

# A CENSUS OF SMALL TRANSITIVE GROUPS AND VERTEX-TRANSITIVE GRAPHS

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ABSTRACT. We describe two similar but independently-coded computations used to construct a complete catalogue of the transitive groups of degree less than 48, thereby verifying, unifying and extending the catalogues previously available. From this list, we construct all the vertex-transitive graphs of order less than 48. We then present a variety of summary data regarding the transitive groups and vertex-transitive graphs, focussing on properties that seem to occur most frequently in the study of groups acting on graphs. We illustrate how such catalogues can be used, first by finding a complete list of the elusive groups of order at most 47 and then by completely determining which groups of order at most 47 are CI groups.

## 1. INTRODUCTION

In the study of finite permutation groups and the study of groups acting on graphs, transitive groups play a fundamental role. For well over 100 years, researchers have used catalogues of transitive groups of (necessarily) small degree to provide examples and counterexamples, or simply to identify promising lines of enquiry. G. A. Miller was one of the most prolific of these early cataloguers with many of the 400+ papers in his *Collected Works* [9] listing small groups with particular properties (transitive, primitive, etc). The difficulty of the task is determined by the prime factorisation of the degree, with the most difficult degrees being those with several small prime factors. The first “difficult degree” is 12 and although Miller [8] published a supposedly complete list of the transitive permutation groups of degree 12 as early as 1896, it was later discovered to contain a handful of mistakes (Royle [10]). Miller notwithstanding, constructing catalogues of combinatorial objects is a difficult and error-prone task by hand, yet one particularly amenable to computation. As computers became more widespread and more powerful, the catalogues of transitive groups were extended to larger and larger degrees until by 1996 the lists were complete up to degree 31 (see Hulpke [7] for an overview including references to the various authors who contributed to these extensions).

When the degree is a power of a small prime, then we expect the computation to be the most difficult and to yield the largest collections of transitive groups, and so 32 is the next difficult case. This case was resolved by Cannon & Holt [2] who determined that there are 2801324 transitive groups of degree 32, which is two orders of magnitude more than the total number of all transitive groups of degree less than 32. (Throughout this

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paper, when we talk about classifying transitive permutation groups of a given degree  $n$ , then we always mean classifying them up to conjugacy in  $\text{Sym}(n)$ , and when we say, for example, that there are 2801324 transitive groups of degree 32, we really mean that there are 2801324 conjugacy classes of such subgroups in  $\text{Sym}(n)$ . It would not be difficult to count the sizes of each of these classes and thereby count the total number of groups.)

In this paper we extend the catalogues of transitive groups up to degree 47, i.e. just short of the next really difficult degree, namely 48. For “end-users” of a catalogue of combinatorial objects, the primary concern is the extent to which the user has confidence that the catalogue is correct and complete. Increasingly, computational papers in combinatorics are addressing these concerns through redundancy — two or more researchers writing programs that are independent (as far as possible) and then cross-checking the results. Along these lines, we present two computations that were conducted totally independently, and yielded the same output when first compared. (More precisely, we checked that the lists of groups output by the two computations had the same lengths, and that each group on one of the lists was conjugate in  $\text{Sym}(n)$  to exactly one group on the other list.) Both computations were done in MAGMA [1] and so both rely on basic functions such as calculating the maximal subgroups of a finite group and checking whether two groups are conjugate in the symmetric group. As these functions have by now received decades of user-testing, we feel confident that the chance of an error from this source is negligible.

The first author is in the process of computing the transitive groups of degree 48, but with no great urgency, so this computation is not expected to complete in the foreseeable future. Based on the numbers of groups found so far, it is looking as though there could be about 200 million such groups in total, of which all except about 3.4 million will have minimal block size 2.

## 2. FIRST COMPUTATION

The first computation was based around recursive use of the `MaximalSubgroups` command of MAGMA [1], together with partitioning the computation into a large number of disjoint parts that can be run independently (for example, on multiple computers or just multiple cores on a single computer.) It uses only elementary permutation group theory, instead seeking to be as simple and robust as possible. The majority of the effort in this approach involves implementing computational techniques to partition the search, to eliminate as much duplication as possible, and to manage and collate the resulting large data sets; it involves more “data bookkeeping” than mathematics.

The *primitive* permutation groups are known up to degree 4095 (See [3]) and are incorporated into the databases of both MAGMA and GAP, and so we need only consider the imprimitive groups. By definition if a group  $G$  acting transitively on the set  $\Omega$  of size  $n$  is not primitive, then there is at least one partition of  $\Omega$  into a *block system*  $\mathcal{B}$  such that  $G$  permutes the blocks of  $\mathcal{B}$ . If we let  $G^{\mathcal{B}}$  denote the action of  $G$  on the blocks (“the top group”) and if  $\mathcal{B}$  has  $n/k$  blocks of size  $k$ , then  $G^{\mathcal{B}}$  is a transitive permutation group of

degree  $n/k$ . Thus we can associate to each group  $G$  a set of pairs of the form

$$\{(k, G^{\mathcal{B}}) : \mathcal{B} \text{ is a minimal block system for } G \text{ with blocks of size } k\}.$$

If this set contains more than one pair (imprimitive groups may of course have more than one minimal block system), then we wish to distinguish just one of them. Thus we define the *signature* of an imprimitive permutation group to be the *lexicographically least* pair  $(k, G^{\mathcal{B}})$  associated with  $G$ , where the second component is indexed according to its order in the list of transitive groups of degree  $n/k$  already in MAGMA. But note that it can happen that two different minimal block systems of  $G$  define the same signature.

Our aim will be to separate the computation into parts, with each part constructing only the groups with a particular signature. Given an integer  $k$  such that  $1 < k < n$ , and a transitive group  $H$  of degree  $n/k$ , the wreath product  $\text{Sym}(k) \wr H$  contains (a conjugate of) every transitive group of degree  $n$  with signature  $(k, H)$ . Therefore, at least in principle, these groups can all be found by exploring the subgroup lattice of  $\text{Sym}(k) \wr H$ . To do this, we repeatedly use the `MaximalSubgroups` command of MAGMA thereby traversing the subgroup lattice downwards and in a breadth-first fashion, pruning each branch of the search as soon as it produces groups with signature differing from  $H$ , while using conjugacy tests to avoid duplication as far as possible.

More precisely, the program maintains a list of *active* transitive subgroups of  $\text{Sym}(k) \wr H$  in descending group order. This list is initialised with the single group  $\text{Sym}(k) \wr H$  which by default is constructed with the “canonical block system” with blocks  $\{1, 2, \dots, k\}$ ,  $\{k + 1, k + 2, \dots, 2k\}$ , and so on. At each step, the program removes an active subgroup of largest order, say  $G$ , from the list for processing. The processing stage computes the transitive maximal subgroups of  $G$ , and tests each of these maximal subgroups  $M$  to determine if it should be retained or not, using the following rules:

- (1) If  $M$  has a minimal block system with blocks of size smaller than  $k$ , then reject,
- (2) If the action of  $M$  on the canonical block system is not equal to  $H$ , then reject,
- (3) If  $M$  is conjugate (in  $\text{Sym}(k) \wr \text{Sym}(n/k)$ ) to a group on the list of active subgroups, then reject.

If  $M$  passes all these tests, it is then added to the list of active subgroups in the appropriate position (depending on its order).

The rationale behind the first two tests is that if  $M$  fails either of them, then a conjugate of  $M$  will be found during another part of the search, either the search for all transitive groups preserving a block system with strictly smaller blocks, or during the search for transitive groups with a different “top group”. The third test ensures that the groups in each part are pairwise non-conjugate.

Every group that is processed is a transitive group with a minimal block system with blocks of size  $k$ , no block systems with blocks with fewer than  $k$  elements, and with top-group isomorphic to  $H$ . Conversely, every transitive group with these three properties will at some stage enter the list of active subgroups and then be processed. Therefore by adding an output step as the point that a group enters (or leaves) the list of active

subgroups, we can compute all transitive groups associated with a particular  $(k, H)$  pair. By running over all possibilities for  $k$  and letting  $H$  range over all the transitive groups of degree  $n/k$ , every transitive group of degree  $n$  is constructed. As indicated previously, we need to eliminate conjugate groups that occur in more than one part of the computation, which results from groups having multiple minimal block systems. If a group has two minimal block systems that define different signatures, then we only keep it if its canonical block system has minimal signature. But if there is more than one minimal block system with the same minimal signature as the canonical block system, then a final conjugacy check is required to eliminate possible duplicates.

### 3. SECOND COMPUTATION

For many of the calculations, we used essentially the same methods as in the first computation, although these calculations were carried out completely independently. In fact, for all degrees except for 36 and 40, we were able to complete the calculation in a single run, without any need for filtering by size of blocks, by repeated application of the MAGMA commands `MaximalSubgroups` and `IsConjugate`, starting with `Sym(n)`. But for some degrees, such as 42 and 44, it was quicker to use the alternative techniques that we shall now describe for the smaller block sizes.

In the following descriptions, we use ATLAS notation for group structures. In particular, an integer  $k$  in a structure description denotes a cyclic group of order  $k$ . For calculations with  $n$  even and minimal block size 2, we used a method similar to the one described in detail in [2, Section 2.2], which was applied to the enumeration of the transitive groups of degree 32 with minimal block size 2. Suppose that the transitive group  $G$  preserves the block system  $\mathcal{B}$  with blocks of size 2. So  $G \leq W := 2 \wr \text{Sym}(n/2)$ . Then  $\bar{H} := G^{\mathcal{B}}$  is one of the groups in the known list of transitive groups of degree  $n/2$ , and  $G \leq H := 2 \wr \bar{H}$ . As in the first computation, we calculate those groups with signature  $(2, \bar{H})$  for each individual group  $\bar{H}$ .

Let  $K \cong 2^{n/2}$  be the kernel of the action of  $W$  on  $\mathcal{B}$ . Then we can regard  $K$  as a module for  $\bar{H}$  over the field  $\mathbb{F}_2$  of order 2, and  $M := G \cap K$  is an  $\mathbb{F}_2\bar{H}$ -submodule. We can use the MAGMA commands `GModule` and `Submodules` to find all such submodules. In fact, since we are looking for representatives of the conjugacy classes of transitive subgroups of  $W$ , we only want one representative of the conjugation action of  $N := 2 \wr N_{\text{Sym}(n/2)}(\bar{H})$  on the set all  $\mathbb{F}_2\bar{H}$ -submodules  $M$  of  $K$ , and we use the MAGMA command `IsConjugate` to find such representatives.

Now, for each such pair  $(\bar{H}, M)$ , the transitive groups  $G$  with  $\bar{H} = G^{\mathcal{B}}$  and  $M = G \cap K$  correspond to complements of  $K/M$  in  $H/M$ , and the  $H$ -conjugacy classes of such complements correspond to elements of the cohomology group  $H^1(\bar{H}, K/M)$ , which can be computed in MAGMA.

We also need to test these groups  $G$  for conjugacy under the action of  $N_N(M)$ , which can either be done in straightforward fashion using MAGMA's `IsConjugate` function or (with a little more programming but usually faster in terms of computation) using an induced action on the cohomology group. Finally, for each  $G$  that we find, we need

to find all blocks systems with block size 2 preserved by  $G$ , so that we can eliminate occurrences of groups that are conjugate in  $\text{Sym}(n)$  but arise either for distinct pairs  $(\bar{H}, M)$  or more than once for the same pair. We refer the reader to [2, Section 2.2] for further details.

In the case  $n = 36$ , we used a similar method for blocks systems with blocks of size 3. In this case, we have  $G \leq \text{Sym}(3) \wr \text{Sym}(12) \cong 3^{12} : (2 \wr \text{Sym}(12))$ . Let  $H$  be the projection of  $G$  onto the quotient group  $2 \wr \text{Sym}(12)$ . Then  $H \leq \text{Sym}(24)$  and  $H$  preserves a block system with blocks of size 2 and projects onto a transitive subgroup of degree 12. We can find the possible groups  $H$  using the method just described for blocks of size 2 (although there is a minor complication, because  $H$  is not necessarily transitive), and then find the possible groups  $G$  using the same method, but working with modules over  $\mathbb{F}_3$  rather than  $\mathbb{F}_2$ .

In the cases  $n = 36$  and  $n = 40$  with minimal block size 4, we did a corresponding 3-step calculation using  $G \leq \text{Sym}(4) \wr \text{Sym}(n/4) \cong 2^{n/2} : 3^{n/4} : 2^{n/4} : \text{Sym}(n/4)$ .

Finally, for  $n = 40$  with minimal block size 5, the induced action of the stabilizer of a block on that block is transitive of degree 5, and its structure is one of 5, 5:2, 5:4,  $\text{Alt}(5)$ , or  $\text{Sym}(5)$ . We enumerated those groups in the final two of these cases separately using the methods of the first computation. For the first three cases we used a 3-step calculation using  $G \leq 5^8 : 2^8 \cdot 2^8 : \text{Sym}(n/5)$ .

These computations were originally carried out in 2014 on a number of different computers with different specifications, so it is difficult to provide a meaningful estimate of the total cpu-time involved, but this was of the order of 150 hours in total. Perhaps surprisingly, the most time consuming individual computation was of the case  $n = 36$  with block size 9, which took about 47 hours. The calculation requiring the most memory was the case  $n = 40$  with block size 2, which used about 27GB.

#### 4. TRANSITIVE GROUPS

The numbers of transitive groups of each degree (up to conjugacy in  $\text{Sym}(n)$ ) are shown in Table 1. As expected, the number of transitive groups is primarily dependent on the number of repeated prime factors in the degree. The single degree  $n = 32$  provides well over 90% of the transitive groups in the entire catalogue.

For many applications that involve considering all possible transitive actions of a certain degree, it is sufficient to consider only the *minimal transitive groups* i.e., transitive groups with no proper transitive subgroups. (One example of this can be found in the next section, where all vertex-transitive graphs are constructed.) Testing if a transitive graph is minimal can be done by finding all its maximal subgroups and verifying that none are transitive. As most of the groups are not minimal transitive, it proves useful in practice to first construct some random subgroups in an attempt to find a transitive proper subgroup, only undertaking the more expensive step of finding all maximal subgroups if this fails.

$n$	$g(n)$	$n$	$g(n)$	$n$	$g(n)$	$n$	$g(n)$	$n$	$g(n)$
		11	8	21	164	31	12	41	10
2	1	12	301	22	59	32	2801324	42	9491
3	2	13	9	23	7	33	162	43	10
4	5	14	63	24	25000	34	115	44	2113
5	5	15	104	25	211	35	407	45	10923
6	16	16	1954	26	96	36	121279	46	56
7	7	17	10	27	2392	37	11	47	6
8	50	18	983	28	1854	38	76		
9	34	19	8	29	8	39	306		
10	45	20	1117	30	5712	40	315842		

TABLE 1. Numbers  $g(n)$  of transitive groups of degree  $n$ 

$n$	$m(n)$	$n$	$m(n)$	$n$	$m(n)$	$n$	$m(n)$	$n$	$m(n)$
		11	1	21	5	31	1	41	1
2	1	12	17	22	6	32	12033	42	84
3	1	13	1	23	1	33	3	43	1
4	2	14	6	24	213	34	7	44	148
5	1	15	4	25	2	35	4	45	41
6	4	16	75	26	7	36	436	46	4
7	1	17	1	27	20	37	1	47	1
8	5	18	23	28	30	38	5		
9	2	19	1	29	1	39	4		
10	6	20	47	30	79	40	1963		

TABLE 2. Numbers  $m(n)$  of minimal transitive groups of degree  $n$ 

The numbers of minimal transitive groups of each order are given in Table 2, which shows that the numbers of minimal transitive groups vary in much the same way as the numbers of all transitive groups.

## 5. VERTEX-TRANSITIVE GRAPHS

If  $G$  is a group acting transitively on a set  $\Omega$ , then it is straightforward to construct all the  $G$ -invariant graphs or digraphs with vertex set  $\Omega$ . The orbits of  $G$  on  $\Omega \times \Omega$  are called the *orbitals* of  $G$  and it is immediate that the arc set of a  $G$ -invariant digraph is a union of these orbitals. If  $\mathcal{O}$  is an orbital containing a pair  $(a, b)$  with  $a \neq b$ , then

we denote by  $\mathcal{O}'$  the orbital containing  $(b, a)$ . It is possible that  $\mathcal{O}'$  is equal to  $\mathcal{O}$ , in which case  $\mathcal{O}$  is called *self-paired*, and otherwise  $\mathcal{O}$  and  $\mathcal{O}'$  are *paired*. Any subset of the orbitals determines a  $G$ -invariant digraph, and any subset of the orbitals closed under taking pairs determines a  $G$ -invariant *graph*. (We view a graph simply as a digraph that happens to have the property that if  $(a, b)$  is an arc, then so is  $(b, a)$ , and thus “digraphs” includes “graphs”.) The set of  $G$ -invariant digraphs arising in this way will usually contain isomorphic digraphs, but for the small sizes that we are considering, it is easy to filter these out, thus yielding a complete list of the pairwise non-isomorphic  $G$ -invariant digraphs.

The complete list of vertex-transitive digraphs can be computed by repeating this computation for each of the transitive groups of degree  $n$ , combining the resulting lists, and then performing one final filtering process to remove all but one copy of each digraph. To construct only *graphs*, the process is modified slightly to ensure that the orbitals are included/excluded in pairs in the arc-set of the digraph under construction.

If  $H, G$  are transitive groups such that  $H \leq G$ , then the orbitals of  $G$  are unions of the orbitals of  $H$  and so the set of  $H$ -invariant digraphs contains the set of  $G$ -invariant digraphs. Thus it is sufficient to perform the construction only for the minimal transitive groups. The *regular* groups of degree  $n$  (i.e., those with degree equal to order) are necessarily minimal transitive, and the digraphs arising from these groups are exactly the *Cayley digraphs* of that order. Any non-Cayley digraphs can *only* be created when the larger groups are processed, though these groups will usually produce Cayley digraphs as well.

The numbers of transitive (resp. Cayley) graphs peak at degree 44 even though there are far fewer groups of degree 44 than, say, degree 32. We can give a heuristic argument as to why this is to be expected as follows. For this range of degrees, the majority of the vertex-transitive graphs are Cayley graphs, and so groups that contribute large numbers of Cayley graphs dominate the enumeration. If a group  $G$  has  $a$  involutions and  $b$  non-involutions, then a first approximation to the number of distinct Cayley sets (i.e. inverse-closed subsets of  $G$  that are pairwise inequivalent under  $\text{Aut}(G)$ ) is given by

$$\frac{2^{a+b/2}}{|\text{Aut}(G)|}.$$

For a fixed degree, this value will be greatest when  $a$  is large and  $|\text{Aut}(G)|$  is small. For the range of degrees currently under consideration, the *dihedral groups* with relatively large  $a$  and relatively small  $b$  give the greatest value. If the degree is a power of 2 then the elementary abelian 2-group has the largest possible value of  $a$ , because every non-identity element is an involution. However the automorphism group of  $\mathbb{Z}_2^n$  is  $GL(n, 2)$ , which is very large, and so elementary abelian groups contribute relatively few Cayley graphs to the total.

$n$	$t(n)$	$c(n)$	$n$	$t(n)$	$c(n)$	$n$	$t(n)$	$c(n)$
			16	286	278	32	677402	659232
			17	36	36	33	6768	6768
2	2	2	18	380	376	34	132580	131660
3	2	2	19	60	60	35	11150	11144
4	4	4	20	1214	1132	36	1963202	1959040
5	3	3	21	240	240	37	14602	14602
6	8	8	22	816	816	38	814216	814216
7	4	4	23	188	188	39	48462	48462
8	14	14	24	15506	15394	40	13104170	13055904
9	9	9	25	464	464	41	52488	52488
10	22	20	26	4236	4104	42	9462226	9461984
11	8	8	27	1434	1434	43	99880	99880
12	74	74	28	25850	25784	44	39134640	39134544
13	14	14	29	1182	1182	45	399420	399126
14	56	56	30	46308	45184	46	34333800	34333800
15	48	44	31	2192	2192	47	364724	364724

TABLE 3. Numbers  $t(n)$ ,  $c(n)$  of transitive and Cayley graphs of order  $n$ 

## 6. TWO APPLICATIONS

One of the major reasons to construct catalogues of combinatorial objects is to gather evidence relating to conjectures or other open questions. Even if a newly-constructed catalogue does not directly contain a counterexample to a conjecture (thereby immediately resolving it), it can be useful in refining a researcher's intuition regarding both the typical and extremal behaviour of the objects in the catalogue.

In the remainder of this section, we consider two areas in which computational evidence has played a role, and augment that evidence with information derived from the list of transitive groups described in this paper.

**6.1. Elusive Groups.** A permutation group  $G$  is called *elusive* if it contains no *fixed-point-free* elements (i.e., *derangements*) of prime order. Elusive groups are interesting because of their connection to Marušič's *Polycirculant Conjecture* which asserts that the automorphism group of a vertex-transitive digraph is *never elusive*. In principle, a positive resolution of the polycirculant conjecture may simplify the construction and analysis of vertex-transitive graphs and digraphs, as it would then be possible to assume the presence of an automorphism with  $n/p$  cycles of length  $p$  for some prime  $p$ . For example, early catalogues of vertex-transitive graphs relied on ad hoc arguments to



show that all transitive groups of the specific degrees under consideration have a suitable derangement of prime order.

A permutation group  $G$  is called *2-closed* if there is no group properly containing  $G$  with the same orbitals as  $G$ . The automorphism group of a vertex-transitive digraph is necessarily 2-closed, because it is *already* the maximal group (by inclusion) that fixes the set of arcs of the digraph, which is a union of some of the orbitals. The conjecture can thus be strengthened to the assertion that there are no elusive 2-closed transitive groups, yielding a conjecture that was first proposed by Klin.

One might hope that there are simply no elusive groups at all, in which case both conjectures would hold vacuously, but in fact there are a number of sporadic examples of elusive groups and a handful of infinite families. All the known elusive groups are not 2-closed, so do not provide counterexamples for either conjecture.

It is relatively easy to test the groups for the property of being elusive by checking to see if any of the conjugacy class representatives are derangements of prime order. For the larger groups, it is often faster to first generate some number of randomly selected elements inside each of the Sylow subgroups in the hope of stumbling on a suitable derangement without the cost of computing all the conjugacy classes.

**Proposition 6.1.** *A transitive permutation group  $G$  of degree  $n < 48$  is elusive if and only if one of the following holds:*

- (1)  $G$  has degree 12 and is either the group  $M_{11}$  (acting on 12 points), or one of its four proper transitive subgroups,
- (2)  $G$  has degree 24 and is one of the 19 groups described by Giudici [5],
- (3)  $G$  has degree 36 and is either a particular group of shape  $((C_9^2 : Q_8) : C_3) : C_2$ , or one of its five proper transitive subgroups, as shown in Figure 1.

The complete lists of elusive groups for  $n \leq 30$  were previously known (Giudici [5]), and while some of the examples for degree 36 were known, the list was not complete. Prior to this work, the smallest degree for which the existence of an elusive group was undecided was  $n = 40$ , which has now been ruled out. The Appendix contains the indices of the elusive groups in the lists of transitive groups available in MAGMA.

**6.2. CI groups.** Recall that a *Cayley digraph* for the group  $G$  with connection set  $C \subseteq G$  is the graph  $\text{Cay}(G, C)$  with vertex set  $G$ , and where  $(x, xc)$  is an arc of  $G$  for all  $c \in C$ . Clearly  $G$  acts regularly on  $\text{Cay}(G, C)$  by left-multiplication, and any digraph admitting a regular automorphism group  $G$  is a Cayley digraph for  $G$ . A Cayley digraph is loopless if and only if  $\text{id}_G \notin C$  and undirected if and only if  $C = C^{-1}$ . If  $\sigma$  is an automorphism of the group  $G$ , then it is immediate that  $\text{Cay}(G, C)$  is isomorphic to  $\text{Cay}(G, C^\sigma)$ . For some groups, these isomorphisms are the *only* isomorphisms between the Cayley graphs, or digraphs, on that group, in which case the group is called a CI-group or DCI-group respectively. (The acronym CI stands for ‘‘Cayley Isomorphic’’, and D for ‘‘directed’’ — previously the terminology  $\mathcal{G}$ -CI group was used for the undirected case, but this seems to have fallen out of style.) We shall use [6] for background.

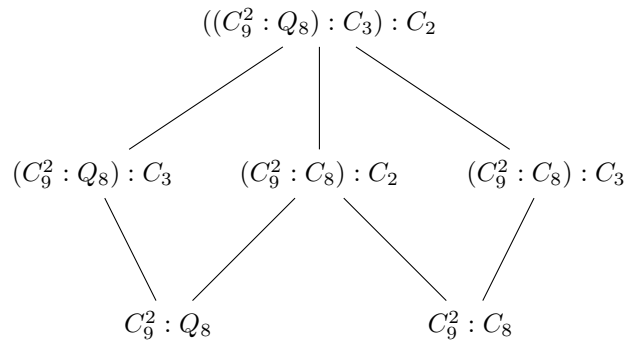


FIGURE 1. The elusive groups of degree 36

One method of identifying the transitive graphs that are *not* Cayley graphs would be to separately process each graph by computing its automorphism group and searching for regular subgroups. However it is considerably easier to precompute the entire collection of Cayley graphs for each of the groups of order less than 48. Then the non-Cayley graphs are simply those that appear in the list of transitive graphs but not in the list of Cayley graphs.

As a side-effect, this process also allowed us to determine the entire collection of CI-groups of order up to 47 in the following fashion. For each group  $G$ , we computed its automorphism group  $A = \text{Aut}(G)$  and then, because we were primarily interested in the undirected case, determined the action of  $A$  on the set

$$S = \{\{g, g^{-1}\} : g \in G, g \neq \text{id}_G\}. \tag{1}$$

We used a straightforward orderly algorithm [11] to calculate one representative from each orbit of  $A$  on the power set  $\mathcal{P}(S)$ , thereby finding all the connection sets that are both inverse-closed and pairwise inequivalent under  $A$ . Finally, we constructed all the Cayley graphs with these pairwise-inequivalent connection sets and checked the lists for isomorphic pairs of graphs. The group  $G$  is a CI-group if and only if this final step finds no isomorphic pairs of graphs. (If we were to repeat this for DCI-graphs, then  $S$  would need to be the set containing all the non-identity elements of  $G$ , and the final step would construct all the Cayley digraphs.)

The result of this is a long list of CI and non-CI groups. However this can be presented in a more compact format by noting that a *subgroup* of a CI-group is a CI-group and a *quotient* of a CI-group is a CI-group (Dobson and Morris [4]), thus permitting us to identify the *minimal* non-CI-groups of order up to 47. In particular the following list of groups is the complete list of minimal non-CI groups of order at most 47.

- (1) The cyclic groups  $C_{16}, C_{24}, C_{25}, C_{27}, C_{36}, C_{40}, C_{45}$ .
- (2) The dihedral groups  $D_{12}, D_{16}, D_{20}, D_{28}, D_{44}$ .
- (3) One of 16 groups listed individually in Table 4.

Order	No.	Structure	Order	No.	Structure
8	2	$C_4 \times C_2$	16	8	$QD_{16}$
16	9	$Q_{16}$	18	3	$C_3 \times S_3$
20	3	$C_5 : C_4$	24	3	$SL(2, 3)$
24	10	$C_3 \times D_8$	24	12	$S_4$
24	13	$C_2 \times A_4$	27	2	$C_9 \times C_3$
27	3	$(C_3 \times C_3) : C_3$	27	4	$C_9 : C_3$
36	9	$(C_3 \times C_3) : C_4$	36	11	$C_3 \times A_4$
40	10	$C_5 \times D_8$	42	1	$(C_7 : C_3) : C_2$

TABLE 4. Minimal non-CI groups with  $|G| < 48$  (not cyclic or dihedral).

The column labelled “Structure” is simply the output of GAP’s `StructureDescription` command. As this is not unique, we also include (in the column labelled “No.”) the number of the group in the list of *small groups* of that particular order. These lists of small groups are found in both MAGMA and GAP and, at least for the orders we are considering here, the numbering is consistent between the two programs. The *regular representations* of these small groups are transitive groups of course, and so they appear in the lists of transitive groups of each degree. However the ordering of the regular transitive groups is **not the same** as the ordering of the small groups. Therefore `SmallGroup(deg,k)` and `TransitiveGroup(deg,k)` are usually not isomorphic.

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## APPENDIX A. CI AND NON-CI GROUPS

In this section, we record in more detail some of the computations underlying the list of CI and non-CI groups.

Recall that a group  $G$  is a CI-group if the only isomorphisms between Cayley graphs for  $G$  are those induced by automorphisms of  $G$  acting on possible connection sets (which in our case are inverse-closed sets without the identity).

Letting the term *Cayley set* refer interchangeably to an  $\text{Aut}(G)$ -orbit of subsets of  $V(G)$  or an arbitrary member of such an orbit, we see that a group is CI if and if it has an equal number of Cayley sets and Cayley graphs.

The number of Cayley sets of a group  $G$  can be calculated using the *cycle index polynomial* of  $A = \text{Aut}(G)$  acting on the set  $S$  (defined above in (1)). This polynomial is the multivariate polynomial in variables  $\{X_1, X_2, \dots\}$  given by

$$Z(A; X_1, X_2, \dots) := \frac{1}{|A|} \sum_{a \in A} \prod_k X_k^{n_k(a)}.$$

where  $n_k(a)$  is the number of cycles of length  $k$  in the permutation  $a$ . The number of Cayley sets is then just an evaluation of this polynomial, in particular the evaluation  $Z(A; 2, 2, \dots)$ . The MAGMA function below performs these computations using the (undocumented) function `CycleIndexPolynomial`.

```

numCayleySets := function(g)

    ptsinv := Setseq({ {x,x^-1} : x in g | Order(x) eq 2 });
    ptsnot := Setseq({ {x,x^-1} : x in g | Order(x) gt 2 });

    pts := ptsinv cat ptsnot; generators := [];

    sym := Sym(#pts);

    autg := AutomorphismGroup(g);

    generators := [];
    for gen in Generators(autg) do
        Append(~generators, [Position(pts,gen(pts[i])) : i in [1..#pts]]);
    end for;

    autonpts := sub<sym|generators>;
    ci := CycleIndexPolynomial(autonpts);

```

```
return Evaluate(ci,[2 : i in [1..Rank(Parent(ci))]]);  
end function;
```

---

By further refining the cycle index polynomial to count separately the numbers of cycles of each length that consist of elements of  $S$  corresponding to involutions, and elements of  $S$  corresponding to a non-involution along with its inverse, it would be possible to count the number of Cayley sets of each valency. This would allow some greater exploration of the more refined property of being  $m$ -CI, which means that the number of Cayley sets and Cayley graphs of degree  $m$  coincide.

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