Signed Nut Graphs

Nino Bašić\textsuperscript{1,2,3}, Patrick W. Fowler\textsuperscript{4}, Tomaž Pisanski\textsuperscript{1,2,3,5}, and Irene Sciriha\textsuperscript{6}

\textsuperscript{1}FAMNIT, University of Primorska, Koper, Slovenia
\textsuperscript{2}IAM, University of Primorska, Koper, Slovenia
\textsuperscript{3}Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia
\textsuperscript{4}Department of Chemistry, University of Sheffield, Sheffield S3 7HF, UK
\textsuperscript{5}Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia
\textsuperscript{6}Department of Mathematics, Faculty of Science, University of Malta, Msida, Malta

September 22, 2020

Abstract

Orders for which regular nut graphs exist have been determined recently for the degrees up to 11. In this paper we extend the notion of nut graphs to signed graphs, i.e. graphs with edges weighted either by $+1$ or $-1$. A signed graph is proper if it is not equivalent to an unsigned graph under an intuitive operation of sign switching, otherwise it is traditional. By including signed nut graphs, we find all pairs $(\rho, n)$ for which a $\rho$-regular nut graph of order $n$ exists with $\rho \leq 11$. In addition, we show how a literature construction for obtaining larger nut graphs can be extended to signed graphs, giving a construction for both proper and traditional $\rho$-regular signed nut graphs.

Keywords: Signed graph, nut graph, singular graph, graph spectrum, Fowler construction.

Math. Subj. Class. (2020): 05C92, 05C50, 05C22

1 Introduction and motivation

Spectral graph theory is an important branch of discrete mathematics that links graphs to linear algebra. Its applications are numerous. For instance, in Chemistry the Hückel molecular orbital theory of conjugated $\pi$ systems \cite{25} is essentially an exercise in applied spectral graph theory \cite{26}. Unlike the adjacency matrix itself, the spectrum of the adjacency matrix is an invariant. Singular graphs, i.e. graphs that have a zero eigenvalue of the adjacency matrix, have been studied extensively. One subclass of singular graphs, known as nut graphs, is of particular interest. A nut graph is a singular graph whose 0-1 adjacency matrix has a one-dimensional kernel (nullity $\eta = 1$) and has a full corresponding eigenvector. Some properties of nut graphs are easily proved. For instance, nut graphs are connected, non-bipartite, and have no vertices of degree one \cite{24}. It is conventional to require that a nut graph has $n \geq 2$ vertices, although some authors consider $K_1$ as the trivial nut. There exist numerous construction rules for making larger nut graphs from smaller \cite{24}. 

1
In this contribution we will consider signed graphs, i.e. graphs with edge weights drawn from \{-1, 1\} and ask whether they can also be nut graphs. Although the problem may appear to be purely mathematical, we were driven to study it by the chemical interest arising from the study of specific properties of conjugated \(\pi\) systems. For example, in electronic structure theory, nut graphs have distributed radical reactivity, since occupation by a single electron of the molecular orbital corresponding to the kernel eigenvector leads to spin density on all carbon centres [23]. In the context of theories of molecular conduction, nut graphs have a unique status as the strong omni-conductors of nullity 1 [8]. Möbius carbon networks, representable by signed graphs, obey different electron counting rules from those of unweighted Hückel networks [6].

For general discussion of signed graphs the reader is referred to recent papers [1, 12] which set out notation and basic properties. For nut graphs, several useful papers are available, for instance [9, 17, 19, 20]. Recently the problem of existence of regular nut graphs was posed, and solved for cubic and quartic graphs [10]. Later, it was solved for degrees \(\rho\), \(\rho \leq 11\) [7]. In this paper we carry the problem of the existence of regular nut graphs over from ordinary graphs to signed graphs. We are able to characterise all cases (\(\rho \leq 11\)) for which a \(\rho\)-regular nut graph of order \(n\) (either signed or unsigned) exists. In addition, we describe a construction, based on work on unsigned nut graphs [7, 10], which produces larger signed nut graphs from smaller.

## 2 Signed graphs, nut graphs and signed nut graphs

### 2.1 Signed graphs

A **signed graph** \(\Gamma = (G, \Sigma)\) is a graph \(G = (V, E)\) with a distinguished subset of edges \(\Sigma \subseteq E\) that we shall call **negative edges**, or more informally Möbius edges. Equivalently, we may consider the signed graph \((G, \sigma)\) to be a graph endowed with a mapping \(\sigma : E \to \{-1, +1\}\) where \(\Sigma = \{e \in E \mid \sigma(e) = -1\}\). The adjacency matrix \(A(\Gamma)\) of a signed graph is a symmetric matrix obtained from the adjacency matrix \(A(G)\) of the underlying graph \(G\) by replacing 1 by \(-1\) for entries \(a_{uv}\) where \(u\) is connected with \(v\) by a negative edge.

Symmetries (automorphisms) of a signed graph \(\Gamma = (G, \Sigma)\) are also symmetries of the underlying graph \(G\). They preserve edge weights:

\[
\text{Aut} \Gamma = \{\alpha \in \text{Aut} G \mid \forall e = uv \in E(G) : e \in \Sigma \iff \alpha(e) = \alpha(u)\alpha(v) \in \Sigma\}.
\]

Hence, the automorphism group \(\text{Aut} \Gamma\) of a signed graph \(\Gamma\) is a subgroup of the automorphism group \(\text{Aut} G\) of the underlying graph \(G\).

### 2.2 Singular graphs, core graphs and nut graphs

A graph that has zero as an eigenvalue is called a **singular graph**, i.e. a graph is singular if and only if its adjacency matrix has a non-trivial kernel. The dimension of the kernel is the **nullity**. An eigenvector \(x\) can be viewed as a weighting of vertices, i.e. a mapping \(x : V \to \mathbb{R}\). A vector \(x\) belongs to the kernel, \(\ker A\), which is denoted by \(x \in \ker A\), if and only if for each vertex \(v\) the sum of entries on the neighbours \(N_G(v)\) equals 0:

\[
\sum_{u \in N_G(v)} x(u) = 0. \tag{1}
\]
The equation (1) is called the local condition. The support, \( \text{supp} \ x \), of a kernel eigenvector \( x \in \ker A \) is the subset of \( V \) at which \( x \) attains non-zero values:

\[
\text{supp} \ x = \{ v \in V \mid x(v) \neq 0 \}.
\]

If \( \text{supp} \ x = V \), we say that vector \( x \) is full. Define \( \text{supp ker} \ A \) as follows:

\[
\text{supp ker} \ A = \bigcup_{x \in \ker A} \text{supp} \ x.
\]

A singular graph \( G \) is a core graph if \( \text{supp ker} \ A = V \). A core graph of nullity 1 is called a nut graph. Although the kernel of a core graph may have a basis that has no full vectors, there exists a basis with all vectors being full.

Proposition 1. Each core graph admits a kernel basis that contains only full vectors.

Proof. Let \( V(G) = \{1, \ldots, n\} \) and let \( x_1, \ldots, x_\eta \) be an arbitrary kernel basis. Let \( \iota \) be the smallest integer (i.e. vertex label), such that at least one of the entries \( x_1(\iota), \ldots, x_\eta(\iota) \) is zero, and let \( x_\ell(\iota) \) be one of those entries. As \( G \) is a core graph, at least one of the entries \( x_1(\iota), \ldots, x_\eta(\iota) \) is non-zero; let us denote the first such encountered entry by \( x_k(\iota) \). We can replace vector \( x_\ell \) by \( x_\ell + \alpha x_k \), where \( \alpha > 0 \). If we pick \( \alpha \) large enough, i.e. if

\[
\alpha > \max \left\{ \frac{|x_\ell(i)|}{|x_k(i)|} \mid i \neq \iota, x_k(i) \neq 0 \right\},
\]

then \( x_\ell(i) + \alpha x_k(i) \) will be non-zero for all \( i \). No new zero entries were created in the replacement process and at least one zero was eliminated. We repeat this process until no more zeros remain.

Corollary 2. Each core graph admits a kernel basis that contains only full vectors with integer entries.

Proof. An integer basis always exists for an integer eigenvalue. The replacement process described in the proof of Proposition 1 will keep all entries integer if we choose an integer for the value of \( \alpha \) at each step.

2.3 Switching equivalence of signed graphs

Let \( \Gamma = (G, \Sigma) \) be a signed graph over \( G = (V, E) \) and let \( U \subseteq V(G) \) be a set of its vertices. A switching at \( U \) is an operation that transforms \( \Gamma = (G, \Sigma) \) to a signed graph \( \Gamma^U = (G, \Sigma \nabla \partial U) \) where \( \nabla \) denotes symmetric difference of sets and

\[
\partial U = \{uv \in E \mid u \in U, v \notin U\}.
\]

Note that \( \partial U = \partial(V(G) \setminus U) \), \( \Gamma^U = \Gamma^{V(G) \setminus U} \) and \( (\Gamma^U)^U = \Gamma \). In fact, switching is an equivalence relation among the signed graphs with the same underlying graph. Any graph \( G \) can be regarded as a traditional signed graph \( \Gamma = (G, \emptyset) \). We extend this definition. Any signed graph is a traditional signed graph if it is switching equivalent to \( \Gamma = (G, \emptyset) \), otherwise it is called a proper signed graph.

As observed, for instance in [1], switching has an obvious linear algebraic description.
Proposition 3 (II). Let $A(\Gamma)$ be the adjacency matrix of signed graph $\Gamma$ and $A(\Gamma^U)$ be the corresponding adjacency matrix of the signed graph switched at $U$. Let $S = \text{diag}(s_1, s_2, \ldots, s_n)$ be the diagonal matrix with $s_i = -1$ if $v_i \in U$ and $s_i = 1$ elsewhere. Then

$$A(\Gamma^U) = SA(\Gamma)S.$$ 

Since $S^T = S^{-1} = S$ we also have:

$$A(\Gamma) = SA(\Gamma^U)S.$$ 

Theorem 4. Let $G$ be a connected graph on $n$ vertices and $m$ edges. There are $2^m$ signed graphs over $G$, there are $2^m - n + 1$ switching equivalence classes, and each class has $2^{n-1}$ signed graphs.

Proof. We divide our argument into four steps.

Step (a): For a given connected graph $G$ (and a spanning tree $T$) there are $2^m$ different signed graphs. Indeed, we may choose any subset $\Sigma$ of edges $E$ and make all edges in $\Sigma$ negative. Some of the signed graphs will have all edges of $T$ positive, while others will have some edges of $T$ negative.

Step (b): Among the $2^m$ signed graphs over $G$ exactly $2^m - n + 1$ will have all edges of $T$ positive. Indeed, while fixing $(n - 1)$ edges of $T$ positive, any selection of the remaining $(m - n + 1)$ non-tree edges determines $\Sigma$. Such a selection can be done in $2^m - n + 1$ ways.

Hence, Step (a) gives the total number of signed graphs while Step (b) gives the number of signed graphs having all edges of $T$ positive.

Step (c): There are $2^{n-1}$ switchings available. Namely, any switching is determined by a pair $(U, V \setminus U)$, but $(U, V \setminus U)$ is the same switching as $(V \setminus U, U)$. Hence we have to divide $2^n$, the number of subsets of $V$, by 2. Thus, each switching equivalence class contains $2^{n-1}$ signed graphs. Dividing the total number of signed graphs $2^m$ by the cardinality of each switching class $2^{n-1}$ we obtain the number of different switching equivalence classes: $2^{m-n+1}$.

Every switching equivalence class of signed graphs over $G$ contains exactly one signed graph with all edges of $T$ positive. Recall that in any tree there is a unique path between any two vertices. Choose any vertex $w$ from $V$. Let $U$ be the set of vertices $v$ in $T$ that have an even number of negative edges on the unique $w - v$ path of $T$. Then $V \setminus U$ contains the vertices $v$ that have an odd number of negative edges on the path from $w$ to $v$ along $T$. The switching $(U, V \setminus U)$ will make $T$ all positive. Hence, each switching class has at least one signed graph that makes $T$ all positive. However, since the cardinality under Step (c) is the same as under Step (b), namely $2^{m-n+1}$, we may deduce that each switching class contains exactly one all-positive $T$.

2.4 Signed singular graphs, signed core graphs and signed nut graphs

One may consider the kernel of the adjacency matrix of a signed graph. Note that definitions (2) and (3) can be extended to signed graph in a natural way. A signed graph is a signed singular graph if it has a zero as an eigenvalue. A signed graph is a signed core graph if
A signed graph is a signed nut graph if its adjacency matrix $A(\Gamma)$ has nullity one and its kernel $\ker A(\Gamma)$ contains a full kernel eigenvector.

A graph $G$ on $n$ vertices and $m$ edges gives rise to $2^m$ distinct signed graphs. If we are interested only in non-isomorphic signed graphs, this number may be reduced by the symmetries preserve signs. However, there is also an equivalence relation, to be described in the next section, among the signed graphs $\Gamma = (G, \sigma)$ over the same underlying graph that is very convenient as it preserves several important signed invariants and reduces the number of graphs to be considered.

### 2.5 Switching equivalence and signed singular graphs

Proposition 3 has the following immediate consequence:

**Proposition 5.** Let $\Gamma$ be a signed graph and let $\mathcal{U} \subseteq V(G)$. If $\Gamma$ is singular and if $x$ is any of its kernel vectors, then $\Gamma^\mathcal{U}$ is singular and the vector $x^\mathcal{U}$ defined as

$$x^\mathcal{U}(v) = \begin{cases} x(v), & \text{if } v \in V(G) \setminus \mathcal{U}, \\ -x(v), & \text{if } v \in \mathcal{U}, \end{cases}$$

is a kernel eigenvector for $\Gamma^\mathcal{U}$.

This proposition is helpful in the study of singular graphs. Namely, it follows that many properties of signed graphs concerning singularity hold for the whole switching equivalence class.

**Corollary 6.** Let $\Gamma$ and $\Gamma'$ be two switching equivalent signed graphs. The following holds:

1. If one of the pair is singular, then the other is also singular. In addition, if both are singular, they have the same nullity.
2. If one of the pair is a core graph, then the other is also a core graph.
3. If one of the pair is a nut graph then the other is also a nut graph.

In particular, this reduces the search for nut graphs to a search over distinct switching equivalence classes. The following fact may be useful.

**Corollary 7.** Every switching equivalence class of signed nut graphs has exactly one representative that has kernel eigenvector with all entries positive.

**Proof.** Let $\Gamma$ be a signed nut graph and let $x$ be its kernel eigenvector. Let

$$\mathcal{U} = \{v \in V \mid x(v) < 0\}$$

The switching at $\mathcal{U}$ gives rise to the switching-equivalent signed nut graph $\Gamma^\mathcal{U}$ with an all-positive kernel eigenvector. □

The above corollary enables us to select for any signed nut graph $\Gamma = (G, \Sigma)$ a unique switching equivalent graph $\Gamma' = (G, \Sigma')$ s.t. the kernel eigenvector $x'$ relative to $\Gamma'$ is given by $x'(v) = |x(v)|$. This canonical choice of switching can be viewed in the more general setting of signed graphs.
Algorithm 1 Given the class of graphs $G_{n,\rho}$, i.e. the class of connected $\rho$-regular graphs of order $n$, find a signed nut graph in this class.

**Input:** $G_{n,\rho}$, the class of all connected $\rho$-regular graphs of order $n$.

**Output:** A signed nut graph in $G_{n,\rho}$ (or report that there is none).

1. for all $G \in G_{n,\rho}$ do
2. $T \leftarrow$ spanning tree of $G$
3. for all $\Sigma \subseteq E(G) \setminus T$ do
4. $\Gamma \leftarrow (G, \Sigma)$
5. if $\Gamma$ is a signed nut graph then
6. return $\Gamma$
7. end if
8. end for
9. end for
10. report there is no signed nut graph in class $G_{n,\rho}$

Using the idea of the proof of Theorem 4 and a database of regular connected graphs of a given order [14] we may search for signed nut graphs of that order.

Let $F(n, \rho)$ be the number of connected graphs of order $n$ and degree $\rho$. In the worst case the algorithm has to check $2^m - n + 1$ signed structures on each. Since $2m = n\rho$ this implies a maximum of $F(n, \rho)2^{m-n+1}$ tests.

### 3 Results

Our contribution here is based on recent interest in the study of families of nut graphs. An efficient strategy for generating nut graphs of small order was published in 2018 [5] and the full collection of nut graphs found there for orders up to 20 was reported in the House of Graphs [2]. For arbitrary simple graphs, the list is complete for orders up to 12, and counts are give up to 13. A list of regular nut graphs for orders from 3 to 8 was deposited in the same place. This list covers orders up to 22 and is complete up to order 14. More recently, the orders for which regular nut graphs of degree $\rho$ exist have been established for $\rho \in \{3, 4, 5, 6, 7, 8, 9, 10, 11\}$. In [10], the set $N(\rho)$ was defined as the set consisting of all integers $n$ for which a $\rho$-regular nut graph of order $n$ exists. There it was shown that

\[
N(1) = N(2) = \emptyset,
\]
\[
N(3) = \{12\} \cup \{2k \mid k \geq 9\},
\]
\[
N(4) = \{8, 10, 12\} \cup \{k \mid k \geq 14\}.
\]

In [7], $N(\rho)$ was determined for every $\rho$, $5 \leq \rho \leq 11$. Combining these results, we obtain the following theorem.

**Theorem 8.** The following holds:

1. $N(1) = \emptyset$
2. $N(2) = \emptyset$
3. \( N(3) = \{12\} \cup \{2k \mid k \geq 9\} \)
4. \( N(4) = \{8, 10, 12\} \cup \{k \mid k \geq 14\} \)
5. \( N(5) = \{2k \mid k \geq 5\} \)
6. \( N(6) = \{k \mid k \geq 12\} \)
7. \( N(7) = \{2k \mid k \geq 6\} \)
8. \( N(8) = \{12\} \cup \{k \mid k \geq 14\} \)
9. \( N(9) = \{2k \mid k \geq 8\} \)
10. \( N(10) = \{k \mid k \geq 15\} \)
11. \( N(11) = \{2k \mid k \geq 8\} \)

Note that for each \( \rho, 3 \leq \rho \leq 11 \), the set \( N(d) \) misses only a finite number of integer values. The question we tackle here is: which of the missing numbers can be covered by regular signed nut graphs? The main result of this paper is embodied in Table 1 and stated formally in Theorems 8, 9 and 10.

| \( \rho \) | \( n \) | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3 | | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ |
| 4 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ |
| 5 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ |
| 6 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ |
| 7 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ |
| 8 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ |
| 9 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ |
| 10 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ |
| 11 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ |

Table 1: Existence of small regular signed nut graphs of order \( n \) and degree \( \rho \). Notation: ✓...there exists a traditional signed nut graph; ✗...there exists a proper signed nut graph (but no traditional signed nut graph); ✗...there exists no signed nut graph (by Theorem 10); ✗...there exists no signed nut graph (proof by exhaustion).

**Theorem 9.** Let \( N_s(\rho) \) denote the set of orders \( n \) for which no \( \rho \)-regular nut graph exists but there exists a (proper) signed nut graph.

1. \( N_s(3) = \{14, 16\} \)
2. \( N_s(4) = \{5, 7, 9, 11, 13\} \)
3. $N_s(5) = \emptyset$

4. $N_s(6) = \{8, 9, 10, 11\}$

5. $N_s(7) = \{10\}$

6. $N_s(8) = \{9, 10, 11, 13\}$

7. $N_s(9) = \{12, 14\}$

8. $N_s(10) = \{12, 13, 14\}$

9. $N_s(11) = \{14\}$

Proof. In the proof we first used computer search based on the data about regular nut graphs from the House of Graphs [2]. For some set of parameters $n, d$, we were able to prove existence and non-existence by search using the straightforward Algorithm 1. For some sets the search was unfeasible, but in these cases an example was generated by a heuristic approach. In some cases this involved planting a small number of negative edges. In others, a negative hamiltonian cycle was added to an ordinary nut graph.

A further theorem extends the results of Theorem 9 to infinity along the leading diagonal of the table.

**Theorem 10.** Let $\Gamma$ be a signed graph whose underlying graph is $K_n$. If $\Gamma$ is a signed nut graph then $n \equiv 1 \pmod{4}$. Moreover, for each $n \equiv 1 \pmod{4}$, there exists a signed nut graph with underlying graph $K_n$.

Proof. Let $n = 4k + q$, where $0 \leq q \leq 3$. We divide the proof into three parts: (a) $q \in \{0, 2\}$, (b) $q = 3$, and (c) $q = 1$.

Assume that $\Gamma$ is singular. Let $x$ be a full kernel eigenvector (existence established by Proposition [1]). We may assume that $x$ is a non-zero integer vector. If $x$ has no odd coordinate, we may multiply $x$ by an appropriate power of $\frac{1}{2}$ so that at least one coordinate becomes odd. We call vertex $s$ even if $x_s \equiv 0 \pmod{2}$ and odd if $x_s \equiv 1 \pmod{2}$. The local condition for a kernel eigenvector $x$ is

$$\sum_{s \sim r} x_s \sigma(rs) = 0$$

for each choice of a pivot vertex $r$, where $\sigma(rs)$ is the weight ($\pm 1$) of the edge between $r$ and $s$. We know that at least one vertex, say $r$, must be odd. The local condition at $r$ implies that there is an even number of odd vertices around $r$ and hence, together with $r$, an odd number of odd vertices in total for a presumed $K_n$ nut graph.

Case (a): $q \in \{0, 2\}$. This means that $n$ is even. The signed graph $\Gamma$ must have an even vertex $t$. The local condition at $t$ implies that there is an even number of odd vertices around $t$, and hence an even number of odd vertices in total, a contradiction. This rules out the existence of signed complete nut graphs for $q \in \{0, 2\}$.

Case (b): $q = 3$. In this case all entries $x_s$ are odd: the parity of the sum in (1) is opposite for even and odd vertices.
Let \( m_+ \) denote the number of edges in \( \Gamma \) with positive sign. For each vertex \( s \), let \( \rho_+(s) \) and \( \rho_-(s) \), respectively, denote the number of edges with positive sign and negative sign that are incident with \( s \). Note that \( \rho_+(s) + \rho_-(s) = n - 1 \). Summing local conditions over all pivots \( r \):

\[
0 = \sum_r \rho_+(r)x_r - \sum_r \rho_-(r)x_r
\]

Hence,

\[
0 = \sum_r \{\rho_+(r) - \rho_-(r)\}x_r = \sum_r \{2\rho_+(r) - n + 1\}x_r
\]

and

\[
\sum_r \rho_+(r)x_r = \frac{n - 1}{2} \sum_r x_r = \{2k + 1\} \sum_r x_r. \tag{5}
\]

The RHS of (5) is an odd number since it is a product of two odd numbers, hence \( \sum_r \rho_+(r)x_r \) is odd. Therefore, the subgraph with positive edges only has an odd number of vertices with odd degree. By the Handshaking Lemma this is impossible.

Case (c): \( q = 1 \) is the only remaining possibility and the first part of the theorem follows, provided such nut graphs exist.

Now we construct a signed nut graph for each \( n \) of the form \( n = 4k + 1 \). A signed graph (call it \( \Gamma \)) is constructed from \( K_{4k+1} \) as follows. Partition the vertex set of \( K_{4k+1} \) into a single vertex \( r = 0 \) and \( k \) subsets of 4 vertices for \( k \) copies of the path graph \( P_4 \). Change the signs of all edges internal to each \( P_4 \) to \( -1 \). To construct a kernel eigenvector \( x \) of \( \Gamma \) for \( \lambda = 0 \) place +1 on vertex 0, then entries \(-1, +1, +1, -1\) on each \( P_4 \). We denote by 1, 2, 3, 4 the vertices of the first \( P_4 \), by 5, 6, 7, 8 the vertices of the second \( P_4 \), etc. Owing to the symmetry of \( \Gamma \) (since automorphisms of \( \Gamma \) preserve edge-weights) there are only three vertex types to be considered.

1. For \( r = 0 \) all weights \( \sigma(rs) = 1 \) and exactly half of the \( x_s \) are equal to 1 and the other half are equal to \(-1 \). Hence, (1) is true in this case.

2. The vertex \( r \) may be an end-vertex of any of the \( k \) paths \( P_4 \). The net contribution of the three remaining vertices of \( P_4 \) is \(-1 \), and all contributions of other paths cancel out. Taking into account the edge to vertex 0, the weighted sum in (1) is indeed equal to 0.

3. The vertex \( r \) may be an inner vertex of any of the \( k \) paths \( P_4 \). Again, the net contribution of the three remaining vertices of \( P_4 \) is \(-1 \), and by the same argument, the weighted sum in (1) is again equal to 0.

As \( x \) is a full kernel eigenvector, \( \Gamma \) is a signed core graph.

It remains to prove that \( \Gamma \) is a signed nut graph, i.e. with nullity \( \eta(\Gamma) = 1 \). This is done by showing that the constructed full kernel eigenvector \( x \) is the only eigenvector for \( \lambda = 0 \) (up to a scalar multiple). First, note that all edges incident with vertex 0 have weight +1. Hence for \( r = 0 \), (1) becomes:

\[
\sum_{s \neq 0} x_s = 0 \tag{6}
\]
It follows that
\[ \sum_{s=0}^{n} x_s = x_0 \quad (7) \]

Now consider any path \( P_4 \) with vertices, say, 1, 2, 3, 4. Note that vertices 1 and 4 fall into one symmetry class while vertices 2 and 3 are in the other symmetry class. The local conditions are:

\[
\begin{align*}
0 &= x_0 - x_2 + \sum_{s \neq 0,1,2} x_s = x_0 - x_1 - 2x_2 \\
0 &= x_0 - x_1 - x_3 + \sum_{s \neq 0,1,2,3} x_s = x_0 - 2x_1 - x_2 - 2x_3 \\
0 &= x_0 - x_2 - x_4 + \sum_{s \neq 0,2,3,4} x_s = x_0 - 2x_2 - x_3 - 2x_4 \\
0 &= x_0 - x_3 + \sum_{s \neq 0,3,4} x_s = x_0 - 2x_3 - x_4
\end{align*}
\]

(8) \( \quad (9) \quad (10) \quad (11) \)

It is straightforward to show that \( x_1 \) to \( x_4 \) are related to \( x_0 \) as:

\[ x_1 = x_4 = -x_0, x_2 = x_3 = x_0 \quad (12) \]

Since this holds for all \( k \) path graphs \( P_4 \) it follows that \( \Gamma \) is indeed a signed nut graph.

The spectrum of \( \Gamma \) is easily described. The eigenvalues, with multiplicities, are:

\[
(2(k-1) \pm \sqrt{4k(k-1) + 5})^1, (\pm \sqrt{5})^k, (\pm \sqrt{5} - 2)^{k-1}, 0^1.
\]

(13)

For \( k = 1 \), this reduces to five distinct eigenvalues.

4 A construction for proper signed nut graphs

Theorem 9 has answered our initial question, in that if we consider ordinary graphs as special cases of signed graphs and \( \rho \leq 11 \) we need only to perform a computer search for existence of signed nut graphs for those values of \( n \) for which no ordinary nut graph exists. However, if we wanted to search for proper signed nut graphs with the intention of determining the orders for which a proper signed graph exists, then methods would be needed for generating larger signed nut graphs. There are several known constructions that take a nut graph and produce a larger nut graph. We will revisit one construction here and extend it to signed graphs. This is the so-called Fowler construction for enlarging unweighted nut graphs.

Recall that \( \Gamma \) is a proper signed nut graph if and only if it is not switching equivalent to an ordinary unweighted nut graph.

Let \( G \) be a graph and \( v \) a vertex of degree \( \rho \). Let \( N(v) = \{ u_1, u_2, \ldots, u_\rho \} \). Recall [10] [7] that the Fowler Construction, denoted \( F(G, v) \), is a graph with

\[
V(F(G, v)) = V(G) \sqcup \{ q_1, \ldots, q_\rho \} \sqcup \{ p_1, \ldots, p_\rho \}
\]

10
Figure 1: A construction for expansion of a signed nut graph $\Gamma$ about vertex $v$ of degree $\rho$, to give $F(\Gamma, v)$. The labelling of vertices in $\Gamma$ and $F(\Gamma, v)$ is shown within the circles that represent vertices. Shown beside each vertex is the corresponding entry of the unique kernel eigenvector of the respective graph. Panel (a) shows the neighbourhood of vertex $v$ in $\Gamma$. Edges from vertex $v$ to its neighbours have weights $\sigma(vu_i)$ which are either $+1$ or $-1$. In the figure, edges with weight $-1$ are indicated in red, as an illustration. Edges of the remainder of the graph, indicated by the shaded bubble, may take arbitrary signs. Panel (b) shows additional vertices and edges in $F(\Gamma, v)$. Vertices $q_i$ inherit their entries from $\Gamma$ as described in Equation (15). Edges $p_iu_i$ inherit their weights (signs) from $\Gamma$. All other explicit edges in Panel (b) have weights $+1$. 
Since \( u \) conditions at vertices

Moreover, \( x \)

Proof. Let \( v \) that is not a neighbour of

Let \( \Gamma = (G, \sigma) \) be any two non-adjacent vertices, having the same degree, say \( u \), \( v \) is the Fowler Construction for signed graphs.

\[
\text{Definition 1. Let } \Gamma = (G, \sigma) \text{ be a signed graph and } v \text{ a vertex of } G \text{ that has degree } \rho. \text{ Then } F(\Gamma, v) = (F(G, v), \sigma'), \text{ where for } 1 \leq i, j \leq \rho,
\]

\[
\sigma'(e) = \begin{cases} 
1 & \text{if } e = vq_i, \\
1 & \text{if } e = qp_j, \\
\sigma(vu_i) & \text{if } e = pu_i, \\
\sigma(e) & \text{otherwise,}
\end{cases}
\]

is the Fowler Construction for signed graphs.

\[
\text{Lemma 11. Let } \Gamma = (G, \sigma) \text{ be a signed graph and } v \text{ a vertex of } G \text{ that has degree } \rho \text{ and let } x \text{ be a kernel eigenvector for } \Gamma. \text{ Then } x', \text{ defined as}
\]

\[
x'(w) = \begin{cases} 
-(\rho - 1)x(v) & \text{if } w = v, \\
\sigma(vu_i)x(u_i) & \text{if } w = q_i, \\
x(v) & \text{if } w = p_i, \\
x(w) & \text{otherwise,}
\end{cases}
\]

for \( w \in V(F(\Gamma, v)) \), is a kernel eigenvector for \( F(\Gamma, v) \).

The local structures in the signed graphs \( \Gamma \) and \( F(\Gamma, v) \) are shown in Figure 1, which also indicates the local relationships between kernel eigenvectors in these graphs.

\[
\text{Lemma 12. Let } \Gamma \text{ be a singular signed graph, and let } x \text{ be a kernel eigenvector. Let } u, v \in V \text{ be any two non-adjacent vertices, having the same degree, say } \rho, \text{ and sharing } \rho - 1 \text{ neighbours. Let } u' \text{ denote the neighbour of } u \text{ that is not a neighbour of } v, \text{ and let } v' \text{ denote the neighbour of } v \text{ that is not a neighbour of } u. \text{ If } \sigma(uw) = \sigma(vw) \text{ for all } w \in N(u) \setminus \{u'\}, \text{ then } |x(u')| = |x(v')|. \text{ Moreover, } x(u') = x(v') \text{ if and only if } \sigma(uv') = \sigma(uu').
\]

Proof. Let \( N(u) \setminus \{u'\} = N(v) \setminus \{v'\} = \{w_2, \ldots, w_\rho\} \) (see Figure 2). The respective local conditions at vertices \( u \) and \( v \) are

\[
\sigma(uu')x(u') + \sum_{i=2}^{\rho} \sigma(uw_i)x(w_i) = 0, \tag{16}
\]

\[
\sigma(vv')x(v') + \sum_{i=2}^{\rho} \sigma(w_i v)x(w_i) = 0. \tag{17}
\]

Since \( \sigma(uw_i) = \sigma(w_i v) \) for all \( 2 \leq i \leq \rho \), we get that

\[
\sigma(uu')x(u') = \sigma(vv')x(v'), \tag{18}
\]

12
Figure 2: The neighbourhood of vertices $u$ and $v$ from Lemma 12. The red edges indicate a possible selection of edges with weight $-1$.

by taking the difference of (16) and (17). Clearly,
\[ |x(u')| = |\sigma(uu')x(u')| = |\sigma(vv')x(v')| = |x(v')|. \]

If $\sigma(uu') = \sigma(vv')$, then (18) implies $x(u') = x(v')$. Similarly, if $x(u') = x(v')$, then (18) implies $\sigma(uu') = \sigma(vv')$. \qed

**Lemma 13.** Let $\Gamma$ and $\Gamma'$ be signed graphs over the same base graph $G$, i.e. $\Gamma = (G, \sigma)$ and $\Gamma' = (G, \sigma')$. Let $v$ be a vertex of $G$. Then $\Gamma$ is switching equivalent to $\Gamma'$ if and only if $F(\Gamma, v)$ is switching equivalent to $F(\Gamma', v)$.

**Proof.** Let $\Gamma$ and $\Gamma'$ be two signed graphs over graph $G$, say $\Gamma = (G, \Sigma)$ and $\Gamma' = (G, \Sigma')$. Let $v \in V(G)$ and let $F(\Gamma, v)$ and $F(\Gamma', v)$ be the corresponding Fowler constructions. Let $\Gamma$ and $\Gamma'$ be switching equivalent. This means that there exists $S \subset V(G)$, such that $\Gamma' = \Gamma_S$. We know that $\Gamma'^S = \Gamma^V(G) \setminus S$. Without loss of generality we may assume that $v \notin S$. Let the vertex labelling of $F(\Gamma, v)$, $F(\Gamma', v)$ and $F(G, v)$ be the same as in Figure 1. In particular, this means that all vertices of $G$ belong also to $F(G, v)$. Since $v \notin S$ we have:
\[ F(\Gamma', v) = F(\Gamma^S, v) = F(\Gamma, v)^S. \]

Hence it follows:
\[ \Gamma \sim \Gamma' \Rightarrow F(\Gamma, v) \sim F(\Gamma', v). \]

To prove the converse assume the following: $F(\Gamma, v) \sim F(\Gamma', v)$, where $\Gamma = (G, \Sigma)$ and $\Gamma' = (G, \Sigma')$. Let $S \subset V(F(G, v))$ such that $v \notin S$. Since all edges above $u_1, u_2, \ldots, u_s$ in Figure 1(b) are positive in both signed graphs, it is clear that $S \subset V(G)$ and the result follows. \qed

**Theorem 14.** Let $\Gamma$ be a signed graph and $v$ any one of its vertices. Then the nullities of $\Gamma$ and $F(\Gamma, v)$ are equal, i.e. $\eta(\Gamma) = \eta(F(\Gamma, v))$. Moreover, ker $\Gamma$ admits a full eigenvector if and only if ker $F(\Gamma, v)$ admits a full eigenvector.

**Proof.** Let $u_1, \ldots, u_\rho$ be the neighbours of vertex $v$ in $G$. Assume first that $G$ is a core graph and that $x$ is an admissible eigenvector. Let $x(w)$ denote the entry of $x$ at vertex $w$. Let $a = x(v)$ and let $b_i = x(u_i)$. We now produce a vertex labelling $x'$ of $F(\Gamma, v)$ as above. It
follows that if \( x \) is a valid assignment of \( G \) then \( x' \) is a valid assignment on \( F(\Gamma, v) \). Thus \( \eta(F(\Gamma, v)) \geq \eta(\Gamma) \).

On the other hand, apply Lemma 12 to \( F(\Gamma, v) \) and an admissible assignment \( x' \). First consider vertices \( q_i \) and \( q_j \) and their neighbourhoods. Lemma 12 implies that \( x'(p_i) = x'(p_j) \). Hence \( x' \) is constant on \( p_i \), say \( x'(p_i) = a \). Thus, it follows that \( x'(v) = -(\rho - 1)a \). The second application of the lemma goes to vertices \( v \) and \( p_i \). It implies that for each \( i \) the values \( x'(q_i) \) and \( x'(u_i) \) are equal, namely \( x'(q_i) = x'(u_i) \). Finally, let \( x(w) = x'(w) \) for every \( w \in V(G) \setminus \{v\} \) and let \( x(v) = a \). Hence, the existence of an admissible \( x' \) on \( F(\Gamma, v) \) implies the existence of an admissible \( x \) on \( \Gamma \). Thus \( \eta(F(\Gamma, v)) \leq \eta(\Gamma) \). □

An alternative proof of \( \eta(F(\Gamma, v)) \leq \eta(\Gamma) \). One may work out the rank of \( F(\Gamma, v) \) directly. Let \( N_G(v) = \{u_1, \ldots, u_\rho\} \) and \( V(G) \setminus N[v] = \{w_1, \ldots, w_{\rho-1}\} \), where \( n = |V(G)| \). The adjacency matrix \( A(\Gamma) \) can be partitioned into block matrices as follows:

\[
A(\Gamma) = \begin{pmatrix}
0 & w_1 & \cdots & w_{\rho-1} & u_1 & \cdots & u_\rho \\
\vdots & \vdots & & \vdots & \vdots & & \vdots \\
0 & \sigma(vu_1) & \cdots & \sigma(vu_\rho) & 0 & \cdots & 0
\end{pmatrix}
\]

where submatrices \( B, C \) and \( D \) encode the signed edges between the respective vertex-sets. The adjacency matrix of \( A(F(\Gamma, v)) \) can similarly be partitioned as follows:

\[
\begin{pmatrix}
v & u_1 & \cdots & u_{\rho-1} & u_1 & \cdots & u_\rho & q_1 & \cdots & q_\rho & p_1 & \cdots & p_\rho \\
0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 1 & \cdots & 1 & 0 & \cdots & 0
\end{pmatrix}
\]

where \( I \) is the identity matrix, \( J \) is the all-one matrix and \( K = \text{diag}(\sigma(vu_1), \ldots, \sigma(vu_\rho)) = \text{diag}(\sigma'(p_1u_1), \ldots, \sigma'(p_\rho u_\rho)) \) is a modified identity matrix in which weights of edges from the
neighbourhood of the original vertex $v$ replace the unit entries. Elementary row and corresponding column operations that leave the rank unchanged are performed by replacing the rows and columns corresponding to $u_1, \ldots, u_\rho$ by $u_1 + \sigma(vu_1)q_1, \ldots, u_\rho + \sigma(vu_\rho)q_\rho$, respectively (where by abuse of notation $u_i$ and $q_i$ stand for rows/columns corresponding to $u_i$ and $q_i$, respectively), to obtain the matrix

$$
\begin{pmatrix}
v & w_1 & \cdots & w_{n-\rho-1} & u_1 & \cdots & u_\rho & q_1 & \cdots & q_\rho & p_1 & \cdots & p_\rho \\
0 & 0 & \cdots & 0 & \sigma(vu_1) & \cdots & \sigma(vu_\rho) & 1 & \cdots & 1 & 0 & \cdots & 0
\end{pmatrix}
$$

where $J'$ is a $\rho \times \rho$ matrix defined as $(J')_{i,j} = \sigma(vu_i)$ and all other symbols have their previous meanings.

We remark that the block $J - I$ is of full rank. We now pre-multiply the blocked matrix for $F(\Gamma, v)$ by a non-singular matrix that is chosen to transform the first $J - I$ block of (21) to $I$. The transformation matrix is

$$
\begin{pmatrix}
v & w_1 & \cdots & w_{n-\rho-1} & u_1 & \cdots & u_\rho & q_1 & \cdots & q_\rho & p_1 & \cdots & p_\rho \\
1 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 & \cdots & 0
\end{pmatrix}
$$

The matrix $(J_\rho - I_\rho)^{-1}$ has diagonal entries $\frac{1}{\rho-1} - 1$ and off-diagonal entries $\frac{1}{\rho-1}$. Since
the matrix (22) is non-singular, the matrix resulting from the premultiplication has the same rank as before, and is

\[
\begin{pmatrix}
v & w_1 & \ldots & w_{n-\rho-1} & u_1 & \ldots & u_\rho & q_1 & \ldots & q_\rho & p_1 & \ldots & p_\rho \\
0 & 0 & \ldots & 0 & \sigma(vu_1) & \ldots & \sigma(vu_\rho) & 1 & \ldots & 1 & 0 & \ldots & 0 \\
0 & \vdots & & \vdots & B & C & 0 & 0 \\
0 & \vdots & & \vdots & \sigma(vu_1) & \vdots & \vdots & \vdots & C^T & D & 0 & 0 & J' \\
0 & \vdots & & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\frac{1}{\rho-1} & 0 & \ldots & 0 & (J')^T & 0 & 0 \\
\frac{1}{\rho-1} & \vdots & & \vdots & J_{\rho} & -I_\rho & 0 \\
1 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & I_\rho \\
1 & \vdots & & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
1 & \vdots & & \vdots & p_1 & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
1 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_\rho \\
\end{pmatrix}
\]

Now consider the rank of the red block of this matrix. Before this last transformation, it was equal to \( A(\Gamma) \) and had \( \eta = 1 \), as \( \Gamma \) is a signed nut graph. After the transformation, the
red block differs only by the replacement of $\sigma(vu_i)$ with $-\sigma(vu_i)/(\rho - 1)$. The block now has nullity 0 or nullity 1. (We know that the submatrix $\begin{bmatrix} B & C \\ C^T & D \end{bmatrix}$ is non-singular, as deletion of any vertex (here $v$) from a nut graph reduces the nullity to zero [21, 22].) Hence, the rank of the red block is $\geq n - 1$ and the inequality follows:

$$\text{rk}(\mathbf{A}(F(\Gamma, v))) \geq \text{rk}(\mathbf{A}(\Gamma)) + 2\rho = n - 1 + 2\rho,$$

since the last $2\rho$ rows are linearly independent of all the other rows. Thus, $\eta(F(\Gamma, v)) \leq \eta(\Gamma)$, as before.

**Corollary 15.** Let $\Gamma = (G, \sigma)$ be a signed graph and $v \in V(G)$ any one of its vertices. The following statements hold:

1. $F(\Gamma, v)$ is a signed nut graph if and only if $\Gamma$ is a signed nut graph.
2. $F(\Gamma, v)$ is a proper signed nut graph if and only if $\Gamma$ is a proper signed nut graph.

**Proof.** Follows directly from Lemma 13 and Theorem 14. Namely, if $\Gamma$ is proper then it is switching equivalent to the all-positive (traditional) signed nut graph $\Gamma' = (G, \emptyset)$. However, in this case $F(\Gamma', v) = F((G, \emptyset), v) = (F(G, v), \emptyset)$. Virtually the same argument can be used in the opposite direction.

## 5 Conclusion

Invocation of signed graphs as candidates for nut graphs allows extension of the orders at which a nut graph exists, and allows proof of all cases for regular nut graphs (signed and unsigned) with degree at most 11. As with unweighted nut graphs, signed nut graphs can be generated by a generic construction in which the order of a smaller signed nut graph increases from $n$ to $n + 2\rho$, where $\rho$ is the degree of the vertex chosen as the focus of this vertex-expansion construction.

## Acknowledgements

The work of Tomaž Pisanski is supported in part by the Slovenian Research Agency (research program P1-0294 and research projects N1-0032, J1-9187, J1-1690, N1-0140 and J1-2481), and in part by H2020 Teaming InnoRenew CoE. The work of Nino Bašić is supported in part by the Slovenian Research Agency (research program P1-0294 and research projects J1-9187, J1-1691, N1-0140 and J1-2481). The work of Irene Sciriha and Patrick W. Fowler is supported by The University of Malta under the project Graph Spectra, Computer Network Design and Electrical Conductivity in Nano-Structures MATRP01-20.

## References

[1] F. Belardo, S. M. Cioabă, J. Koolen and J. Wang, Open problems in the spectral theory of signed graphs, *Art Discrete Appl. Math.* 1 (2018), #P2.10, doi:10.26493/2590-9770.1286.d7b.
[2] G. Brinkmann, K. Coolsaet, J. Goedgebeur and H. Mélot, House of Graphs: A database of interesting graphs, *Discrete Appl. Math.* **161** (2013), 311–314, doi:10.1016/j.dam.2012.07.018, available at [https://hog.grinvin.org/](https://hog.grinvin.org/).

[3] G. Brinkmann, J. Goedgebeur and B. D. McKay, Generation of cubic graphs, *Discrete Math. Theor. Comput. Sci.* **13** (2011), 69–80, [https://dmtcs.episciences.org/551](https://dmtcs.episciences.org/551).

[4] K. Coolsaet, P. W. Fowler and J. Goedgebeur, Nut graphs, homepage of Nutgen, [http://caagt.ugent.be/nutgen/](http://caagt.ugent.be/nutgen/).

[5] K. Coolsaet, P. W. Fowler and J. Goedgebeur, Generation and properties of nut graphs, *MATCH Commun. Math. Comput. Chem.* **80** (2018), 423–444, [http://match.pmf.kg.ac.rs/electronic_versions/Match80/n2/match80n2_423-444.pdf](http://match.pmf.kg.ac.rs/electronic_versions/Match80/n2/match80n2_423-444.pdf).

[6] P. W. Fowler, Hückel spectra of Möbius π systems, *Phys. Chem. Chem. Phys.* **4** (2002), 2878–2883, doi:10.1039/b201850k.

[7] P. W. Fowler, J. B. Gauci, J. Goedgebeur, T. Pisanski and I. Sciriha, Existence of regular nut graphs for degree at most 11, *Discuss. Math. Graph Theory* **40** (2020), 533–557, doi: 10.7151/dmgt.2283.

[8] P. W. Fowler, B. T. Pickup, T. Z. Todorova, M. Borg and I. Sciriha, Omni-conducting and omni-insulating molecules, *J. Chem. Phys.* **140** (2014), 054115, doi:10.1063/1.4863559.

[9] P. W. Fowler, T. Pisanski and N. Bašić, Charting the space of chemical nut graphs, *MATCH Commun. Math. Comput. Chem.* (2020), in press.

[10] J. B. Gauci, T. Pisanski and I. Sciriha, Existence of regular nut graphs and the Fowler construction, *Appl. Anal. Discrete Math.* (2020), in press.

[11] I. Gutman and I. Sciriha, Graphs with maximum singularity, *Graph Theory Notes N. Y.* **30** (1996), 17–20.

[12] W. H. Haemers, E. Ghorbani, H. R. Maimani and L. P. Majd, On sign-symmetric signed graphs, *Ars Math. Contemp.* (2020), doi:10.26493/1855-3974.2161.55, in press.

[13] D. Holt and G. Royle, A census of small transitive groups and vertex-transitive graphs, *J. Symb. Comput.* **101** (2020), 51–60, doi:10.1016/j.jsc.2019.06.006.

[14] B. D. McKay and A. Piperno, Practical graph isomorphism, II, *J. Symb. Comput.* **60** (2014), 94–112, doi:10.1016/j.jsc.2013.09.003.

[15] B. D. McKay and G. F. Royle, The transitive graphs with at most 26 vertices, *Ars Combinatoria* **30** (1990), 161–176.

[16] M. Meringer, Fast generation of regular graphs and construction of cages, *J. Graph Theory* **30** (1999), 137–146, doi:10.1002/(sici)1097-0118(199902)30:2<137::aid-jgt7>3.0.co;2-g.}
[17] I. Sciriha, On the construction of graphs of nullity one, *Discrete Math.* 181 (1998), 193–211, doi:10.1016/s0012-365x(97)00036-8.

[18] I. Sciriha, On the rank of graphs, in: *Combinatorics, Graph Theory, and Algorithms, Volume II*, New Issues Press, Kalamazoo, MI, 1999 pp. 769–778, Proceedings of the 8th Quadrennial International Conference on Graph Theory, Combinatorics, Algorithms, and Applications, dedicated to the memory of Paul Erdős, held at Western Michigan University, Kalamazoo, MI, June 3 – 7, 1996.

[19] I. Sciriha, A characterization of singular graphs, *Electron. J. Linear Algebra* 16 (2007), 451–462, doi:10.13001/1081-3810.1215.

[20] I. Sciriha, Coalesced and embedded nut graphs in singular graphs, *Ars Math. Contemp.* 1 (2008), 20–31, doi:10.26493/1855-3974.20.7cc.

[21] I. Sciriha, Graphs with a common eigenvalue deck, *Linear Algebra Appl.* 430 (2009), 78–85, doi:10.1016/j.laa.2008.06.033.

[22] I. Sciriha, Maximal core size in singular graphs, *Ars Math. Contemp.* 2 (2009), 217–229, doi:10.26493/1855-3974.115.891.

[23] I. Sciriha and P. W. Fowler, Nonbonding orbitals in fullerenes: Nuts and cores in singular polyhedral graphs, *J. Chem. Inf. Model.* 47 (2007), 1763–1775, doi:10.1021/ci700097j.

[24] I. Sciriha and I. Gutman, Nut graphs: Maximally extending cores, *Util. Math.* 54 (1998), 257–272.

[25] A. Streitwieser, *Molecular Orbital Theory for Organic Chemists*, Wiley International Edition, Wiley, 1961.

[26] N. Trinajstić, *Chemical Graph Theory*, Mathematical Chemistry Series, CRC Press, Boca Raton, FL, 2nd edition, 1992, doi:10.1007/s10910-008-9464-6.