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A novel method to construct NSSD molecular graphs

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Abstract: A graph is said to be NSSD (=non-singular with a singular deck) if it has no eigenvalue equal to zero, whereas all its vertex-deleted subgraphs have eigenvalues equal to zero. NSSD graphs are of importance in the theory of conductance of organic compounds. In this paper, a novel method is described for constructing NSSD molecular graphs from the commuting graphs of the H_v-group. An algorithm is presented to construct the NSSD graphs from these commuting graphs.

Keywords: H_v-group, commuting graph, non-singular graph with singular deck

MSC: 20N20

1 Introduction

Beginning in 1970s, graph spectra found noteworthy applications in chemistry, mainly in the area of molecular orbital theory [1, 2]. One of the most recent developments along these lines are the model of Fowler et al. [3], describing the electrical current created by the injection of ballistic electrons via external contacts into an unsaturated conjugated molecule. Within this model, the considered molecule is predicted to be an insulator for all single-π-electron connections, if the underlying molecular graph belongs to the class of NSSD graphs. Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. Its adjacency matrix $\mathbf{A} = (a_{ij})$ is defined so that $a_{ij} = 1$ if the vertices v_i and v_j are adjacent, and $a_{ij} = 0$ otherwise [4]. The eigenvalues of $\mathbf{A}$, denoted by $\lambda_1, \lambda_2, \dots, \lambda_n$ are said to be the eigenvalues of the graph G and to form the spectrum of G [4]. The nullity of a graph G, denoted by $\eta(G)$, is the number of eigenvalue that are equal to zero. If none of these eigenvalues is equal to zero, $i.e.$, $\eta(G) = 0$ then the graph is said to be non-singular. Otherwise, it is singular. The graph G is an NSSD graph (a **N**on-**S**ingular graph with a **S**ingular **D**eck) if it is non-singular, and if all its vertex-deleted subgraphs $G-v_i$, $i = 1, 2, \dots, n$ are singular [5–7]. The term NSSD was introduced in [8], motivated by the search for carbon molecules in the Huckel model. The first step in the history of the development of hyperstructure theory was the 8th congress of Scandinavian mathematician from 1934, when Marty [9] put forward the concept of hypergroup, analyzed its properties and showed its utility in the study of groups, algebraic functions, and rational fractions. Eventually, hyperstructure theory found applications in the field of cryptography, geometry, graphs, hypergraphs, binary relations, theory of fuzzy sets, coding theory, automata theory, etc. The correspondence between hyperstructure and binary relations is implicity

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contained in Nieminen [10] who associated hypergroups to connected simple graphs; for further work in this direction see [11–14]. In 1990, Vougiouklis introduced the concept of H_v-structure [13]. The main idea of H_v-structures is in establishing a generalization of the other algebraic hyperstructures. In fact, some axioms related to these hyperstructures are replaced by their corresponding weak axioms.

Various classes of NSSD graphs and their construction are described in recent articles [6, 15]. Some necessary and sufficient conditions are obtained for a two-vertex-deleted subgraph of an NSSD graph G to remain an NSSD by considering triangles in the inverse NSSD G^{-1} [16]. In this paper, we present a new method for constructing NSSD graphs, utilizing hyperstructure theory and commuting graphs. We also present an algorithm written in *GAP* language to construct NSSD graphs from these commuting graphs. The paper is structured as follows. In Section 2, we consider an H_v-group. We discuss its commuting graphs and establish some NSSD graphs. We present some algorithms. Using these algorithms we determine NSSD graphs. In Section 3, we find some NSSD molecular graphs from these commuting graphs. Conclusions are made in Section 4.

2 Commuting graphs on H_v-group and an algorithm to determine NSSD graphs

In this section we discuss some metric properties of commuting graphs on H_v-group. Recall that in a commuting graph, two elements are joined by an edge if they commute with each other. For further study of commuting graphs see [17–22].

Let J be a non-empty set. A hyperoperation on a non-empty set J is a mapping $\circ : J \times J \to \mathcal{P}^{\star}(J)$, where $\mathcal{P}^{\star}(J)$ denotes the set of all non-empty subsets of J. If U, V are non-empty subsets of J and $x \in J$, then we define

$$U \circ V = \bigcup_{\substack{x \in U \\ y \in V}} x \circ y, \;\; x \circ V = \{x\} \circ V \text{ and } V \circ x = V \circ \{x\} .$$

An algebraic hyperstructure $(J, \circ)$ is said to be an H_v-group if it satisfies the following properties

(1) $(J, \circ)$ is weakly associative, i.e., $s \circ (t \circ u) \cap (s \circ t) \circ u \neq \emptyset$, for all $s, t, u \in J$.
(2) $x \circ J = J = J \circ x$, for all $x \in J$.

The dihedral group of order $2n$ is given by, $D_{2n} = \langle a, b : a^n = b^2 = 1, ab = ba^{-1} \rangle$. We have constructed an H_v-group $(D_{2n}, \circ)$, where D_{2n} is the dihedral group and $\circ$ is the hyperoperation such that $\circ : D_{2n} \times D_{2n} \to \mathcal{P}^{\star}(D_{2n})$ defined by

$$x \circ y = \left\{xy, xy^{-1}, a, a^{-1}, a^2, a^{-2}, b\right\} \text{ for all } x, y \in D_{2n} , \tag{1}$$

where on the right–hand side, a, a^{-1}, a^2, a^{-2}, and b are fixed elements of D_{2n}, while x, y are any two general elements of D_{2n}. In what follows, we discuss the properties of commuting graph of this H_v-group. In the remaining part of this paper, the H_v-group $(D_{2n}, \circ)$ is denoted by $H^{\natural}$. First of all, we have to find those elements that commute with each other. The elements of D_{2n} are of the type a^i, a^ib, for $i \in \{1, 2, \ldots, n\}$. Therefore, the compositions of the elements of this H_v-group are possibly of the types $a^i \circ a^j$, $a^i \circ a^jb$, $a^ib \circ a^jb$, for $i, j \in \{1, 2, \ldots, n\}$. We first consider the compositions $a^i \circ a^j$, $a^j \circ a^i$ and find those elements that commute with each other. Note that

$$\begin{aligned} a^i \circ a^j &= \left\{a^i \cdot a^j, a^i \cdot a^{-j}, a, a^{-1}, a^2, a^{-2}, b\right\} \\ &= \left\{a^{i+j}, a^{i-j}, a, a^{-1}, a^2, a^{-2}, b\right\} , \end{aligned} \tag{2}$$

and

$$\begin{aligned} a^j \circ a^i &= \left\{a^j \cdot a^i, a^j \cdot a^{-i}, a, a^{-1}, a^2, a^{-2}, b\right\} \\ &= \left\{a^{j+i}, a^{j-i}, a, a^{-1}, a^2, a^{-2}, b\right\} . \end{aligned} \tag{3}$$

If $j = i + 1$, then the equations (2) and (3) become

$$a^i \circ a^j = \left\{a^{2i+1}, a, a^{-1}, a^2, a^{-2}, b\right\}, \tag{4}$$

$$a^j \circ a^i = \left\{a^{2i+1}, a, a^{-1}, a^2, a^{-2}, b\right\}. \tag{5}$$

Thus a^i commutes with a^{i+1} for all $i \in \{1, 2, \ldots, n\}$. Similarly, for each $i \in \{1, 2, \ldots, n\}$, we can see that a^i commutes with a^j, where $j = i+1, i-1, i+2, i-2$, and also for $j = \frac{n}{2}+i$, if n is an even integer. In an analogous manner, one can check the other compositions and find the elements that commute with each other.

Let Γ be a subset of the H_V-group $(D_{2n}, \circ)$. The vertices of the commuting graph are the elements of Γ, where any two different vertices $s, t \in \Gamma$ are joined by an edge if $s \circ t = t \circ s$. The degree $deg_G(s)$ of a vertex $s \in V(G)$ of a graph G is the number of first neighbors of s. The following two theorems explain about the degree of each vertex in the commuting graph $G = C(H^\natural, H^\natural)$.

Theorem 1. *Let $H^\natural = (D_{2n}, \circ)$ be an H_V-group for an even integer $n \geq 6$ and $G = C(H^\natural, H^\natural)$ be a commuting graph. Then*

(1) $\deg_G(a^i) = \begin{cases} 6 & \text{if } i \neq n, n/2, \\ n+5 & \text{if } i = n, n/2. \end{cases}$

(2) $\deg_G(a^i b) = \begin{cases} 8 & \text{if } i \neq n, n/2, \\ 7 & \text{if } i = n, n/2. \end{cases}$

Proof. (1) For an even integer $n \geq 6$, each a^i commutes with $a^{i+1}, a^{i-1}, a^{i+2}, a^{i-2}, a^{\frac{n}{2}+i}$. Also a^i commutes with $a^i b$ if $i \neq n, \frac{n}{2}$ whereas $e, a^{\frac{n}{2}}$ commute with $a^i b$ for all $i \in \{1, 2, \ldots, n\}$.

(2) Each $a^i b$ commutes with $a^{i+1}b, a^{i-1}b, a^{i+2}b, a^{i-2}b, a^{\frac{n}{2}+i}b, a^i, e$, and $a^{\frac{n}{2}}$. Therefore, $\deg_G(a^i b) = 8$ if $i \neq n, \frac{n}{2}$ and $\deg_G(a^i b) = 7$ if $i = n, \frac{n}{2}$. □

Theorem 2. *Let $H^\natural = (D_{2n}, \circ)$ be an H_V-group for an odd integer $n \geq 5$ and $G = C(H^\natural, H^\natural)$ be a commuting graph. Then*

(1) $\deg_G(a^i) = \begin{cases} 5 & \text{if } i \neq n, \\ n+4 & \text{if } i = n. \end{cases}$

(2) $\deg_G(a^i b) = \begin{cases} 6 & \text{if } i \neq n, \\ 5 & \text{if } i = n. \end{cases}$

Proof. Relations (1) and (2) follow by straightforward calculations. □

Now, we present some algorithms to construct NSSD graphs from these commuting graphs. These algorithms are written in the *GAP* language.

Algorithm 1 Dihedral Group

Input : n

Output : Dihedral group of order $2n$

1. f := FreeGroup("a", "b");
2. g := $f/[f.1^n, f.2^2, (f.1 * f.2)^2]$;
3. Unbind(a);
4. a := g.1; b := g.2; assign variables

Algorithm (1) gives us dihedral group of order $2n$. Here in this algorithm we have to give the input value of n and we get the dihedral group of order $2n$. Now, we give an algorithm to define the hyperoperation given in Eq. (1). This Algorithm (2) gives us the product of two elements under the hyperopeation defined in Eq. (1).

Algorithm 2 Hyperoperation

Input : two elements $x, y \in g$

Output : The image of (x,y) under the hyperoperation " $\circ$ ", $i.e.$, $x \circ y$.

```
H := The function of (x, y)
Define the local variable " ∘ "
if x in g and y in g then
∘ := The hyperoperation defined as in Eq. (1);
fi;     return ∘;     end;
```

Algorithm 3 Adjacency Matrix

Input : Any subset U of this H_v-group

Output : The adjacency matrix for the commuting graph of U.

```
T := function(U)
local S, M, n, i, j, k;
n is the order of the subset U;
M is the identity matrix of order n;
for i in [1..n-1] do
for j in [i+1..n] do
if the elements at ith and jth position in U commutes then
M[i][j] := 1;
M[j][i] := 1;     fi;
od;     od;
for k in [1..n] do
M[k][k] := 0;
od;     return M;     end;
```

Algorithm (3) presents the pseudo-code for the adjacency matrix of a commuting graph $G = C(H^\natural, U)$. Here subset U is the input value and the output value is the adjacency matrix for the commuting graph of U. Now, the following algorithm (4) shows that wether the commuting graph is NSSD graph or not.

Algorithm (4) is the pseudo-code for NSSD graph. In this algorithm the input value is the adjacency matrix of a commuting graph and it returns true if the corresponding graph is NSSD graph otherwise it returns false. Using these algorithms present in this paper, we can find the NSSD graphs. For example, if we consider the dihedral group for an integer $n = 4$ and define the hyperoperation using algorithm (2). Now, consider the subset $U = \{a, a^3, b, ab\}$ of the H_v-group $H^\natural = (D_8, \circ)$ and find the adjacency matrix for the commuting graph $G = C(H^\natural, U)$ using algorithm (3), we get

$$M = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}.$$

When we use algorithm (4) to check wether it is NSSD graph or not, it returns "$true$". The corresponding graph is depicted in Figure 1.

Now, consider the H_v-group $H^\natural = (D_{2n}, \circ)$, for an integer $n \geq 2$. In Table 1, we present the number of NSSD graphs, obtained from the commuting graphs of the H_v-group $H^\natural = (D_{2n}, \circ)$, with the help of Algorithm 4.

Algorithm 4 NSSD Graph

Input : An adjacency matrix

Output : Is corresponding graph NSSD graph or not.

```
RemRowCol := function(M,c)
local A, i;    A := StructuralCopy(M);
for i in [1..Length(A)] do
Remove ith Row and ith Column of matrix M;
od;    return A;    end;
IsNSSD := function(M)    local A, eig, eigsp, c, i, j;
"c" is the counter;
"eig" are the Eigenvalues of M;
if 0 is an eigenvalue of M then    return false;
else c := c+1;    fi;
for i in [1..Length(M)] do
"A" is the matrix obtained by deleting ith Row and ith Column of M;
"eigsp" are the Eigenvalues of A;
if 0 is an eigenvalue of A then    c := c+1;    fi;
od;    if c=Length(M)+1 then
return true;    else return false;
fi;    end;
```

Table 1: Number of NSSD graphs for different values of n.

n	Order of graph	No. of subsets who's commuting graph is NSSD	No. of NSSD graphs
2	2	6	1
3	2	11	1
	4	2	1
4	2	22	1
	4	5	2
5	2	29	1
	4	54	2
6	2	46	1
	4	84	2
7	2	41	1
	4	262	2
	6	374	7
	8	130	15
	10	4	1
8	2	62	1
	4	409	2
	6	416	7
	8	80	11
	10	4	1

Figure 1: NSSD graphs.

By using Table 1, we calculate the number of NSSD graphs of different orders for different values of n. In addition, we compute the number of subsets, who's commuting graph is NSSD. Similarly, from these commuting graphs one can find more NSSD graphs of higher order by choosing greater value of n. Now, we present some NSSD molecular graphs obtained from these commuting graphs.

3 NSSD molecular graphs

As mentioned in previous section, NSSD graphs are encountered within a theory of conductivity of organic substances [3, 6]. In view of this, it is of particular interest to design NSSD graph that are molecular graphs, i.e., graphs whose vertices and edges pertain to carbon atoms and carbon–carbon bonds, respectively [1, 23, 24]. Hyperstructure theory has been earlier much used in the chemistry, see [25–28]. In this section our main purpose is to construct NSSD molecular graphs from the above described commuting graphs. The following theorems related to construct NSSD graphs from the commuting graphs of a non-abelian group Ω.

Theorem 3. *Let $G_1 = C(\Omega, U)$ and $G_2 = C(\Omega, V)$ be two commuting graphs, such that G_2 is an empty graph and $|G_1| = |G_2|$. If each element of V commutes with exactly one element of U, then the commuting graph $G' = C(\Omega, U \cup V)$ is an NSSD graph.*

Proof. Since each element of the subset V commutes with exactly one element of U and G_2 is an empty graph, it follows that each vertex in V is a pendent vertex of the commuting graph G'. If v is a pendent vertex of a graph G', adjacent to the vertex u, then [29, 30]

$$\eta(G') = \eta(G' - v - u). \tag{6}$$

If we apply Eq. (6) to each but one pendent vertex of the graph G', then we get a connected graph with two vertices. Therefore, nullity of the graph G' is zero. So G' is a non-singular graph.

Now, consider the vertex deleted subgraph $G' - x$. If $x \in V$, then x is a pendent vertex, so applying the Eq. (6) to each pendent vertex of the graph $G' - x$, we obtain a graph with single vertex. Therefore, the nullity of $G' - x$ is 1. If $x \in U$, then there exists an isolated vertex of the graph $G' - x$, Therefore, the nullity of $G' - x$ is 1. Hence G' is a non-singular graph with a singular deck. □

Theorem 4. *If the commuting graphs $G_1 = C(\Omega, U)$ and $G_2 = C(\Omega, V)$ are two NSSD graphs, such that there exists exactly one element $u \in U$ that commutes with exactly one element $v \in V$, then the commuting graph $G' = C(\Omega, T)$ is an NSSD graph, where $T = U \cup V$.*

Proof. Clearly, G' is obtained by joining a vertex $u \in G_1$ with a vertex $v \in G_2$. The following relation gives the characteristic polynomial [23, 24]

$$P(G', \lambda) = P(G_1, \lambda)P(G_2, \lambda) - P(G_1 - u, \lambda)P(G_2 - v, \lambda). \tag{7}$$

Both graphs G_1 and G_2 are NSSD graphs, so they are non-singular, i.e., $P(G_1, 0) \neq 0$, $P(G_2, 0) \neq 0$. Moreover, each vertex deleted subgraph is singular, so $P(G_1 - u, 0) = 0$ and $P(G_2 - v, 0) = 0$. Consequently, we get $P(G', 0) \neq 0$, and this implies that G' is non-singular. Now, consider the vertex deleted subgraph $G' - x$. If $x = u$, then $G' - u$ is singular, because $G_1 - u$ is singular. Similarly, if $x = v$, then the subgraph $G' - v$ is singular. Let $x \in T$, such that $x \neq u, v$. Assume that $x \in U$, then from Eq. (7)

$$P(G' - x, \lambda) = P(G_1 - x, \lambda)P(G_2, \lambda) - P(G_1 - x - u), \lambda)P(G_2 - v, \lambda).$$

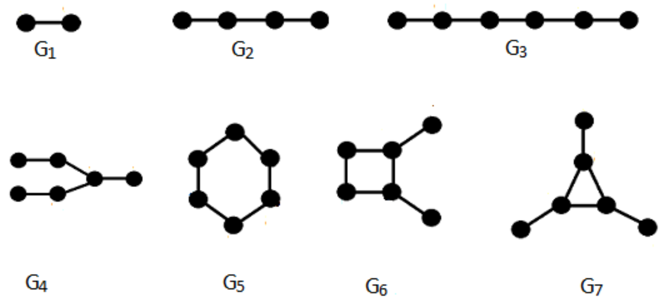

Figure 2: NSSD graphs with 2, 4, and 6 vertices.

We have $P(G_1 - x, 0) = 0$, because G_1 is an NSSD graph. Therefore, $P(G' - x, 0) = 0$, which shows that the subgraph $G' - x$ is singular. Hence G' is an NSSD graph. □

Now, using these results and the algorithms presented in section (2), we construct the NSSD molecular graphs from the commuting graphs of the H_v-group $H^\natural$. Consider the H_v-group $H^\natural = (D_{2n}, \circ)$, where D_{2n} is the dihedral group for $n = 16$ and $\circ$ is the hyperoperation defined as in Eq. (1). In addition, define the following sets of vertices for which the commuting graphs give NSSD molecular graphs with 2, 4, and 6 vertices:

$$\begin{aligned}
\Gamma_1 &= \left\{a, a^3\right\}, \\
\Gamma_2 &= \left\{a^5, a^7, a^8, a^{10}\right\}, \\
\Gamma_3 &= \left\{a, a^3, a^5, a^7, a^8, a^{10}\right\}, \\
\Gamma_4 &= \left\{a, a^3, a^5, a^6, a^5b, a^7b\right\}, \\
\Gamma_5 &= \left\{a^2, a^3, a^5, a^7, a^9, a^{10}\right\}, \\
\Gamma_6 &= \left\{a, a^2, a^{10}, ab, a^2b, a^4b\right\}, \\
\Gamma_7 &= \left\{a, a^2, a^3, a^5, a^{15}, a^2b\right\}.
\end{aligned}$$

Here the commuting graphs $G_i = C(H^\natural, \Gamma_i)$, $i = 1, 2, \ldots, 7$, result the NSSD graphs given in Figure 2.

For instance, we specify the construction of the graph G_3, whose vertex set is Γ_3. Since the graphs G_1, G_2 are NSSD and only one element $a^3 \in \Gamma_1$ commutes with exactly one element $a^5 \in \Gamma_2$. So, the commuting graph corresponding to $\Gamma_3 = \Gamma_1 \cup \Gamma_2$ is NSSD. Thus, the graph G_3 is the path of the form $a - a^3 - a^5 - a^7 - a^8 - a^{10}$. In an analogous manner, one can establish the structure of the remaining graphs from the set $\{\Gamma_i \mid i = 1, 2, \ldots, 7\}$. One can determine these graphs using algorithm (4). We now list the sets of vertices for which the commuting graphs yield NSSD graphs with 8 vertices.

$$\begin{aligned}
\Gamma_8 &= \left\{a, a^2, a^3, a^5, a^{15}, a^2b, a^5b, a^7b\right\}, \\
\Gamma_9 &= \left\{a, a^3, a^5, a^7, a^9, a^{10}, a^3b, a^5b\right\}, \\
\Gamma_{10} &= \left\{a^5, a^6, a^5b, a^6b, a^{13}b, a^{14}b, a^{12}b, a^{12}\right\}, \\
\Gamma_{11} &= \left\{a^2, a^3, a^5, a^7, a^9, a^{10}, a^2b, a^7b\right\}, \\
\Gamma_{12} &= \left\{a, a^3, a^5, a^7, a^9, a^{10}, ab, a^7b\right\}.
\end{aligned}$$

For these sets of vertices the commuting graphs $G_i = C(H^\natural, \Gamma_i)$, $i = 8, 9, \ldots, 12$, are the NSSD graphs depicted in Figure 3.

For instance, $\Gamma_8 = \left\{a, a^2, a^3, a^5, a^{15}, a^2b, a^5b, a^7b\right\}$ is the set of vertices for the commuting graph G_8. Since the commuting graphs of the subsets Γ_7 and $\Gamma' = \{a^5b, a^7b\}$ NSSD. Also there exists only one element

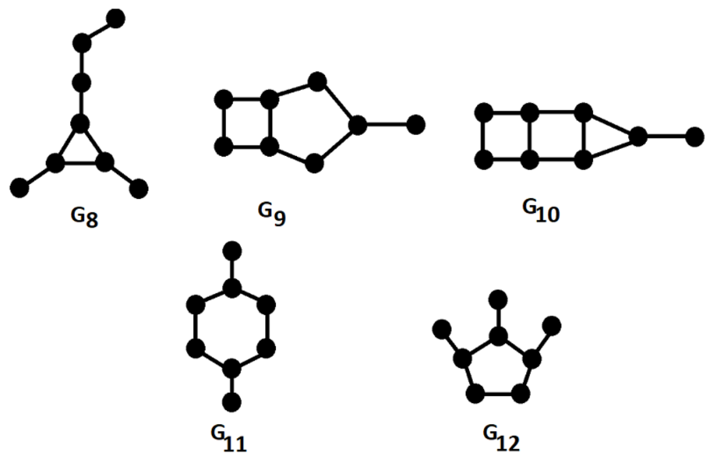

Figure 3: NSSD graphs with 8 vertices.

$a^5b \in \Gamma'$ that commutes with only one element $a^2b \in \Gamma_7$. Thus the commuting graph of the subset $\Gamma_8 = \Gamma_7 \cup \Gamma'$ is NSSD. These structural features fully determine the NSSD graph G_8. The other graphs can be analysed and determined in a similar manner.

The following sets of vertices pertain to commuting graphs resulting in NSSD molecular graphs with 10 vertices.

$$\Gamma_{13} = \left\{a, a^3, a^5, a^7, a^9, a^{10}, ab, a^5b, a^7b, a^{13}b\right\},$$
$$\Gamma_{14} = \left\{a, a^3, a^5, a^7, a^9, a^{10}, a^3b, a^5b, a^{11}b, a^{13}b\right\},$$
$$\Gamma_{15} = \left\{a^2, a^3, a^5, a^6, a^7, a^9, a^{10}, a^2b, a^3b, a^{14}\right\},$$
$$\Gamma_{16} = \left\{a^5, a^6, a^7, a^9, a^{12}, a^5b, a^6b, a^{13}b, a^{14}b, a^{12}b\right\},$$
$$\Gamma_{17} = \left\{a^2, a^3, a^5, a^7, a^9, a^{10}, a^{12}, a^{13}, a^{15}, a^{12}b\right\},$$
$$\Gamma_{18} = \left\{a, a^3, a^4, a^6, a^7, a^9, a^{11}, a^{13}, a^{14}, a^{14}b\right\}.$$

Consider now the H_v-group $H^\natural = (D_{2n}, \circ)$, where D_{2n} is the dihedral group for $n = 20$ and $\circ$ is the hyperoperation, and define the following set of vertices of this H_v-group for which the commuting graphs give NSSD graphs with 10 vertices.

$$\Gamma_{19} = \left\{a^3, a^5, a^7, a^9, a^{11}, a^{12}, a^{14}, a^{15}, a^9b, a^{11}b\right\},$$
$$\Gamma_{20} = \left\{a, a^2, a^3, a^5, a^6, a^7, a^9, a^{12}, ab, a^6b\right\},$$
$$\Gamma_{21} = \left\{a, a^2, a^3, a^5, a^6, a^8, a^{19}, a^2b, a^5b, a^6b\right\},$$
$$\Gamma_{22} = \left\{a, a^2, a^4, a^5, a^{11}, a^2b, a^3b, a^5b, a^{11}b, a^{12}b\right\},$$
$$\Gamma_{23} = \left\{a^3, a^5, a^7, a^9, a^{11}, a^{12}, a^{14}, a^{15}, a^{19}, a^7b\right\},$$
$$\Gamma_{24} = \left\{a^3, a^5, a^7, a^9, a^{11}, a^{12}, a^{14}, a^{15}, a^7b, , a^{12}b\right\}.$$

The commuting graphs $G_i = C(H^\natural, \Gamma_i)$, $i = 13, 14, \ldots, 24$, lead to the NSSD graphs depicted in Figures 4 and 5.

In order to construct NSSD graphs with 12 vertices from these commuting graphs, consider the H_v-group $H^\natural = (D_{2n}, \circ)$, for $n = 20$ and define the following sets of vertices.

$$\Gamma_{25} = \left\{a, a^2, a^3, a^5, a^{19}, a^2b, a^5b, a^7b, a^9b, a^{11}b, a^{13}b, a^{14}b\right\},$$

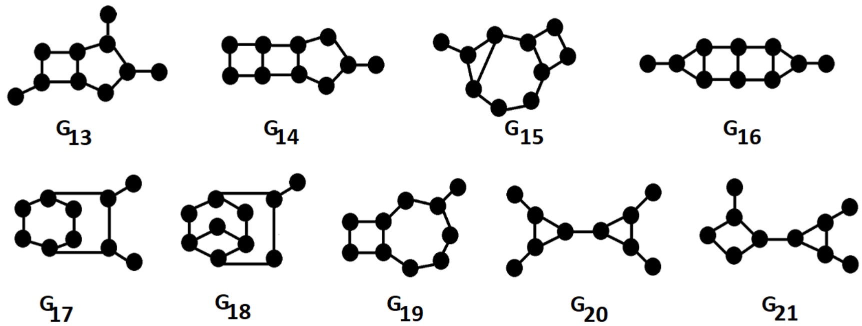

Figure 4: NSSD graphs with 10 vertices.

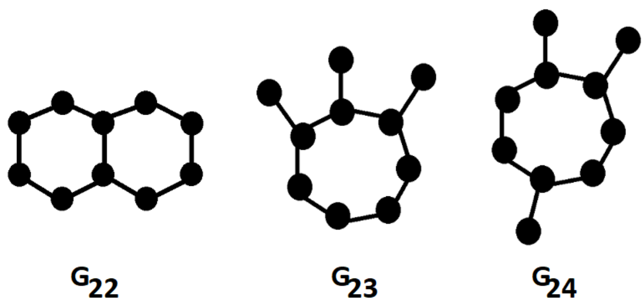

Figure 5: NSSD graphs with 10 vertices.

$$\Gamma_{26} = \left\{a, a^2, a^3, a^5, a^6, a^8, a^{16}, a^{19}, a^2b, a^8b, a^9b, a^{11}b\right\},$$
$$\Gamma_{27} = \left\{a, a^2, a^3, a^5, a^6, a^8, a^{16}, a^{19}, a^2b, a^8b, a^9b, a^{16}b\right\},$$
$$\Gamma_{28} = \left\{a, a^2, a^3, a^5, a^6, a^8, a^{19}, a^2b, a^8b, a^9b, a^{11}b, a^{18}b\right\},$$
$$\Gamma_{29} = \left\{a, a^2, a^3, a^5, a^6, a^{19}, a^2b, a^6b, a^8b, a^9b, a^{16}b, a^{17}b\right\},$$
$$\Gamma_{30} = \left\{a, a^2, a^3, a^5, a^6, a^8, a^{19}, a^2b, a^6b, a^7b, a^9b, a^{16}b\right\},$$
$$\Gamma_{31} = \left\{a, a^2, a^3, a^5, a^6, a^{15}, a^{19}, a^2b, a^6b, a^8b, a^9b, a^{15}b\right\},$$
$$\Gamma_{32} = \left\{a, a^2, a^3, a^5, a^7, a^{19}, a^2b, a^4b, a^7b, a^9b, a^{11}b, a^{14}b\right\},$$
$$\Gamma_{33} = \left\{a, a^2, a^3, a^5, a^6, a^8, a^{15}, a^{19}, a^2b, a^6b, a^7b, a^{15}b\right\},$$
$$\Gamma_{34} = \left\{a, a^2, a^3, a^5, a^7, a^{15}, a^{16}, a^{19}, a^2b, a^4b, a^7b, a^{14}b\right\},$$
$$\Gamma_{35} = \left\{a, a^2, a^3, a^5, a^7, a^{18}, a^{19}, a^2b, a^4b, a^7b, a^{14}b, a^{18}b\right\}$$
$$\Gamma_{36} = \left\{a, a^2, a^3, a^5, a^6, a^{11}, a^{17}, a^2b, a^6b, a^7b, a^8b, a^{10}b\right\},$$
$$\Gamma_{37} = \left\{a, a^2, a^3, a^5, a^7, a^8, a^{11}, a^{17}, a^2b, a^8b, a^{17}b, a^{18}b\right\},$$
$$\Gamma_{38} = \left\{a, a^2, a^3, a^5, a^7, a^8, a^{19}, a^2b, a^7b, a^8b, a^{10}b, a^{17}b\right\},$$
$$\Gamma_{39} = \left\{a^2, a^5, a^6, a^7, a^9, a^{11}, a^{12}, a^{15}, a^2b, a^6b, a^{12}b, a^{14}b\right\}.$$

The commuting graphs $G_i = C(H^{\natural}, \Gamma_i)$, $i = 25, 26, \ldots, 39$, yield the NSSD graphs with 12 vertices depicted in Figures 6 and 7.

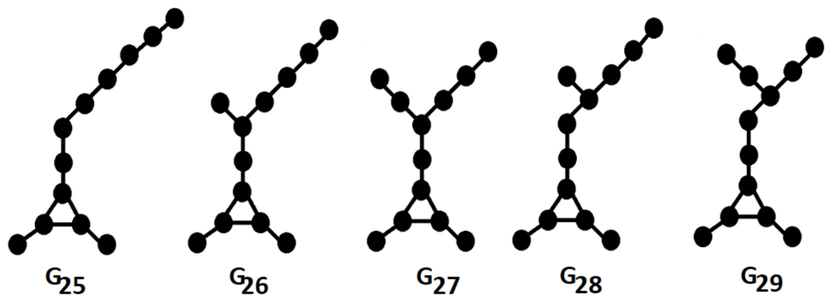

Figure 6: NSSD graphs with 12 vertices.

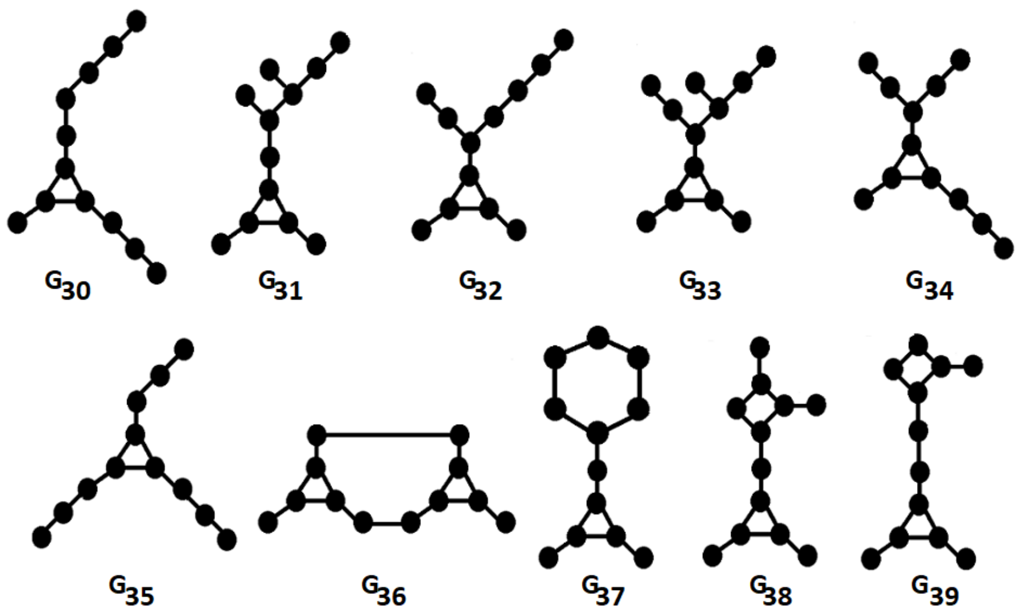

Figure 7: NSSD graphs with 12 vertices.

At the end, consider the H_v-group $H^\natural = (D_{2n}, \circ)$, for $n = 20$, and define the following sets of vertices to construct the NSSD graphs with 12 and 14 vertices.

$$\begin{aligned}
\Gamma_{40} &= \left\{a, a^2, a^3, a^5, a^8, a^{11}, a^2b, a^7b, a^8b, a^9b, a^{11}b, a^{17}b\right\},\\
\Gamma_{41} &= \left\{a^3, a^5, a^7, a^9, a^{11}, a^{12}, a^{14}, a^{15}, a^{19}, a^7b, a^{11}b, a^{15}b\right\},\\
\Gamma_{42} &= \left\{a^2, a^3, a^7, a^8, a^{12}, a^{13}, a^7b, a^8b, a^{12}b, a^{13}b, a^{14}b, a^{16}b, a^{17}b, a^{18}b\right\}.
\end{aligned}$$

Also, consider the H_v-group $H^\natural = (D_{2n}, \circ)$, for $n = 24$ and define the following set of vertices to construct an NSSD graph with 16 vertices:

$$\Gamma_{43} = \left\{a^3, a^4, a^9, a^{10}, a^{15}, a^{16}, a^{17}, a^3b, a^4b, a^9b, a^{10}b, a^{17}b, a^{18}b, a^{20}b, a^{21}b, a^{22}b\right\}$$

The commuting graphs $G_i = C(H^\natural, \Gamma_i)$, $i = 40, \ldots, 43$, are the NSSD molecular graphs with 12, 14, and 16 vertices, given in Figure 8.

Remark 1. *There are a lot of NSSD graphs but we have shown only a few here. One can find NSSD graphs of higher order by choosing high values of n.*

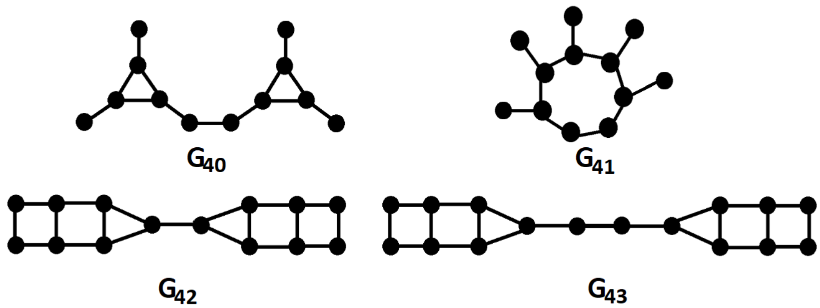

Figure 8: NSSD graphs with 12, 14, and 16 vertices.

4 Conclusion

In this article we have defined an H_v-group and discussed its commuting graph. We have constructed NSSD molecular graphs from the commuting graph of this H_v-group. Also we have defined an algorithm that can construct NSSD graphs. In this paper, we have considered a hyperoperation on dihedral group given in Eq. (1). For feature work in this direction on can use another hyperoperation and determine different NSSD graphs.

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