

This is a repository copy of Nut graphs with a given automorphism group.

White Rose Research Online URL for this paper: <u>https://eprints.whiterose.ac.uk/223690/</u>

Version: Published Version

Article:

Bašić, N. orcid.org/0000-0002-6555-8668 and Fowler, P.W. orcid.org/0000-0003-2106-1104 (2025) Nut graphs with a given automorphism group. Journal of Algebraic Combinatorics, 61 (2). 17. ISSN 0925-9899

https://doi.org/10.1007/s10801-025-01389-4

Reuse

This article is distributed under the terms of the Creative Commons Attribution (CC BY) licence. This licence allows you to distribute, remix, tweak, and build upon the work, even commercially, as long as you credit the authors for the original work. More information and the full terms of the licence here: https://creativecommons.org/licenses/

Takedown

If you consider content in White Rose Research Online to be in breach of UK law, please notify us by emailing eprints@whiterose.ac.uk including the URL of the record and the reason for the withdrawal request.



eprints@whiterose.ac.uk https://eprints.whiterose.ac.uk/



Nut graphs with a given automorphism group

Nino Bašić^{1,2,3} · Patrick W. Fowler⁴

Received: 23 May 2024 / Accepted: 22 January 2025 $\ensuremath{\mathbb{C}}$ The Author(s) 2025

Abstract

A *nut graph* is a simple graph of order 2 or more for which the adjacency matrix has a single zero eigenvalue such that all nonzero kernel eigenvectors have no zero entry (i.e. are full). It is shown by construction that every finite group can be represented as the group of automorphisms of infinitely many nut graphs. It is further shown that such nut graphs exist even within the class of regular graphs; the cases where the degree is 8, 12, 16, 20 or 24 are realised explicitly.

Keywords Nut graph \cdot Graph automorphism \cdot Automorphism group \cdot Nullity \cdot Graph spectra \cdot F-universal

Mathematics Subject Classification 05C25 · 05C50

1 Introduction

A problem posed in Kőnig's 1936 book on Graph Theory [35, p. 5] asks when a given abstract group can be represented as the group of automorphisms of a (finite) graph G, and if this is the case, how the graph can be constructed¹. In response, Frucht first solved the problem in its original form [30]. Later, he showed that solution is still possible under the extra requirement that G is a cubic graph [31]. In both cases he gave an explicit construction. Sabidussi [41] refined the question and proved that every group can be represented by a graph with additional properties such as: prescribed chromatic number, prescribed vertex-connectivity, or regularity with prescribed degree. An early survey paper by Babai [5] reviews this research direction and defines the term f-

 $^{^1}$ "Wann kann eine gegebene abstrakte Gruppe als die Gruppe eines Graphen aufgefaßt werden und – ist des der Fall – wie kann die entsprechende Graph konstruoert werden?"

[⊠] Nino Bašić Nino.Basic@famnit.upr.si

¹ FAMNIT, University of Primorska, Koper, Slovenia

² IAM, University of Primorska, Koper, Slovenia

³ Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia

⁴ Department of Chemistry, University of Sheffield, Sheffield S3 7HF, UK

universal: a class of graphs C is f-universal if for every finite group \mathfrak{G} there exists a graph $G \in C$ such that $\operatorname{Aut}(G) \cong \mathfrak{G}$. Not all famous graph classes are f-universal; for example, Babai has shown that there are infinitely many finite groups which cannot be realised by a *planar* graph [2, 3]. Kőnig's question has also been extended from graphs to other combinatorial objects, such as tournaments [38], Steiner triple and quadruple systems [37], and cycle systems [33, 36]. Here, we consider Kőnig's original question, but for *nut graphs*.

The *nullity*, $\eta(G)$, of a graph *G* is the dimension of the kernel of its adjacency matrix $\mathbf{A}(G)$, i.e. $\eta(G) = \dim \ker \mathbf{A}(G)$. A nut graph is a singular simple graph *G* with nullity 1, where in addition every non-trivial kernel eigenvector of the adjacency matrix $\mathbf{A}(G)$ has only nonzero entries. Nut graphs occur in several chemical applications [43]: they are connected, leafless and non-bipartite [47]. Catalogues have been constructed [11, 14–16]: nut graphs may be regular, vertex-transitive [7, 28] (including GRRs [39, 40] and non-Cayley graphs), but are not edge-transitive [8]. Recently, a comprehensive theory of circulant nut graphs has been developed [20–23]. The study of polycirculant nut graphs [24] has also been initiated.

The graphs that can be used to model conjugated carbon frameworks in Hückel theory and similar applications [48] are known as chemical graphs. A *chemical graph* in this definition is connected and subcubic. Cubic chemical graphs form an important subclass that includes the fullerene carbon cages [27]. Nut graphs can be found among chemical graphs [29], including some cubic polyhedra [45] and, in particular, fullerenes [46]. Applications of nut graphs in theories of radical chemistry and molecular conduction are described in [43].

Here, we prove a Sabidussi-type result for the class of nut graphs: we show that the graph G that realises a given automorphism group can be chosen to satisfy the requirements of the nut-graph definition; hence, nut graphs are f-universal (in the sense of [5]). We prove that:

Theorem 1 For every finite group \mathfrak{G} there exist infinitely many finite nut graphs G, such that $\operatorname{Aut}(G) \cong \mathfrak{G}$.

Furthermore, we can require that the graph G is also regular.

Theorem 2 For every finite group \mathfrak{G} and $d \in \{8, 12, 16, 20, 24\}$ there exist infinitely many finite *d*-regular nut graphs *G*, such that $\operatorname{Aut}(G) \cong \mathfrak{G}$.

2 Preliminaries

All graphs considered in this paper are finite, simple and connected. The adjacency matrix of graph *G* is $\mathbf{A}(G)$ and the dimension of the nullspace of $\mathbf{A}(G)$ is the *nullity*, $\eta(G)$. An *automorphism* α of a graph *G* is a permutation $\alpha : V(G) \rightarrow V(G)$ of the vertices of *G* that maps edges to edges and non-edges to non-edges. The set of all automorphisms of a graph *G* forms a group, the (*full*) *automorphism* group of *G*, denoted by $\operatorname{Aut}(G)$. The image of a vertex $v \in V(G)$ under automorphism α will be denoted v^{α} . We use the notation $\mathfrak{H} \leq \mathfrak{G}$ to indicate that graph *H* is a subgraph of *G*. We use C_n to denote the

cyclic group of order *n*. For other standard definitions we refer the reader to one of the many comprehensive treatments of the theory of graph spectra (e.g. [12, 13, 17–19]) and algebraic graph theory (e.g. [9, 26, 32]).

Nut graphs [47] are graphs that have a one-dimensional nullspace (i.e., $\eta(G) = 1$), where every non-trivial kernel eigenvector $\mathbf{x} = [x_1 \dots x_n]^{\mathsf{T}} \in \ker \mathbf{A}(G)$ is full (i.e., $|x_i| > 0$ for all $i = 1, \dots, n$). As the defining paper considered the isolated vertex to be a trivial case [47], non-trivial nut graphs have seven or more vertices. If *G* is a *regular* nut graph, then $\delta(G) = \Delta(G) \ge 3$. Note that there are no nut graphs with $\Delta(G) = 2$, as no cycle has nullity 1.

In what follows, it will be useful to have constructions that are guaranteed to produce a nut graph, when applied to a starting graph of specified type. For example, let Gbe a nut graph and $e \in E(G)$ an arbitrary edge. Then the graph obtained from Gby subdividing the edge e four times is again a nut graph; this is the *subdivision construction* [47]. Two further constructions that will prove useful in what follows are now described.

The first is the coalescence construction: Let G_1 and G_2 be graphs and let $v_1 \in V(G_1)$ and $v_2 \in V(G_2)$. The *coalescence of* (G_1, v_1) and (G_2, v_2) , which we denote here as $(G_1, v_1) \odot (G_2, v_2)$, is the graph obtained from the disjoint union of G_1 and G_2 by identifying root vertices v_1 and v_2 . Sciriha obtained the following result [44, Corollary 21].

Lemma 3 ([44]) Let G_1 and G_2 be nut graphs. Then the coalescence $(G_1, v_1) \odot (G_2, v_2)$ is a nut graph.

The coalescence construction must be provided with an initial collection of nut graphs. The second construction is different in that it produces a nut graph from any (2t)-regular graph.

Proposition 4 ([8]) Let G be a connected (2t)-regular graph, where $t \ge 1$. Let $\mathcal{M}_3(G)$ be the graph obtained from G by fusing a bouquet of t triangles to every vertex of G. Then $\mathcal{M}_3(G)$ is a nut graph.

The construction $\mathcal{M}_3(G)$ is called the *triangle-multiplier construction* [8]. The choice of name is justified by the fact that $|V(\mathcal{M}_3(G))| = (2t + 1)|V(G)|$. Its effect on the automorphism group is described by the following proposition.

Proposition 5 ([8]) Let G be a connected (2t)-regular graph, where $t \ge 1$. Then $\operatorname{Aut}(G) \le \operatorname{Aut}(\mathcal{M}_3(G))$ and $|\operatorname{Aut}(\mathcal{M}_3(G))| = (2^t t!)^{|V(G)|} |\operatorname{Aut}(G)|$.

The group $\operatorname{Aut}(G)$ also acts on $\mathcal{M}_3(G)$. The additional automorphisms in $\operatorname{Aut}(\mathcal{M}_3(G))$ are well-understood. They arise from swapping the two degree-2 endvertices of the attached triangles and from permuting the triangles attached to a given vertex of graph *G*.

As mentioned above, Sabidussi showed for a range of properties that they can be required of the graph that realises a given finite group. Theorem 3.7 in [41] is more general than we need here; in a version tailored for our purposes, it is:

Theorem 6 ([41]) For every finite group \mathfrak{G} of order $|\mathfrak{G}| > 1$ and $d \ge 3$ there exist infinitely many connected *d*-regular graphs *G*, such that $\operatorname{Aut}(G) \cong \mathfrak{G}$.

Fig. 1 The graph $\mathcal{M}_3(H)$



The theorem of Sabidussi requires the group \mathfrak{G} to be non-trivial. However, as Bollobás has shown, a consequence of [10, Theorem 6] is that for $d \ge 3$ almost every *d*-regular graph is asymmetric. Thus it is easy to incorporate the trivial case into Theorem 6 and the requirement $|\mathfrak{G}| > 1$ could be omitted. Theorem 6 is the jumping-off point for our proofs.

3 Proof of Theorem 1

We are now ready to prove the main theorem. We will exploit a combination of the triangle-multiplier and coalescence constructions.

Proof of Theorem 1 If $|\mathfrak{G}| > 1$, then by Theorem 6, there exists a 4-regular graph H, such that $\operatorname{Aut}(H) \cong \mathfrak{G}$. In the case $|\mathfrak{G}| = 1$, simply take H to be the graph from Fig. 3a, i.e. an asymmetric 4-regular graph of the minimum order. By Proposition 4, the graph $\mathcal{M}_3(H)$ is a nut graph such that $\operatorname{Aut}(H) \leq \operatorname{Aut}(\mathcal{M}_3(H))$. By Proposition 5, $|\operatorname{Aut}(\mathcal{M}_3(H))| = 8^{|V(H)|} |\operatorname{Aut}(H)|$.

Let us denote $\theta = |V(H)|$ and $V(H) = \{h_1, h_2, \dots, h_\theta\}$. By definition, $H \subset \mathcal{M}_3(H)$. Let the extra vertices be denoted $t_i^{(j,k)}$ for $1 \le i \le \theta$ and $j, k \in \{1, 2\}$ such that the new neighbours of h_i are $t_i^{(1,1)}, t_i^{(1,2)}, t_i^{(2,1)}$ and $t_i^{(2,2)}$. Moreover, $t_i^{(j,1)}$ and $t_i^{(j,2)}$ are adjacent; see Fig. 1.

The automorphisms of $\mathcal{M}_3(H)$ are well-understood. Every $\alpha \in \operatorname{Aut}(H)$ is extended to an automorphism $\widehat{\alpha} \in \operatorname{Aut}(\mathcal{M}_3(H))$ by the following natural definition:

$$v^{\widehat{\alpha}} = \begin{cases} v^{\alpha}, & \text{if } v \in V(H); \\ t_{\ell}^{(j,k)}, & \text{if } v = t_i^{(j,k)} \text{ and } h_{\ell} = h_i^{\alpha}. \end{cases}$$
(1)

In addition to $\hat{\alpha}$ for $\alpha \in Aut(H)$, there are the following extra automorphisms in $Aut(\mathcal{M}_3(H))$:

$$\beta_{i,j} = (t_i^{(j,1)} t_i^{(j,2)}), \tag{2}$$

$$\gamma_i = (t_i^{(1,1)} \ t_i^{(2,1)})(t_i^{(1,2)} \ t_i^{(2,2)}), \tag{3}$$

for $i = 1, ..., \theta$ and j = 1, 2.

Fig. 2 The gadget graph Q_0 . The root vertices used in the first and second attachment are labelled q_1 and q_2 , respectively



We will remove the extra automorphisms by attaching 'gadgets' to vertices $t_i^{(1,1)}$ and $t_i^{(2,1)}$ for $i = 1, ..., \theta$.

Consider the graph Q_0 in Fig. 2. It is easy to verify that Q_0 is a nut graph of order 8 with $|\operatorname{Aut}(Q_0)| = 2$, and that vertices labelled q_1 and q_2 belong to different vertex orbits. Moreover, the respective stabilisers $\operatorname{Aut}(Q_0)_{q_1}$ and $\operatorname{Aut}(Q_0)_{q_2}$ are trivial.

Let *G* be the graph obtained from $\mathcal{M}_3(H)$ by a series of coalescence constructions. Start with $G_0:=\mathcal{M}_3(H)$. For $i = 1, \ldots, \theta$ define $G_i:=(G_{i-1}, t_i^{(1,1)}) \odot (Q_0, q_1)$. (The graph G_i is obtained from G_{i-1} by adding a new copy of Q_0 to G_{i-1} and identifying q_1 with the vertex $t_i^{(1,1)}$.) For $i = 1, \ldots, \theta$ define $G_{i+\theta}:=(G_{i+\theta-1}, t_i^{(2,1)}) \odot (Q_0, q_2)$. By Lemma 3, $G_1, G_2, \ldots, G_{2\theta}$ are all nut graphs. Let $G:=G_{2\theta}$.

Next, observe that automorphisms $\widehat{\alpha}$ can be extended naturally from $\mathcal{M}_3(H)$ to G. However, all automorphisms $\beta_{i,j}$ have been removed, since vertices $t_i^{(j,1)}$ now carry gadgets, while vertices $t_i^{(j,2)}$ do not (they are still of degree 2). Similarly, all automorphisms γ_i have been removed, since the gadget attached to $t_i^{(1,1)}$ does not map to the gadget attached to $t_i^{(1,2)}$, as vertices q_1 and q_2 are in different vertex orbits of Q_0 . Moreover, no new automorphisms have been introduced, as vertices $q_1, q_2 \in V(Q_0)$ have trivial stabilisers. Therefore, $\operatorname{Aut}(G) \cong \operatorname{Aut}(H) \cong \mathfrak{G}$.

We provided one nut graph G which realises the group \mathfrak{G} . To obtain an infinite family, we can subdivide each edge from $\{h_i t_i^{(1,2)} \mid i = 1, \ldots, \theta\}$ with 4σ vertices for any choice of $\sigma \ge 0$, i.e. we use the subdivision construction on these edges. \Box

Note that there are many 'degrees of freedom' in the proof of Theorem 1. In our construction, we could have taken H to be *any* 4-regular graph that realises the given group \mathfrak{G} . In case $|\mathfrak{G}| > 1$, Theorem 6 already provides infinitely many starting graphs H (which in turn produce infinitely many non-isomorphic nut graphs G). If $|\mathfrak{G}| = 1$, by [10], there are also infinitely many starting graphs H. At the coalescence stage, we could have picked different vertices as q_1 and q_2 in Q_0 (so long as they are in different vertex orbits). We could also have chosen a different gadget graph for Q_0 , or taken two different gadget graphs. We could have decorated both triangles with the same gadget and taken $q_1 = q_2$; that choice would have removed only elements $\beta_{i,j}$; to further remove elements γ_i , we could have used the subdivision construction on edges $h_i t_i^{(1,2)}$.

The multiplier-coalescence construction is prodigal in terms of the number of vertices of the nut graphs obtained. The order of graph *G* provided by the proof of Theorem 1 is 19|V(H)|, where |V(H)| is the order of the graph *H*. For a given group \mathfrak{G} , $|\mathfrak{G}| > 3$, with ν generators, the smallest 4-regular graph of the family constructed



Fig. 3 Graphs that realise the minimum order among 4-regular graphs with automorphism groups C_1 , C_2 and C_3 , respectively. These graphs are not uniquely determined; they are selected from sets of 4, 3 and 8 candidates, respectively

by Sabidussi in [41] is of order $4(\nu + 2)|\mathfrak{G}|$. Therefore, the order of the smallest graph obtained from Sabidussi's starting graph is $76(\nu + 2)|\mathfrak{G}|$. Code to compute this graph for any given finite group is supplied in [6].

Typically, much smaller examples can exist. Instead of the graph provided by the construction in the proof by Sabidussi, we could take the starting graph H to be a minimal 4-regular graph that realises \mathfrak{G} . For groups C_1 , C_2 and C_3 , minimal graphs H are shown in Fig.3. These have orders 10, 9 and 14, respectively. Application of the multiplier-coalescence construction gives rise to nut graphs of respective orders 190, 171 and 266.

4 Proof of Theorem 2

Proof of Theorem 2 The proof proceeds as for Theorem 1 to the point where gadgets are attached to $\mathcal{M}_3(H)$.

First, we prove the case d = 8. Consider the graphs P_1 , P_2 and P_3 in Fig. 4. They are non-isomorphic graphs; each of them contains six degree-3 vertices and six degree-4 vertices. The gadget Q_i , $1 \le i \le 3$, is obtained from P_i by adding a new vertex w_i to its complement $\overline{P_i}$ and joining w_i to all degree-7 vertices of $\overline{P_i}$. Observe that Q_1 , Q_2 and Q_3 are non-isomorphic graphs of order 13. All vertices of Q_i are of degree 8, except for w_i which is of degree 6. It is easy to verify that Q_1 , Q_2 and Q_3 are nut graphs and that their automorphism groups are trivial.

As in the proof of Theorem 1, we obtain G by a series of coalescence constructions. Start with $G_0:=\mathcal{M}_3(H)$. For $i = 1, \ldots, \theta$ define $G_i:=(G_{i-1}, t_i^{(1,1)}) \odot$ (Q_1, w_1) . For $i = 1, \ldots, \theta$ define $G_{i+\theta}:=(G_{i+\theta-1}, t_i^{(2,1)}) \odot (Q_1, w_1)$. For $i = 1, \ldots, \theta$ define $G_{i+2\theta}:=(G_{i+2\theta-1}, t_i^{(1,2)}) \odot (Q_2, w_2)$. For $i = 1, \ldots, \theta$ define $G_{i+3\theta}:=(G_{i+3\theta-1}, t_i^{(2,2)}) \odot (Q_3, w_3)$. In other words, gadgets Q_1, Q_2 and Q_3 are attached to degree-2 vertices of the triangles as indicated schematically in Fig. 5a. By Lemma 3, $G_1, G_2, \ldots, G_{4\theta}$ are all nut graphs. Let $G:=G_{4\theta}$.

By similar reasoning to that used in the proof of Theorem 1, we can see that automorphisms $\hat{\alpha}$ can be extended naturally from $\mathcal{M}_3(H)$ to G. Moreover, the gadgets



Fig. 4 The proto-gadget graphs for the proof of Theorem 2 in the case d = 8



 Q_1 , Q_2 and Q_3 were attached in a manner such that automorphisms $\beta_{i,j}$ and γ_i were removed. Further, attachment has introduced no new automorphisms, as these gadgets all have trivial symmetry. Hence, $\operatorname{Aut}(G) \cong \operatorname{Aut}(H) \cong \mathfrak{G}$. Finally, observe that all vertices of *G* are of degree 8. This proves the case d = 8. For higher values of *d* the proof is similar, but the search for the requisite number of proto-gadgets becomes rapidly more tedious.

To prove the result for a given *d*, we start with a (d/2)-regular graph *H* that realises the group \mathfrak{G} . If $|\mathfrak{G}| > 1$, Theorem 6 provides us with infinitely many such graphs *H*. If $|\mathfrak{G}| = 1$, by [10], there are also infinitely many such graphs *H*. By Proposition 4, $\mathcal{M}_3(H)$ is a nut graph. In this graph, there are d/4 triangles attached at every vertex of *H*. To remove the unwanted symmetries, every triangle is decorated by a different pair of gadgets. (See Fig. 5.) With *s* gadgets, we can form $\binom{s}{2}$ different pairs. We choose the smallest *s* such that $\binom{s}{2} \ge d/4$.

Figure 6 tabulates a sufficient set of proto-gadgets for degrees 12, 16, 20 and 24. The complement of $P_i^{(d)}$ contains d - 2 vertices of degree d - 1, and the remaining vertices are of degree d. To obtain $Q_i^{(d)}$, add a new vertex to the complement of $P_i^{(d)}$ and connect it to all vertices of degree d - 1. Graph $Q_i^{(d)}$ has exactly one vertex of degree d - 1, while the rest are of degree d. It is easy to verify that graphs $Q_1^{(d)}$, $Q_2^{(d)}$, ... are non-isomorphic and that they all have trivial symmetry.

We note that there are other strategies for the choice of gadgets in the proof. For example, one may prefer to find one gadget and then, to generate the others,



Fig. 6 The proto-gadget graphs for the proof of Theorem 2 for cases $d \in \{12, 16, 20, 24\}$. The set $P_i^{(d)}$ is used to construct the decorating gadgets Q_i , as described in the proof

repeatedly apply a construction that preserves symmetry but does not produce vertices of unwanted degree. One candidate is the so-called Fowler construction [8]. This approach would lead to a nut graph of yet larger order than the one generated by the present proof. The order of graph *G* constructed in the proof of Theorem 2 is $\omega(d)|V(H)|$, where $\omega(8) = 53$, $\omega(12) = 99$, $\omega(16) = 161$, $\omega(20) = 241$, and $\omega(24) = 337$. Recall that *H* denotes a (d/2)-regular starting graph that realises \mathfrak{G} .

5 Discussion

Constructive methods used to answer Kőnig's question typically do not provide minimal examples. Let $\alpha(\mathfrak{G})$ be the smallest order of the graphs representing the group \mathfrak{G} . Sabidussi [42] opened the question by studying the relationship between the values $\alpha(\mathfrak{G})$ and $|\mathfrak{G}|$. The value $\alpha(\mathfrak{G})$ has been determined for various families of groups (see [1] for abelian groups and a survey in [50]). Babai [4] gave $\alpha(\mathfrak{G}) \leq 2|\mathfrak{G}|$ provided



Fig. 7 a The smallest 4-regular graph, and b the smallest nut graph, that respectively represent the group \mathfrak{G}_{288}

that $\mathfrak{G} \notin \{C_3, C_4, C_5\}$; Deligeorgaki [25] improved this to $\alpha(\mathfrak{G}) \leq |\mathfrak{G}|$, with a longer list of exceptions that includes some infinite families. Planar graphs have also been considered from this point of view (for a survey see [34]).

Nut graphs raise analogous questions. It is clear that the constructions used in proving Theorems 1 and 2 are far from minimal. As an example, consider the group \mathfrak{G}_{288} of order 288, defined by its permutation representation

$$\mathfrak{G}_{288} = \langle (1, 2, 3)(4, 5)(6, 7, 8), (1, 8)(2, 7)(3, 6)(4, 9)(5, 10), (7, 8) \rangle.$$

In GAP [49], this group can be obtained by calling SmallGroup (288, 889). The smallest 4-regular graph representing this group that is given by Sabidussi's construction (Theorem 6) is of order 5760. Expansion to a nut graph by the construction used in the proof of Theorem 1 gives order 109440. A much smaller 4-regular parent graph could have been used as the basis for that construction, since the smallest 4-regular graph representing \mathfrak{G}_{288} is of order 11; see Fig. 7a, leading to a nut graph of order 209. However, the database obtained by nutgen [14] reveals that the smallest nut graph that represents \mathfrak{G}_{288} has only 10 vertices; see Fig. 7b.

Let $\beta(\mathfrak{G})$ be the smallest order of the nut graphs representing the group \mathfrak{G} . It is evident that $\beta(\mathfrak{G}) \ge \alpha(\mathfrak{G})$. For groups up to order 6, the values are

$$\begin{aligned} \alpha(C_1) &= 1, \, \beta(C_1) = 9; & \alpha(C_2) = 2, \, \beta(C_2) = 8; \\ \alpha(C_3) &= 9, \, \beta(C_3) = 11; & \alpha(C_4) = 10, \, \beta(C_4) = 11; \\ \alpha(C_2 \times C_2) &= 4, \, \beta(C_2 \times C_2) = 7; & \alpha(C_5) = 15, \, \beta(C_5) = 15; \\ \alpha(C_3 \times C_2) &= 11, \, \beta(C_3 \times C_2) = 11; & \alpha(C_3 \rtimes C_2) = 3, \, \beta(C_3 \rtimes C_2) = 7. \end{aligned}$$

These numbers were found by computer search of the available censuses of nut graphs [11, 16]. For C_5 , [1, Lemma 5.2] gives us $\alpha(C_5) = 15 \leq \beta(C_5)$. The equality $\beta(C_5) = 15$ was established by finding an example.

Problem 7 Given any finite group \mathfrak{G} , find a nut graph *G* of minimum order, such that Aut(*G*) $\cong \mathfrak{G}$. Find an upper bound on $\beta(\mathfrak{G})$ in terms of $|\mathfrak{G}|$.

Another question relates to the degrees of regular nut graphs that represent groups \mathfrak{G} .

Problem 8 Given a finite group \mathfrak{G} and an integer $d \ge 3$, find a *d*-regular nut graph *G*, such that Aut(*G*) $\cong \mathfrak{G}$.

Theorem 2 supplies the answer for small cases $d \equiv 0 \pmod{4}$, and the same technique could be used to extend the list of degrees obeying that restriction. As the proto-gadget graphs in Fig. 6 were obtained by computer search, this task becomes increasingly onerous with higher degree. But the present strategy, based on the triangle-multiplier construction, still leaves unresolved all cases with $d \not\equiv 0 \pmod{4}$. Extension to an arbitrary degree will need a different approach.

A missing case of particular interest for the chemical applications mentioned in the introduction is d = 3. Interestingly, the eponymous Frucht graph, introduced in [31] as a small graph that has trivial symmetry, is both cubic (in fact polyhedral) and a nut graph. It has order 12 and is the smallest cubic nut graph of trivial symmetry. Frucht also treated the group C_2 separately; his graph that realises this group (see [31, Fig. 2]) is not a nut graph. It is straightforward to show that his general constructions [31] for groups of order greater than 2 do not yield nut graphs. The repeated motifs devised by Frucht (the 'corners' [31]) give rise to at least one non-trivial kernel eigenvector with some zero entries in the constructed graph. Hence, it would be interesting to find a construction that yields cubic nut graphs directly.

Acknowledgements We would like to thank our colleague Prof. Primož Potočnik for fruitful discussion and for drawing our attention to [31] during a research visit to Sheffield. The work of Nino Bašić is supported in part by the Slovenian Research Agency (research program P1-0294 and research projects N1-0140 and J1-2481). PWF thanks the Leverhulme Trust for an Emeritus Fellowship on the theme of 'Modelling molecular currents, conduction and aromaticity' and the Francqui Foundation for the award of an International Francqui Professorship.

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit http://creativecommons.org/licenses/by/4.0/.

References

- Arlinghaus, W.C.: The Classification of Minimal Graphs with Given Abelian Automorphism Group, volume 330 of Memoirs of the American Mathematical Society, American Mathematical Society, Providence, RI (1985) doi:https://doi.org/10.1090/memo/0330
- Babai, L.: Automorphism groups of planar graphs. II. In: infinite and finite sets, North-Holland, Amsterdam-London, volume 10 of Colloq. Math. Soc. János Bolyai, pp. 29–84 (1975)
- Babai, L.: Automorphism groups of planar graphs I. Discrete Math. 2, 295–307 (1972). https://doi. org/10.1016/0012-365x(72)90010-6
- Babai, L.: On the minimum order of graphs with given group. Can. Math. Bull. 17, 467–470 (1974). https://doi.org/10.4153/cmb-1974-082-9
- Babai, L.: On the abstract group of automorphisms: combinatorics, pp. 1–40. Cambridge University Press, Cambridge (1981)
- Bašić, N., Fowler, P.W.: Nut graphs with a given automorphism group: supplementary material (GitHub repository), https://github.com/nbasic/nut-graphs-automorphisms
- Bašić, N., Knor, M., Škrekovski, R.: On 12-regular nut graphs. Art Discrete Appl. Math. 5, #P2.01 (2022). https://doi.org/10.26493/2590-9770.1403.1b1

- Bašić, N., Fowler, P.W., Pisanski, T.: Vertex and edge orbits in nut graphs. Electron. J. Comb. 31, #P2.38 (2024). https://doi.org/10.37236/12619
- 9. Biggs, N.: Algebraic Graph Theory Cambridge Mathematical Library, 2nd edn. Cambridge University Press, Cambridge (1993)
- Bollobás, B.: Distinguishing vertices of random graphs. In: graph Theory, North-Holland, Amsterdam-New York, volume 62 of North-Holland Mathematics Studies, pp. 33–49 (1982)
- Brinkmann, G., Coolsaet, K., Goedgebeur, J., Mélot, H.: House of graphs: a database of interesting graphs. Discrete Appl. Math. 161, 311–314 (2013). https://doi.org/10.1016/j.dam.2012.07.018
- 12. Brouwer, A.E., Haemers, W.H.: Spectra of Graphs, Universitext. Springer, New York (2012)
- Chung, F.R.K.: Spectral Graph Theory. CBMS Regional Conference Series in Mathematics, vol. 92. American Mathematical Society, Providence (1997)
- Coolsaet, K., Fowler, P.W., Goedgebeur, J.: Nut graphs, homepage of Nutgen, http://caagt.ugent.be/ nutgen/
- Coolsaet, K., Fowler, P.W., Goedgebeur, J.: Generation and properties of nut graphs. MATCH Commun. Math. Comput. Chem. 80, 423–444 (2018)
- Coolsaet, K., D'hondt, S., Goedgebeur, J.: House of graphs 2.0: a database of interesting graphs and more. Discrete Appl. Math. 325, 97–107 (2023). https://doi.org/10.1016/j.dam.2022.10.013
- 17. Cvetković, D.M., Doob, M., Sachs, H.: Spectra of Graphs: Theory and Applications, 3rd edn. Johann Ambrosius Barth, Heidelberg (1995)
- Cvetković, D.M., Rowlinson, P., Simić, S.: Eigenspaces of Graphs, volume 66 of Encyclopedia of Mathematics and its Applications. Cambridge University Press, Cambridge (1997)
- Cvetković, D.M., Rowlinson, P., Simić, S.: An Introduction to the Theory of Graph Spectra. London Mathematical Society Student Texts, vol. 75. Cambridge University Press, Cambridge (2010)
- Damnjanović, I.: On the nullities of quartic circulant graphs and their extremal null spaces, (2022). arXiv:2212.12959 [math.CO]
- Damnjanović, I.: Complete resolution of the circulant nut graph order-degree existence problem. Ars. Math. Contemp. (2023). https://doi.org/10.26493/1855-3974.3009.6df
- 22. Damnjanović, I.: Two families of circulant nut graphs. Filomat **37**, 8331–8360 (2023)
- 23. Damnjanović, I., Stevanović, D.: On circulant nut graphs. Linear Algebra Appl. 633, 127–151 (2022). https://doi.org/10.1016/j.laa.2021.10.006
- Damnjanović, I., Bašić, N., Pisanski, T., Žitnik, A.: Classification of cubic tricirculant nut graphs. Electron. J. Comb. 31, #P2.31 (2024). https://doi.org/10.37236/12668
- Deligeorgaki, D.: Smallest graphs with given automorphism group. J. Algebraic Combin. 56, 609–633 (2022). https://doi.org/10.1007/s10801-022-01125-2
- Dobson, T., Malnič, A., Marušič, D.: Symmetry in Graphs, volume 198 of Cambridge Studies in Advanced Mathematics. Cambridge University Press, Cambridge (2022)
- 27. Fowler, P.W., Manolopoulos, D.E.: An Atlas of Fullerenes. Dover Publications, Mineola (2007)
- Fowler, P.W., Gauci, J.B., Goedgebeur, J., Pisanski, T., Sciriha, I.: Existence of regular nut graphs for degree at most 11. Discuss. Math. Graph Theory 40, 533–557 (2020). https://doi.org/10.7151/dmgt. 2283
- Fowler, P.W., Pisanski, T., Bašić, N.: Charting the space of chemical nut graphs. MATCH Commun. Math. Comput. Chem. 86, 519–538 (2021)
- Frucht, R.: Herstellung von Graphen mit vorgegebener abstrakter Gruppe. Compos. Math. 6, 239–250 (1939)
- Frucht, R.: Graphs of degree three with a given abstract group. Can. J. Math. 1, 365–378 (1949). https:// doi.org/10.4153/cjm-1949-033-6
- 32. Godsil, C., Royle, G.: Algebraic Graph Theory, volume 207 of Graduate Texts in Mathematics. Springer-Verlag, New York (2001)
- Grannell, M.J., Griggs, T.S., Lovegrove, G.J.: Even-cycle systems with prescribed automorphism groups. J. Combin. Des. 21, 142–156 (2013). https://doi.org/10.1002/jcd.21334
- Jones, C.J., Lauderdale, L.-K., Lubow, S.E., Triplitt, C.J.: Vertex-minimal planar graphs with a prescribed automorphism group. J. Algebraic Combin. 53, 355–367 (2021). https://doi.org/10.1007/ s10801-019-00932-4
- Kőnig, D.: Theorie Der Endlichen Und Unendlichen Graphen. American Mathematical Society, Providence (2001)
- Lovegrove, G.J.: Odd-cycle systems with prescribed automorphism groups. Discrete Math. 314, 6–13 (2014). https://doi.org/10.1016/j.disc.2013.09.006

- Mendelsohn, E.: On the groups of automorphisms of Steiner triple and quadruple systems. J. Combin. Theory Ser. A 25, 97–104 (1978). https://doi.org/10.1016/0097-3165(78)90072-9
- Moon, J.W.: Tournaments with a given automorphism group. Can. J. Math. 16, 485–489 (1964). https:// doi.org/10.4153/cjm-1964-050-9
- Nowitz, L.A., Watkins, M.E.: Graphical regular representations of non-abelian groups. I. Can. J. Math. 24, 993–1008 (1972). https://doi.org/10.4153/cjm-1972-101-5
- Nowitz, L.A., Watkins, M.E.: Graphical regular representations of non-abelian groups. II. Can. J. Math. 24, 1009–1018 (1972). https://doi.org/10.4153/cjm-1972-102-3
- Sabidussi, G.: Graphs with given group and given graph-theoretical properties. Can. J. Math. 9, 515– 525 (1957). https://doi.org/10.4153/cjm-1957-060-7
- Sabidussi, G.: On the minimum order of graphs with given automorphism group. Monatsh. Math. 63, 124–127 (1959). https://doi.org/10.1007/bf01299094
- Sciriha, I., Farrugia, A.: From nut graphs to molecular structure and conductivity. Mathematical chemistry monographs, vol. 23. University of Kragujevac and Faculty of Science Kragujevac, Kragujevac (2021)
- Sciriha, I.: Coalesced and embedded nut graphs in singular graphs. ARS Math. Contemp. 1, 20–31 (2008). https://doi.org/10.26493/1855-3974.20.7cc
- Sciriha, I., Fowler, P.W.: Nonbonding orbitals in fullerenes: nuts and cores in singular polyhedral graphs. J. Chem. Inf. Model. 47, 1763–1775 (2007). https://doi.org/10.1021/ci700097j
- Sciriha, I., Fowler, P.W.: On nut and core singular fullerenes. Discrete Math. 308, 267–276 (2008). https://doi.org/10.1016/j.disc.2006.11.040
- 47. Sciriha, I., Gutman, I.: Nut graphs: maximally extending cores. Util. Math. 54, 257-272 (1998)
- 48. Streitwieser, A.: Molecular Orbital Theory for Organic Chemists. Wiley, Hoboken (1961)
- The GAP Group, GAP groups, algorithms, and programming, Version 4.13.0 (2024). https://www.gap-system.org
- Woodruff, J.A.: A survey of graphs of minimum order with given automorphism group, Master's thesis, The University of Texas at Tyler, (2016). http://hdl.handle.net/10950/423

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.