any other edge than $\{u_1, v_1\}$ in $G$ and we have $v_1 \in N_G(\sigma'_{i-1})$ since $v_1$ has a neighbor $v_2$ in $V(\sigma'_{i-1})$, and hence it holds that $N_G(\sigma_i) = N_G(\sigma'_{i-2})$ and $d_G(\sigma_i) = d_G(\sigma'_{i-2})$.

Case 2. $i_2 < i_3$ (see Fig. 5(b)): Firstly it holds that $v_2 \notin N_G(\sigma'_{i-1})$ since the two neighbors $v_1$ and $v_3$ of $v_2$ are not in $V(\sigma'_{i-1})$. Secondly we have $v_2 \in N_G(\sigma'_{i-1})$ since there is an edge $\{v_1, v_2\}$ in $G'$. Finally $v_1$ has no neighbor in $V(\sigma'_{i-1})$ since the two neighbors $v_2$ and $v_3$ of $v_2$ appear after $v_1$, and hence any vertex in $N_G(\sigma'_{i-1})$ also belongs to $N_G(\sigma_i)$. As a consequence of these, the numbers $d_G(\sigma'_{i-1})$ and $d_G(\sigma'_{i-1})$ of neighbors of the sequences $\sigma'_{i-1}$ and $\sigma_i'$ satisfy $d_G(\sigma'_{i-1}) < d_G(\sigma_i')$. Since there is an edge $\{u_1, v_1\}$ in $G$, the number of neighbors of the sequence $\sigma_i$ satisfies that $d_G(\sigma_i) = d_G(\sigma'_{i-1}) + 1 \leq d_G(\sigma_i')$. □

Next, to prove Theorem 6, the following lemma is used.

**Lemma 5:** Let $G$ be an undirected graph and let $\sigma' \in \text{PW}(G)$ be a sequence in which a vertex $v$ of degree at least 2 appears after all its neighbors and the last two neighbors of $v$ are adjacent. Let $\sigma \in \Sigma(V(G))$ be the sequence constructed from $\sigma'$ by moving $v$ at the position immediately before the last neighbor of $v$ in $\sigma'$ (see Fig. 6). Then $\text{pw}(\sigma) = \text{pw}(\sigma')$.

**Proof.** Since clearly $\text{pw}(\sigma) \geq \text{pw}(G) = \text{pw}(\sigma')$ holds, we prove $\text{pw}(\sigma) \leq \text{pw}(\sigma')$. Let $n = |V(G)|$ and let $v_0$, $v_1$, and $v_2$ be the last two neighbors of $v$ which appear in $\sigma'$ in this order. Let $i_0$, $i_1$, and $i_2$ denote the positions of the vertices $v_0$, $v_1$, and $v$ in $\sigma'$, respectively; i.e., $\sigma'(i_0) = v_0$, $\sigma'(i_1) = v_1$, and $\sigma'(i_2) = v$. By assumption, $i_0 < i_1 < i_2$. The sequence $\sigma \in \Sigma(V(G))$ obtained from $\sigma'$ by moving $v$ immediately before $v_0$ is given by

$$
\sigma(i) = \begin{cases} 
\sigma'(i) & (1 \leq i \leq i_0 - 1) \\
v & (i = i_0) \\
\sigma'(i - 1) & (i_0 + 1 \leq i \leq i_1) \\
\sigma'(i) & (i_1 + 1 \leq i \leq n).
\end{cases}
$$

To prove $\text{pw}(\sigma) \leq \text{pw}(\sigma')$, it suffices to show that for each $i \in [1, n]$ there is a $j \in [1, n]$ such that $d_G(\sigma_i) \leq d_G(\sigma'_j)$ or $|N_G(\sigma_i) \setminus N_G(\sigma'_j)| \leq |N_G(\sigma'_j) \setminus N_G(\sigma_i)|$.

For each $i \in [1, i_0 - 1] \cup [i_3, n]$, it holds that $N_G(\sigma_i) = N_G(\sigma'_i)$ and $d_G(\sigma_i) = d_G(\sigma'_i)$. For $i \in [i_0 + 1, i_3 - 1]$, we have $N_G(\sigma_i) \setminus N_G(\sigma'_i) \subseteq \{v\}$ since $v$ is not adjacent to any other vertex than $v_0$ in $V(G) \setminus V(\sigma'_{i-1})$, while we have $N_G(\sigma'_i) \setminus N_G(\sigma_i) \subseteq \{v\}$ since $v \notin N_G(\sigma'_i)$ and $v \notin N_G(\sigma_i)$, indicating that $d_G(\sigma_i) \leq d_G(\sigma'_i)$. Finally we show that $d_G(\sigma_i) \leq d_G(\sigma'_i)$. We have $N_G(\sigma'_i) \setminus N_G(\sigma_i) \supseteq \{v\}$ since $v \in N_G(\sigma'_i)$ and $v \notin N_G(\sigma_i)$. On the other hand, the unique vertex $v_0$ in $(N_G(\sigma_i) \cap N(v)) \setminus \{v\}$ is also in $N_G(\sigma'_i)$ because the last two neighbors $v_0$ and $v_0$ of $v$ in $\sigma'$ are adjacent. From this, each vertex in $N_G(\sigma_i) \setminus \{v\}$ also belongs to $N_G(\sigma'_i)$. In addition, since we have $v_0 \in N_G(\sigma_i)$ and $v_0 \notin N_G(\sigma'_i)$, it holds that $N_G(\sigma_i) \setminus N_G(\sigma'_i) = \{v_0\}$. Hence, $d_G(\sigma_i) \leq d_G(\sigma'_i)$. □

Now we prove Theorem 6 using Lemma 5.

**Theorem 6:** Let $G$ be an undirected graph which has three degree-3 vertices $v_0$, $v_1$, and $v_2$ adjacent each other, and let $v_0$ be adjacent to a degree-1 vertex $u$ (see Fig. 7(a)). Then the pathwidth remains unchanged after removing $u$.

**Proof.** Let $n = |V(G)|$. Let $G'$ be the subgraph obtained from $G$ by removing $u$ (see Fig. 7(b)). Since clearly $\text{pw}(G) \geq \text{pw}(G')$ holds, we prove that $\text{pw}(G) \leq \text{pw}(G')$. Let $v_0$ be the other neighbor of $v_1$ than $v_0$ and $v_2$, and let $v_2$ be the other neighbor of $v_0$ than $v_0$ and $v_2$, where possibly $w_1 = w_2$. We here claim that there is a sequence $\sigma' \in \text{PW}(G')$ such that $v_0$ appears between $v_1$ and $v_2$; or $v_0$ appears before $v_1$ and $v_2$, and $v_0$ or $v_0$ appears after $v_0$. If there exists a sequence in $\text{PW}(G')$ in which $v_0$ appears after $v_1$ and $v_2$, then by applying Lemma 5 with $v := v_0$ and adjacent degree-2 neighbors $v_1$ and $v_2$ of $v_0$, we can obtain a sequence in $\text{PW}(G')$ such that $v_0$ appears before $v_1$ and $v_2$. Let $\sigma' \in \text{PW}(G')$ be a sequence in which $v_0$ appears after $v_1$ and $v_2$. Let $\sigma'' \in \text{PW}(G')$ be a sequence in which $v_0$ appears before $v_1$ and $v_2$. If $\sigma''$ appears after $v_0$ in $\sigma'$, then let $\sigma' = \sigma''$. If both $\sigma_1$ and $\sigma_2$ appear before $v_0$ in $\sigma'$ (see Fig. 8), then by applying Lemma 5 with $v := v_1$ or $v := v_2$, we can obtain a sequence $\sigma'' \in \text{PW}(G')$ such that $v_0$ appears between $v_1$ and $v_2$. This proves the claim.

Let $i_0, i_1$, and $i_2$ denote the positions of the vertices $v_0$, $v_1$, and $v_2$ in $\sigma'$, respectively; i.e., $\sigma'(i_0) = v_0$, $\sigma'(i_1) = v_1$, and $\sigma'(i_2) = v_2$, where $i_1 < i_2$ is assumed without loss of generality.

To prove that $\text{pw}(G) \leq \text{pw}(G')$, it suffices to show that

![Fig. 6](image-url)

**Fig. 6** Illustrations for the proof of Lemma 5.

![Fig. 7](image-url)

**Fig. 7** Illustrations for (a) a given graph $G$ and (b) the subgraph $G'$ reduced from $G$ by Theorem 6.
To prove $\text{pw}(\sigma) \leq \text{pw}(\sigma')$ holds for the sequence $\sigma$ obtained from $\sigma'$ by inserting the vertex $u$ immediately before $v_0$ in $\sigma'$. Then $\sigma$ is given by

$$\sigma(i) = \begin{cases} 
\sigma'(i) & (1 \leq i \leq i_0 - 1) \\
u & (i = i_0) \\
\sigma'(i - 1) & (i_0 + 1 \leq i \leq n).
\end{cases}$$

To prove $\text{pw}(\sigma) \leq \text{pw}(\sigma')$, we show that for each $i \in [1, n]$ there is a $j \in [1, n]$ such that $d_G(\sigma_i) \leq d_G(\sigma'_j)$ or $|N_G(\sigma_i) \setminus N'_G(\sigma'_j)| \leq |N_G(\sigma'_j) \setminus N'_G(\sigma_i)|$.

For each $i \in [1, i_0 - 1]$, it holds that $N_G(\sigma_i) = N'_G(\sigma'_i)$ and $d_G(\sigma_i) = d_G(\sigma'_i)$. For each $i \in [i_0 + 1, n]$, we have that $N_G(\sigma_i) = N'_G(\sigma'_{i-1})$ and $d_G(\sigma_i) = d_G(\sigma'_{i-1})$. For $i = i_0$, we distinguish two cases.

Case 1. $i_0 < i_1$ (see Fig. 9(b)): In this case, by the choice of $\sigma'$, $w_1$ or $w_2$ appears after $v_0$ in $\sigma'$. Hence $v_1$ or $v_2$ has no neighbor before $v_0$ in $\sigma'$ since $d_G(v_1) = 3$ and $d_G(v_2) = 3$. Firstly it holds that $v_1 \notin N_G(\sigma'_{i_0-1})$ or $v_2 \notin N_G(\sigma'_{i_0-1})$ since either $v_1$ or $v_2$ has no neighbor before $v_0$. Secondly we have $v_1, v_2 \in N_G(\sigma'_{i_0})$. Since there are edges $\{v_0, v_1\}$ and $\{v_0, v_2\}$ in $G'$. Finally any vertex in $N_G(\sigma'_{i_0-1})$ also belongs to $N_G(\sigma'_{i_0})$ since $v_0$ has no neighbor in $V(\sigma'_{i_0-1})$. As a consequence of these, the numbers $d_G(\sigma'_{i_0-1})$ and $d_G(\sigma'_{i_0})$ of neighbors of the sequence $\sigma'_{i_0-1}$ and $\sigma'_{i_0}$ satisfy that $d_G(\sigma'_{i_0-1}) < d_G(\sigma'_{i_0})$. Since there is an edge $\{v_0, u\}$ in $G$, the number of neighbors of the sequence $\sigma'_{i_0}$ satisfies that

$$d_G(\sigma_{i_0}) = d_G(\sigma'_{i_0-1}) + 1 \leq d_G(\sigma'_{i_0}). \quad \Box$$

To prove Theorem 9, the following two lemmas are used.

**Lemma 7:** Let $G$ be an undirected graph and $u$ be a degree-1 vertex in $G$. For a sequence $\sigma' \in \text{PW}(G)$, let $\sigma \in \Sigma(V(G))$ be the sequence constructed from $\sigma'$ by moving $u$ at the position immediately before its unique neighbor. Then $\text{pw}(\sigma) = \text{pw}(\sigma')$.

**Proof.** Since clearly $\text{pw}(\sigma) \geq \text{pw}(G) = \text{pw}(\sigma')$, we prove $\text{pw}(\sigma) \leq \text{pw}(\sigma')$. Let $n = |V(G)|$. Let $v$ be the unique neighbor of $u$ and $\sigma' \in \text{PW}(G)$ be a sequence in which $u$ does not appear immediately before $v$. Let $i_u$ and $i_v$ denote the positions of the vertices $u$ and $v$ in the sequence $\sigma'$, respectively; i.e., $\sigma'(i_u) = u$ and $\sigma'(i_v) = v$. We distinguish two cases.

Case 1. $i_u < i_v$ (see Fig. 10(a)): The sequence $\sigma$ obtained from $\sigma'$ by moving $u$ immediately before $v$ is given by

$$\sigma(i) = \begin{cases} 
\sigma'(i) & (1 \leq i \leq i_u - 1) \\
u & (i = i_u) \\
\sigma'(i+1) & (i_u \leq i \leq i_v - 2) \\
u & (i = i_v - 1) \\
\sigma'(i) & (i_v \leq i \leq n).
\end{cases}$$

To prove $\text{pw}(\sigma) \leq \text{pw}(\sigma')$, we show that for each $i \in [1, n]$ there is a $j \in [1, n]$ such that $d_G(\sigma_i) \leq d_G(\sigma'_j)$ or $|N_G(\sigma_i) \setminus N'_G(\sigma'_j)| \leq |N_G(\sigma'_j) \setminus N'_G(\sigma_i)|$.

For each $i \in [1, i_u - 1] \cup [i_u - 1, n]$, it holds that $N_G(\sigma_i) = N'_G(\sigma'_j)$ and $d_G(\sigma_i) = d_G(\sigma'_j)$.

For $i \in [i_u, i_v - 2]$, $u$ has no neighbor before itself in $\sigma$ since $u$ is degree-1 vertex and appears before $v$, and hence
each vertex in $N_G(\sigma_i)$ also belongs to $N_G(\sigma'_{i+1})$. From this, since we have $N_G(\sigma_i) \cap N_G(\sigma'_{i+1}) = \emptyset$, we conclude $d_G(\sigma_i) \leq d_G(\sigma'_{i+1})$.

Case 2. $i_u < i_v$ (see Fig. 10(b)): The sequence $\sigma$ obtained from $\sigma'$ by moving $u$ immediately before $v$ is given by

$$\sigma(i) = \begin{cases} 
\sigma'(i) & (1 \leq i \leq i_u - 1) \\
u & (i = i_u) \\
\sigma'(i-1) & (i_u + 1 \leq i \leq i_v) \\
\sigma'(i) & (i_v + 1 \leq i \leq n).
\end{cases}$$

To prove $pw(\sigma) \leq pw(\sigma')$, we show that for each $i \in [1,n]$ there is a $j \in [1,n]$ such that $d_G(\sigma_i) \leq d_G(\sigma'_j)$ or $|N_G(\sigma_i) \cap N_G(\sigma'_j)| \leq |N_G(\sigma'_j) \cap N_G(\sigma_i)|$.

For each $i \in [1,i_u - 1] \cup [i_v,n]$, it holds that $N_G(\sigma_i) = N_G(\sigma'_i)$ and $d_G(\sigma_i) = d_G(\sigma'_i)$.

For $i \in [i_u + 1,i_v - 1]$, $u$ has no neighbor after $v$ in $\sigma$ since $u$ is degree-1 vertex and appears after $v$, and hence each vertex in $N_G(\sigma_i)$ also belongs to $N_G(\sigma'_{i-1})$. From this, since we have $N_G(\sigma_i) \cap N_G(\sigma'_{i-1}) = \emptyset$, we conclude $d_G(\sigma_i) \leq d_G(\sigma'_{i-1})$.

For $i = i_u$, we have $N_G(\sigma'_{i-1}) \cap N_G(\sigma_{i_u}) \subseteq \{u\}$ since $u \in N_G(\sigma'_{i-1})$ and $u \notin N_G(\sigma_{i_u})$, while we have $N_G(\sigma_{i_u}) \cap N_G(\sigma'_{i-1}) = \emptyset$ since $u$ has the unique neighbor $v$ in $V(G) \setminus V(\sigma_{i_u})$, and hence it holds $d_G(\sigma_{i_u}) \leq d_G(\sigma'_{i-1})$. $\square$

**Lemma 8:** Let $G$ be an undirected graph which has a vertex $v$ of degree at least 3 adjacent to a degree-1 vertex $u$ (see Fig. 11 (a)) and let $\sigma' \in PW(G)$ be a sequence in which $v$ appears after all neighbors of $v$ and $u$ appears immediately before $v$. Let $\sigma = \Sigma(V(G))$ be the sequence constructed from $\sigma'$ by moving $v$ at the position immediately before the last vertex in $N_G(v) \setminus \{u\}$ and moving $u$ at the position immediately before $v$ in $\sigma'$ (see Fig. 11 (b)). Then $pw(\sigma) = pw(\sigma')$.

**Proof.** Since clearly $pw(\sigma) \geq pw(G) = pw(\sigma')$, we prove $pw(\sigma) \leq pw(\sigma')$. Let $n = |V(G)|$ and let $v_u$ and $v_b$ be the last other two neighbors of $v$ than $u$ which appear in $\sigma'$ in this order. Let $i_u$, $i_v$, and $i_b$ denote the positions of the vertices $v_u$, $v_b$, and $v$ in the sequence $\sigma'$, respectively; i.e., $\sigma'(i_u) = v_u$, $\sigma'(i_b) = v_b$, and $\sigma'(i_v) = v$, where $i_u < i_b < i_v$ is assumed without loss of generality. The sequence $\sigma$ obtained from $\sigma'$ by moving $v$ immediately before $v_b$ and moving $u$ immediately before $v$ is given by

$$\sigma(i) = \begin{cases} 
\sigma'(i) & (1 \leq i \leq i_u - 1) \\
u & (i = i_u) \\
\sigma'(i-2) & (i_u + 2 \leq i \leq i_v) \\
\sigma'(i) & (i_v + 1 \leq i \leq n).
\end{cases}$$

To prove $pw(\sigma) \leq pw(\sigma')$, it suffices to show that for each $i \in [1,n]$ there is a $j \in [1,n]$ such that $d_G(\sigma_i) \leq d_G(\sigma'_j)$ or $|N_G(\sigma_i) \cap N_G(\sigma'_j)| \leq |N_G(\sigma'_j) \cap N_G(\sigma_i)|$.

For each $i \in [1,i_u - 1] \cup [i_v,n]$, it holds that $N_G(\sigma_i) = N_G(\sigma'_i)$ and $d_G(\sigma_i) = d_G(\sigma'_i)$.

For $i = i_u$, since $v \in N_G(\sigma_{i_u-1})$ and $u$ is not incident to any other edge than $[u,v]$ in $G$, we have $N_G(\sigma_{i_u}) = N_G(\sigma_{i_u-1})$ and $d_G(\sigma_{i_u}) = d_G(\sigma_{i_u-1}) = d_G(\sigma'_{i_u})$.

Finally for $i \in [i_u + 1,i_v - 1]$, we show that $d_G(\sigma_i) \leq d_G(\sigma'_{i-2})$. For $i \in [i_u + 1,i_v - 1]$, we have $N_G(\sigma_{i-2}) \setminus (N_G(\sigma_{i-2}) \subseteq \{v\}$ since $v \in N_G(\sigma_{i-2})$ and $v \notin N_G(\sigma_{i})$, while we have $N_G(\sigma_{i-2}) \cap N_G(\sigma_{i+1}) \subseteq \{v\}$ since each vertex in $N_G(\sigma_i) \setminus \{v\}$ also belongs to $N_G(\sigma'_{i+1})$. From this, we can conclude that $d_G(\sigma_{i+1}) \leq d_G(\sigma'_{i+1})$. $\square$

Now we prove Theorem 9 using Lemmas 7 and 8.

**Theorem 9:** Let $G$ be an undirected graph and $v_1$ be a degree-3 vertex adjacent to a degree-1 vertex $u_1$, a degree-3 vertex $v_2$, and a vertex $v_3$ such that $v_2$ has a degree-1 neighbor $u_2$ and a neighbor $v_4 \neq v_3$ (see Fig. 12 (a)). Then the pathwidth remains unchanged after contracting the vertices $v_1$, $u_2$, and $v_2$ to $v_1$.

**Proof.** Let $n = |V(G)|$. Let $G'$ be the subgraph obtained from $G$ by contracting the vertices $v_1$, $u_2$, and $v_2$ to $v_1$ (see Fig. 12 (b)).

We first claim that $pw(G) \geq pw(G')$ holds. Since the graph $\tilde{G} = G - \{u_2\}$ clearly satisfies $pw(G) \geq pw(G')$, we show that $pw(\tilde{G}) \geq pw(G')$ holds. We choose a sequence $\tilde{\sigma} \in PW(\tilde{G})$ wherein a neighbor $v_3$ of $v_2$ appears before the other neighbor $v_4$ of $v_3$, where $\{v_3,v_4\} = |v_3,v_4| = N_\tilde{G}(v_2)$. By applying Lemma 2 with $v := v_3$, we can assume that $v_2$ appears before $v_3$ in $\sigma$. When $v_2$, $v_4$, and $v_b$ appear in this order in $\tilde{\sigma}$, $pw(\tilde{\sigma})$ remains unchanged in the graph $G'$ obtained from $G$ by adding a new edge $[v_3,v_b]$, and $pw(\tilde{\sigma}) \geq pw(G'^*)$ holds, implying that $pw(G) = pw(\tilde{\sigma}) \geq pw(G') \geq pw(G'^*)$ since $G'$ is obtained from $G^*$ by removing vertex $v_2$.

![Fig. 11](image1.png)  Illustrations for (a) a given graph $G$ and (b) a sequence $\sigma'$ and the sequence $\sigma$ constructed from $\sigma'$ by Lemma 8.

![Fig. 12](image2.png)  Illustrations for (a) a given graph $G$ and (b) the graph $G'$ reduced from $G$ by Theorem 9.
Consider the other case where $v_2$, $v_3$ and $v_6$ appear in this order in $\tilde{G}$. In this case, $\text{pw}(\tilde{G})$ remains unchanged in the graph $G'$ obtained from $G$ by removing edges $\{u_1, v_2\}$ and $\{v_2, v_6\}$ and adding a new edge $\{v_6, v_3\}$, and $\text{pw}(\tilde{G}) \geq \text{pw}(G')$ holds, implying that $\text{pw}(G) = \text{pw}(\tilde{G}) \geq \text{pw}(G') \geq \text{pw}(G)$ since $G'$ is obtained from $G$ by removing vertex $v_2$. This proves the claim.

By applying Lemma 7 with $u := u_1$, there exists a sequence $\sigma^* \in \text{PW}(G')$ in which the degree-1 vertex $u_1$ appears immediately before its unique neighbor $v_1$. If $u_1$ appears after $v_3$ and $v_4$ in $\sigma^*$, then by applying Lemma 8 with $u := u_1$ and $v := v_1$ we can obtain a sequence in $\text{PW}(G')$ such that $v_1$ appears immediately before the last vertex in $NG(v_1) \setminus \{u_1\}$ and $u_1$ appears immediately before $v_1$. Hence there is a sequence $\sigma' \in \text{PW}(G')$, where $u_1$ appears immediately before $v_1$ and $v_1$ appears before $v_3$ or $v_4$.

Let $i_1$, $i_2$, and $i_4$ denote the positions of the vertices $v_1, v_3$, and $v_4$ in the sequence $\sigma'$, respectively; i.e., $\sigma'(i_1) = v_1, \sigma'(i_2) = v_3$, and $\sigma'(i_4) = v_4$, where $i_3 < i_4$ is assumed without loss of generality. By assumption on $\sigma'$, $i_1 < i_4$. We distinguish two cases.

Case 1. $i_1 < i_2$ and at least one vertex $u \in NG(v_2) \setminus \{v_1\}$ appears before $u_1$ in $\sigma'$ (see Fig. 13 (a)): To prove that $\text{pw}(G) \leq \text{pw}(G')$, it suffices to show that $\text{pw}(\sigma^1) \leq \text{pw}(\sigma')$ holds for the sequence $\sigma'$ obtained from $\sigma^1$ by inserting the vertex $v_2$ immediately before $u_1$ and inserting the vertex $u_2$ immediately before $v_2$ in $\sigma'$. Then $\sigma^1$ is given by

$$\sigma^1(i) = \begin{cases} 
\sigma'(i) & (1 \leq i \leq i_1 - 2) \\
u_2 & (i = i_1 - 1) \\
v_1 & (i = i_1) \\
\sigma'(i - 2) & (i_1 + 1 \leq i \leq n).
\end{cases}$$

To prove $\text{pw}(\sigma^1) \leq \text{pw}(\sigma')$, we show that for each $i \in [1, n]$ there is a $j \in [1, n]$ such that $d_G(\sigma^1_i) \leq d_G(\sigma'_i)$ or $|N_G(\sigma^1_i) \setminus N_G(\sigma'_i)| \leq |N_G(\sigma'_i) \setminus N_G(\sigma^1_i)|$.

For each $i \in [1, i_1 - 2]$, it holds that $N_G(\sigma^1_i) = N_G(\sigma'_i)$ and $d_G(\sigma^1_i) = d_G(\sigma'_i)$. For $i \in [i_1, i_1 + 1]$, since at least one vertex in $NG(v_4) \setminus \{u_1\}$ appears before $u_1$, we have $N_G(\sigma^1_i) = N_G(\sigma'_i) \setminus \{v_1\}$ and $d_G(\sigma^1_i) = d_G(\sigma'_i)$. For each $i \in [i_1 + 2, n]$, we have $N_G(\sigma^1_i) = N_G(\sigma'_i) \setminus \{v_1\}$ and $d_G(\sigma^1_i) = d_G(\sigma'_i)$.

Finally we show that $d_G(\sigma^1_{i_1 - 1}) \leq d_G(\sigma'_{i_1 - 1})$. We have $N_G(\sigma^1_{i_1 - 1}) \setminus N_G(\sigma'_{i_1 - 1}) \supseteq \{v_1\}$ since $v_1 \in N_G(\sigma'_{i_1 - 1})$ and $v_1 \notin N_G(\sigma^1_{i_1 - 1})$. On the other hand, each vertex in $N_G(\sigma^1_{i_1 - 1}) \setminus \{v_1\}$ also belongs to $N_G(\sigma'_{i_1 - 1})$ since $v_2$ is not incident to any other edge than $\{u_2, v_2\}$. As a consequence, it holds $N_G(\sigma^1_{i_1 - 1}) \setminus N_G(\sigma'_{i_1 - 1}) = \{v_2\}$. From this, we can conclude that $d_G(\sigma^1_{i_1 - 1}) \leq d_G(\sigma'_{i_1 - 1})$.

Case 2. $i_3 < i_2$ or no vertex in $NG(v_4) \setminus \{u_1\}$ appears before $u_1$ in $\sigma'$ (see Fig. 13 (b)): To prove that $\text{pw}(G) \leq \text{pw}(G')$, it suffices to show that $\text{pw}(\sigma^2) \leq \text{pw}(\sigma')$ holds for the sequence $\sigma^2 = \Sigma(u_1, v_2, v_1) \subseteq \Sigma(v_1, v_2)$ obtained from $\sigma'$ by inserting the vertex $u_2$ immediately after $v_1$ and inserting the vertex $v_2$ immediately after $u_2$ in $\sigma'$. Then $\sigma^2$ is given by

$$\sigma^2(i) = \begin{cases} 
\sigma'(i) & (1 \leq i \leq i_1) \\
u_2 & (i = i_1 + 1) \\
v_1 & (i = i_1 + 2) \\
\sigma'(i - 2) & (i_1 + 3 \leq i \leq n).
\end{cases}$$

To prove $\text{pw}(\sigma^2) \leq \text{pw}(\sigma')$, we show that for each $i \in [1, n]$ there is a $j \in [1, n]$ such that $d_G(\sigma^2_i) \leq d_G(\sigma'_i)$ or $|N_G(\sigma^2_i) \setminus N_G(\sigma'_i)| \leq |N_G(\sigma'_i) \setminus N_G(\sigma^2_i)|$.

For each $i \in [1, i_1 - 1]$, it holds that $N_G(\sigma^2_i) = N_G(\sigma'_i)$ and $d_G(\sigma^2_i) = d_G(\sigma'_i)$. For $i \in [i_1, i_1 + 1]$, we have that $N_G(\sigma^2_i) = N_G(\sigma'_{i - 1})$ and $d_G(\sigma^2_i) = d_G(\sigma'_{i - 1})$. For $i \in [i_1, i_1 + 1]$, we distinguish two cases.

Case 2.1. $i_3 < i_2$ (see Fig. 13 (c)): We have $N_G(\sigma^2_{i_1 - 1}) \setminus N_G(\sigma'_i)^2 \supseteq \{v_1\}$ since $v_1 \in N_G(\sigma'_i) \setminus \{v_2\}$ and $v_1 \notin N_G(\sigma^2_i) \setminus \{v_1\}$. On the other hand, each vertex in $N_G(\sigma^2_i) \setminus \{v_2\}$ also belongs to $N_G(\sigma'_i)$ since we have $N_G(\sigma^2_i) \cap N_G(v_1) = \{v_2\}$, and hence it holds that $N_G(\sigma^2_i) \setminus N_G(\sigma'_i) = \{v_2\}$.

Case 2.2. $i_3 < i_2$ (see Fig. 13 (e)): We have $v_4 \in N_G(\sigma'_i)$ and $v_4 \notin N_G(\sigma^2_i)$ because no vertex in $NG(v_4) \setminus \{v_1\}$ appears before $u_1$, and hence it holds $N_G(\sigma'_i) \setminus N_G(\sigma^2_i) \supseteq \{v_4\}$. On the other hand, each vertex in $N_G(\sigma^2_i) \setminus \{v_2\}$ also belongs to $N_G(\sigma'_i)$ since the unique vertex $v_3$ in $(N_G(\sigma^2_i) \cap N_G(v_1)) \setminus \{v_2\}$ is in $N_G(\sigma'_i)$, and hence it holds that $N_G(\sigma^2_i) \setminus N_G(\sigma'_i) = \{v_2\}$. $\square$

Each of the above theorems provides a reduction method, which reduces a given graph that satisfies the condition of the theorem. We apply any of the reduction methods
as long as it is applicable. For example, we first choose a maximal set of degree-1 vertices that satisfy the sufficient conditions of Theorems 3, 4, and 6 in a given graph and remove the degree-1 vertices in the set from the graph. Moreover we choose a maximal set of pairs of a degree-3 vertex and a degree-1 vertex that satisfy the sufficient condition of Theorem 9 in the resulting given graph and contract the vertices in the set. We repeat the operations until there is no vertex which satisfies the sufficient conditions of Theorems 3, 4, 6, and 9. This does not change the pathwidth of the original graph while reducing the instance size.

4. Experimental Results

This section reports the result of computational experiments for testing how effectively our reduction methods can reduce the instance size of chemical graphs. To determine the pathwidth of an instance, we implemented the exact algorithm by Nagamochi [10]. The tests were carried out on a PC with CPU Intel Core i5-2500K 3.30GHz using chemical graphs generated from the chemical compounds in NCI database (http://cactus.nci.nih.gov/index.html). We conducted the following three kinds of computational experiments.

4.1 Decrease Rate of the Number of Vertices by Reductions

In the first experiment, we make a comparison of the number of vertices between the original chemical graphs and those obtained by applying our reduction methods. We first categorize the original chemical graphs in NCI database into groups by every 50 vertices and compute the distribution of the number of chemical graphs in each group. Next we compute the rate of decrease in the number of vertices in the reduced graphs. Table 1 indicates the distribution of the number of chemical graphs with 20, 30, 40, and 50 vertices in NCI database. Table 2 shows the computation time for the original chemical graphs with 20, 30, 40, and 50 vertices and that for the reduced graphs based on Theorems 3, 4, 6, and 9.

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<th>The number of vertices in chemical graphs in NCI.</th>
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<td>50</td>
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<tr>
<td>3 50</td>
<td>50</td>
</tr>
<tr>
<td>3 50</td>
<td>50</td>
</tr>
<tr>
<td>3 50</td>
<td>53</td>
</tr>
<tr>
<td>3 50</td>
<td>54</td>
</tr>
<tr>
<td>3 50</td>
<td>55</td>
</tr>
<tr>
<td>T.O.</td>
<td>50</td>
</tr>
</tbody>
</table>

Note: (1) Instances are chemical graphs in NCI; (2) “pw” is the pathwidth of a given graph; (3) “Original” is a chemical graph without any reductions; (4) “n” and “m” are the numbers of vertices and edges in a given graph; (5) “time(s)” is the CPU time in seconds; (6) “Our Algorithm” is the reduced graph based on Theorems 3, 4, 6, and 9; (7) “reduction” is the number of vertices reduced by “Our Algorithm;” (8) “m"" is the number of vertices in the reduced graph based on “Our Algorithm;” (9) “T.O.” means “time over” (time limit is set to be 300 seconds); and (10) for any real numbers x and y, let xEy denote x × 10^y.

4.2 Computation Time for Determining Pathwidth

In the second experiment, we compare the computation time to determine the pathwidth of the original chemical graphs and that of the reduced graphs by our reduction methods, where the time by our algorithm includes the preprocessing time for our reduction method. We compute the pathwidth of chemical graphs with 20, 30, 40, and 50 vertices in NCI database. Table 2 shows the computation time for the original chemical graphs with 20, 30, 40, and 50 vertices and that for the reduced graphs based on Theorems 3, 4, 6, and 9.
Table 3  The pathwidth analysis of chemical graphs with at most 50 vertices in NCI.

<table>
<thead>
<tr>
<th>Pathwidth</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>≥ 5</th>
<th>T.O.</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Graphs</td>
<td>15</td>
<td>6,685</td>
<td>152,000</td>
<td>35,185</td>
<td>212</td>
<td>50</td>
<td>1,439</td>
<td>199,509</td>
</tr>
<tr>
<td>Ratio (%)</td>
<td>0.007</td>
<td>2.83</td>
<td>76.7</td>
<td>19.6</td>
<td>0.106</td>
<td>0.029</td>
<td>0.721</td>
<td>100</td>
</tr>
</tbody>
</table>

Note: (1) “T.O.” is the number of chemical graphs with “time over” (the time limit is set to be 300 seconds); (2) “Graphs” is the number of chemical graphs with each pathwidth, where ≥ 5 means that the pathwidth is at least 5; and (3) “Ratio” is the ratio of the number of chemical graphs with each pathwidth to that of all chemical graphs.

4.3 Distribution of Pathwidth over Chemical Graphs with at Most 50 Vertices

In the third experiment, we use all 199,509 chemical graphs with at most 50 vertices in NCI database to try to compute their pathwidth under the time limit set to be 300 seconds, where we first apply our reductions to get smaller instances before we use the algorithm in [10] to compute the pathwidth, and the time includes the preprocessing time for our reduction method. Table 3 shows the distribution of the pathwidth of chemical graphs with at most 50 vertices which can be computed within 300 seconds, where we halt the computation when the pathwidth turns out to be at least 5. There are some enumol files in the NCI which indicate the corresponding chemical graphs are disconnected or consists of a single vertex and the pathwidth of such instances is 0. From this table, we observe that there are 1,439 out of 199,509 chemical graphs whose pathwidth could not be computed in 300 seconds.

5. Conclusions

In this paper, we proposed reduction methods that remove or contract some degree-1 vertices without changing the pathwidth. Our experimental results show that the average number of vertices in the chemical graphs in NCI database is reduced to 46.19% and we observe that the reduction rules of some vertices without changing the pathwidth is effective to reduce the computation time. However, there are some undirected chemical graphs with at most 50 vertices in NCI database for which the pathwidth could not be computed in 300 seconds by our implementation. One interesting future work is to devise a reduction method for digraphs.

References