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Chemical Graphs with the Minimum Value of Wiener Index

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Abstract

Wiener index, defined as the sum of distances between all unordered pairs of vertices in a graph, is one of the oldest and the most popular molecular descriptors. In the paper, we would like to point to an "overlooked" problem of determining the minimum value of this index and corresponding extremes among chemical graphs with prescribed number of vertices. It turned out that the problem is far from tractable, and surprisingly related to the cages and the famous degree-diameter problem. Thus, for example, the Petersen graph, the Flower snark J_5, the Heawood graph, and other highly symmetric graphs are encountered as extremes. In the paper, we give some remarks regarding this problem.

1 Introduction

Wiener index, introduced by Wiener [15], is one of the oldest and most important topological indices. Wiener index not only correlates well with many physicochemical properties of organic compounds, it has a wide application also outside chemistry, and it became the topic of countless studies also from the mathematical point of view. Details can be found in some of many surveys [1, 9, 10, 16].

Denote by $d(u,v)$ the distance between vertices u and v in a graph G. The *Wiener index* (i.e. the *total distance* of the *transmission number*) of a graph G, denoted by $W(G)$, is the sum of distances between all (unordered) pairs of vertices of G

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v).$$

In [3] and later in many subsequent works (e.g. [6, 7]) it was shown that for trees on n vertices, the maximum Wiener index is obtained for the path P_n, and the minimum for the star S_n. Thus, for every tree T on n vertices, it holds

$$(n-1)^2 = W(S_n) \leq W(T) \leq W(P_n) = \binom{n+1}{3}.$$

Since the distance between any two distinct vertices is at least one, we have that among all graphs on n vertices K_n has the smallest Wiener index. Removing an edge from a connected graph results in increased Wiener index [8], which leads to the observation that Wiener index of a connected graph is less than or equal to Wiener index of its spanning tree. So, for any connected graph G on n vertices, it holds

$$\binom{n}{2} = W(K_n) \leq W(G) \leq W(P_n) = \binom{n+1}{3}.$$

There are many results of this type known for more specific classes of graphs. For instance, among 2-connected graphs on n vertices (or even stronger, among the graphs of minimum degree 2), the n-cycle has the largest Wiener index. Wang and Guo [14] found the tree with minimum Wiener index among all trees of order n and with diameter d. Wang [13] and Zhang et al. [17] determined the tree that minimizes the Wiener index among trees of given degree sequence. See the survey [10] for further extremal graphs in graph classes satisfying certain conditions.

In this paper we consider chemical graphs. Recall that a graph is *chemical* if the degrees of its vertices do not exceed 4. As it is very often practice to study upper and lower bounds for various indices in various graph classes, it is natural to ask for the Wiener index in the class of chemical graphs. The upper bound is obviously attained by the paths, but characterizing the lower bound seems to be much more complicated. Therefore, we state it explicitly as a problem and consider it here in the sequel.

Problem 1. *Find all the chemical graphs on n vertices with the minimum value of Wiener index.*

Since adding of an edge decreases Wiener index, one would expect that its minimum is attained by 4-regular graphs. Though computer results indicate that this is true, we are not able to prove such a statement. However, we prove that a chemical graph with the minimum value of Wiener index has at most 3 vertices of degree smaller than 4, see below. Hence, one can ask what is the minimum value of Wiener index in the class of 4-regular graphs. We extend our research also to 3-regular graphs, but from the mathematical point of view the problem is interesting for k-regular graphs for arbitrary $k \geq 3$. We remark that this problem is generalized to graphs with bounded minimum and/or maximum degree in [10, Section 4].

Problem 2. *Find all k-regular graphs on n vertices with the smallest value of Wiener index.*

Recall the well-known *degree-diameter problem*, see [12] for details:

Problem 3 (The degree-diameter problem)**.** *Determine the largest order $n(k, d)$ of a graph of (a maximum) degree k and diameter d.*

Our computer results showed that among graphs with the minimum Wiener index there are graphs achieving $n(k, d)$ for pairs (k, d) from$\{(3, 2), (3, 3), (4, 2)\}$, see also [11]. There might appear graphs achieving $n(k, d)$ also for higher values of diameter d, but for those we could not search the space of k-regular graphs of order n exhaustively. Anyway, for higher diameters the graphs achieving $n(k, d)$ do not need to be those with the smallest Wiener index.

As mentioned above, among extremal graphs found by a computer there are graphs achieving $n(3, 2)$ and $n(3, 3)$, which are the well-known Petersen graph and the Flower snark J_5. Surprisingly, there appears also the Heawood graph, which is the Cage$(3, 6)$, i.e., the smallest graph of degree 3 and girth 6, see [5].

We conclude the introduction with the following conjectures. (Probably, it suffices to choose $n_k = k + 1$ therein.)

Conjecture 4 (The even case conjecture)**.** *Let $k \geq 3$, and let n be large enough with respect to k, say $n \geq n_k$. Suppose that G is a graph on n vertices with the maximum* *degree k, and with the smallest possible value of Wiener index. If kn is even, then G is k-regular.*

Conjecture 5 (The odd case conjecture)**.** *Let $k \geq 3$, and let n be large enough with respect to k, say $n \geq n_k$. Suppose that G is a graph on n vertices with the maximum degree k, and with the smallest possible value of Wiener index. If kn is odd, then G has a unique vertex of degree smaller than k and in that case this smaller degree is $k-1$.*

As regards notation, for a graph G its vertex and edge sets are denoted by $V(G)$ and $E(G)$, respectively. An edge connecting vertices u and v is denoted by $[u,v]$, or simply by uv. By $d_G(u,v)$ we denote the distance from u to v. The maximum distance from u, i.e. the eccentricity of u, is denoted by $e_G(u)$. The degree of u in G is denoted by $\deg_G(u)$ and the diameter of G is denoted by $\mathrm{diam}(G)$.

2 Preliminaries

As we already mentioned, one would expect that graphs on n vertices with the maximum degree k which have the smallest Wiener index are regular or almost regular. Unfortunately, we are not able to prove such a statement. We can prove only the following result.

Proposition 6. *Let G be a graph on n vertices with the maximum degree k, $n \geq k+1$, with the minimum possible value of Wiener index. Then G contains at most $k-1$ vertices whose degree is strictly smaller than k, and these vertices induce a clique.*

Proof. By way of contradiction, suppose that G has k vertices whose degree is strictly smaller than k, say $x_1, x_2, \ldots, x_k$. Denote $X = \{x_1, x_2, \ldots, x_k\}$. Since adding of an edge, say uv, does not increase any distance, while the distance between u and v is decreased to 1, adding of an edge decreases the Wiener index. But G has the minimum Wiener index, so we cannot add an edge connecting vertices of X. Thus, there are already all possible edges between the vertices of X. That is, X induces a complete graph K_k in G. But this means that the vertices $x_1, x_2, \ldots, x_k$ all have degree $k-1$, and so there is no edge having one endvertex in X and the other outside X. Since any disconnected graph has Wiener index ∞, we conclude that $V(G) = X$. Consequently $n = k$, a contradiction. ∎

Computer experiments show that graphs on n vertices with maximum degree k which have the smallest Wiener index are regular when kn is even. Therefore, we will focus our attention to regular graphs. Hence, denote by $\mathcal{G}(n,k)$ a class of k-regular graphs on n vertices which have the smallest Wiener index. The value of Wiener index of a graph from $\mathcal{G}(n,k)$ is denoted by $w_{n,k}$.

Let G be a graph, and let $u \in V(G)$. Denote

$$d_i(u) = \left|\{v \in V(G);\ d_G(u,v) = i\}\right|,$$

where $0 \le i \le e_G(u)$. Obviously, $d_0(u) = 1$ and $d_1(u) = \deg_G(u)$. The *distance sequence* from u is

$$N_u(d_0(u), d_1(u), \ldots, d_{e_G(u)}(u)).$$

We omit the index u if no confusion is likely. We have the following lemma.

Lemma 7. *Let G be a k-regular graph on n vertices. If all vertices in G have distance sequence $N(n_0, n_1, \ldots, n_{\mathrm{diam}(G)})$, where $n_0 = 1$ and $n_i = k(k-1)^{i-1}$ for all i, $1 \le i <$ $\mathrm{diam}(G)$, then $G \in \mathcal{G}(n,k)$.*

Proof. Let $u \in V(G)$. Then $d_0(u) = 1$ and $d_1(u) = k$. Let $i \ge 1$ and let v contribute to $d_i(u)$. That is, $d_G(u,v) = i$. Then v must have at least one neighbour at distance $i-1$ from u, and so it has at most $k-1$ neighbours at distance $i+1$ from u. Hence, $d_{i+1}(u) \le (k-1)d_i(u)$, and consequently, $d_i(u) \le k(k-1)^{i-1}$. This means that at distance at most t from u there are at most $1 + k\sum_{i=1}^{t}(k-1)^{i-1}$ vertices of G.

Let j satisfy

$$1 + k\sum_{i=1}^{j-1}(k-1)^{i-1} < n \le 1 + k\sum_{i=1}^{j}(k-1)^{i-1}. \tag{1}$$

Denote $m_t = 1 + k\sum_{i=1}^{t-1}(k-1)^{i-1}$. Then $m_j < n \le m_{j+1}$ and G has at least $n - m_j$ vertices whose distance from u is greater than or equal to j.

We have $W(G) = \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} d_G(u,v)$. Hence, $W(G)$ is smallest if for every $u \in V(G)$ the sum $\sum_{v\in V(G)} d_G(u,v)$ is as small as possible. We have

$$\sum_{v\in V(G)} d_G(u,v) = \sum_{i=0}^{e_G(u)} i\cdot d_i(u) \qquad \text{and} \qquad \sum_{i=0}^{e_G(u)} d_i(u) = n.$$

Hence, increasing $d_i(u)$ by one while decreasing $d_q(u)$ by one, where $i < j \le q$, decreases $\sum_{i=0}^{e_G(u)} i\cdot d_i(u)$. Therefore

$$\sum_{v\in V(G)} d_G(u,v) \ge 0 + k\sum_{i=1}^{j-1} i(k-1)^{i-1} + j(n - m_j),$$

and consequently

$$W(G) \geq \frac{1}{2} \sum_{u \in V(G)} \left[k \sum_{i=1}^{j-1} i(k-1)^{i-1} + j(n-m_j) \right],$$

with equality if and only if $d_i(v) = k(k-1)^{i-1}$ for every $v \in V(G)$ and $1 \leq i < e_G(v)$. ■

We remark that if all vertices of G have distance sequence as in Lemma 7, then the value j defined by (1) is the diameter of G. Lemma 7 gives a theoretical lower bound for $w_{n,k}$.

Corollary 8. *Let $n \geq k+1$ and let j satisfy (1). Then*

$$w_{n,k} \geq \frac{n}{2} \left[k \sum_{i=1}^{j-1} i(k-1)^{i-1} + j \Big(n - 1 - k \sum_{i=1}^{j-1} (k-1)^{i-1} \Big) \right].$$

In the next sections we concentrate on small values of n, when the diameter is not big.

3 Symmetric graphs

In this section we consider symmetric graphs, more precisely the Cayley graphs. An automorphism of G is a bijection $\varphi : V(G) \to V(G)$ such that $\big(\varphi(u), \varphi(v)\big) \in E(G)$ if and only if $[u, v] \in E(G)$. Automorphisms of G partition $V(G)$ into orbits. We say that $u, v \in V(G)$ belong to the same orbit if there exists an automorphism φ of G such that $\varphi(u) = v$. If G has a unique orbit, i.e. if for every pair of vertices $u, v \in V(G)$ there is an automorphism of G mapping u to v, then G is *vertex-transitive*.

A special subclass of vertex-transitive graphs is formed by Cayley graphs. Let $(\mathbb{G}, \cdot)$ be a group and let $S \subseteq \mathbb{G}$ such that the unit element id $\notin S$ and S is closed with respect to inverses, that is, $x \in S$ implies $x^{-1} \in S$. Then the *Cayley graph* $G = \mathrm{Cay}(\mathbb{G}, S)$ is a graph with $V(G) = \mathbb{G}$, in which $[u, v] \in E(G)$ if and only if there is $x \in S$ such that $v = u \cdot x$. Since S is closed with respect to inverses, we have also $u = v \cdot x^{-1}$, and so the edges of Cayley graphs can be considered as undirected. Since id $\notin S$, they do not contain loops. For a simpler description, for arbitrary set $S \subseteq \mathbb{G}$ with id $\notin S$, we denote by $\langle S \rangle$ the set $\{x, x^{-1};\ x \in S\}$. Hence, $\langle S \rangle$ is the minimal subset of $\mathbb{G}$ containing S, which is closed with respect to inverses.

For our problem, Cayley graphs have two important advantages. First, they are easy to describe. It suffices to specify the group and the set of generators S. And second, if we check that id (or any other vertex) has some graphical property in $\mathrm{Cay}(\mathbb{G}, S)$, then all vertices of $\mathrm{Cay}(\mathbb{G}, S)$ have this property. This follows from the fact that if $u, v \in V\big(\mathrm{Cay}(\mathbb{G}, S)\big)$, that is if $u, v \in \mathbb{G}$, then $\varphi: \ x \mapsto (v \cdot u^{-1}) \cdot x$ is an automorphism of $\mathrm{Cay}(\mathbb{G}, S)$ mapping u to v. Hence, Cayley graphs are vertex-transitive.

For graphs with diameter 2, Lemma 7 reduces to the following statement.

Proposition 9. *Let G be a k-regular graph on n vertices. If $\mathrm{diam}(G) \le 2$, then $G \in \mathcal{G}(n,k)$ and $w_{n,k} = n^2 - \frac{1}{2}kn - n$.*

Observe that if $n = k+1$, then $\mathrm{diam}(G) = 1$ and $n^2 - \frac{1}{2}kn - n = \binom{n}{2}$ as expected. In the next statement we construct graphs in $\mathcal{G}(n,k)$ when nk is even and k is "small".

Theorem 10. *Let k satisfy $k+2 \le n \le 3k-1$ and let kn be even. Then there is a Cayley graph on a cyclic group, which has degree k, diameter 2 and n vertices. Hence, $w_{n,k} = n^2 - \frac{1}{2}kn - n$ in this case.*

Proof. First suppose that k is even. Let $S' = \{1, 2, 3, \ldots, \lfloor \frac{n}{2} \rfloor - 1\}$. Denote

$$S'' = \{2, 3, 5, 6, 8, 9, \ldots, \lfloor \tfrac{n}{2} \rfloor - \delta\},$$

where $\delta = 3$ if $\lfloor \frac{n}{2} \rfloor - 2 \equiv 1 \pmod 3$ and $\delta = 2$ otherwise. In other words, S'' contains all values of S' except those of the form $3t+1$ and $\lfloor \frac{n}{2} \rfloor - 1$. Now delete from S' exactly $|S'| - \frac{k}{2}$ values of the set S'', and denote the resulting set by S. Then S will be the set of generators of our Cayley graph. Moreover,

$$\{1, 4, 7, \ldots, \lfloor \tfrac{n}{2} \rfloor - 1\} \subseteq S.$$

However, we have to check if one can delete exactly $|S'| - \frac{k}{2}$ values of S'' from S'. That is, we have to check if $|S''| \ge |S'| - \frac{k}{2}$, which is equivalent to $\frac{k}{2} \ge |S' - S''|$. Since $|\{1, 4, 7, \ldots, \lfloor \frac{n}{2} \rfloor - 1\}| = \lceil \frac{n+1}{6} \rceil$ (check all the congruence classes modulo 6, the crucial case is $n \equiv 0 \pmod 6$), we get an inequality $\frac{k}{2} \ge \lceil \frac{n+1}{6} \rceil$, which is true since $3k-1 \ge n$ and k is even. Since $S \subseteq S'$, we get $\frac{k}{2} \le \lfloor \frac{n}{2} \rfloor - 1$, which is equivalent to the assumption $k+2 \le n$. Hence, a required set S exists.

Let $G = \mathrm{Cay}(\mathbb{Z}_n, \langle S \rangle)$. Since $1 \in S$, G contains a Hamiltonian cycle $(0, 1, 2, \ldots, n-1)$. Moreover, since all vertices of the form $3t+1$ from S' are in S, and also $\lfloor \frac{n}{2} \rfloor - 1 \in S$, for every $x \in \mathbb{Z}_n$ either $(0, x)$ or $(0, x-1)$ or $(0, x+1)$ is in $E(G)$. Since $(x-1, x), (x, x+1) \in E(G)$, we conclude that $e_G(0) \le 2$. However, $(0, \lfloor \frac{n}{2} \rfloor) \notin E(G)$, and so $e_G(0) = 2$. Since G is a Cayley graph, we have $e_G(x) = 2$ for every $x \in V(G)$, and consequently $\mathrm{diam}(G) = 2$.

If k is odd, the proof is analogous. In this case n must be even and S must contain $\frac{n}{2}$. Thus, let $S' = \{1, 2, 3, \ldots, \frac{n}{2}\}$. Denote

$$S'' = \{2, 3, 5, 6, 8, 9, \ldots, \tfrac{n}{2} - \delta\},$$

where $\delta = 2$ if $\frac{n}{2} - 1 \equiv 1 \pmod 3$ and $\delta = 1$ otherwise. Now delete from S' exactly $|S'| - \frac{k+1}{2}$ values of the set S'', and denote the resulting set by S. Observe that since $k+2 \leq n$, we have $k+3 \leq n$ due to parities of k and n. Hence, $\frac{n}{2} - \frac{k+1}{2} \geq 1$ and we delete at least one value of S'' from S'. Again, S will be the set of generators of our Cayley graph. Since S contains $\frac{n}{2}$, one generator is an involution.

Analogously as above, $\{1, 4, 7, \ldots, \frac{n}{2}\} \subseteq S$ and $|\{1, 4, 7, \ldots, \frac{n}{2}\}| = \lceil \frac{n+4}{6} \rceil$. Hence, a required set S exists if $|\langle S \rangle| \geq 2\lceil \frac{n+4}{6} \rceil - 1$. This gives an inequality $k \geq 2\lceil \frac{n+4}{6} \rceil - 1$, which is true since $3k - 1 \geq n$ and k is odd (consider n in all three congruence classes of even number modulo 6).

Denote $G = \mathrm{Cay}(\mathbb{Z}_n, \langle S \rangle)$. Analogously as above we get $e_G(0) = 2$, and so $\mathrm{diam}(G) = 2$. The final statement of the corollary is a consequence of Proposition 9. ■

We remark that if S is chosen carefully, sometimes it is possible to find a Cayley graph on cyclic group, which has degree k, diameter 2 and n vertices, even for n larger than $3k - 1$. For instance, $\mathrm{Cay}(\mathbb{Z}_{13}, \langle 1, 5 \rangle)$ has diameter 2 though $13 = 3k + 1$ in this case. However, there does not exist a Cayley graph $\mathrm{Cay}(\mathbb{Z}_{12}, \langle 1, x \rangle)$ of diameter 2, though $\mathrm{Cay}(\mathbb{Z}_{12}, \langle 2, 3 \rangle)$ has diameter 2.

Observe that if $\mathrm{Cay}(\mathbb{G}, \langle S \rangle)$ is 4-regular of diameter 2 and $\mathbb{G}$ is an Abelian group, then $n \leq 13$. This observation was generalized in [12]:

Proposition 11. *Let G be a Cayley graph on Abelian group, which has degree k, diameter 2, and n vertices. Then $n \leq k^2/2 + k + 1$.*

As regards higher diameters we have the following theorem, see [2].

Theorem 12. *Let G be a Cayley graph on Abelian group, which has degree 4, diameter d, and n vertices. Then $n \leq 2d^2 + 2d + 1$ and the equality is attained for all values of d.*

However, Theorem 12 does not mean that if one denotes $n_d = 2d^2 + 2d + 1$, then for all $n \in (n_{d-1}, n_d]$ there exists a Cayley graph on Abelian group, which has degree 4, diameter d and n vertices.

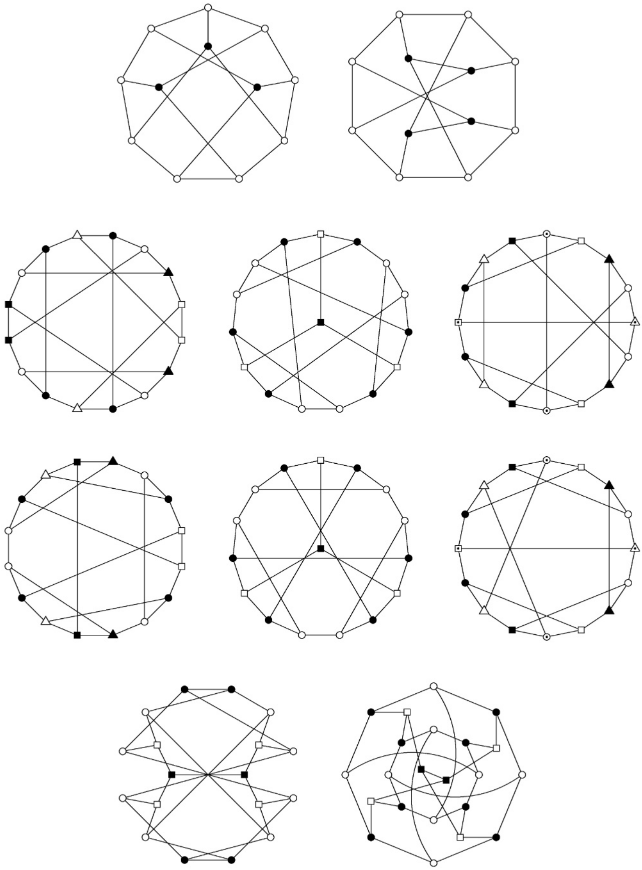

Figure 1. The graphs of $\mathcal{G}(12,3)$, $\mathcal{G}(16,3)$, $\mathcal{G}(18,3)$ and $\mathcal{G}(22,3)$.

4 Computer results

Here we present results obtained by a computer together with some comments. We consider degrees 3 and 4. Using an exhaustive search, for degree 3 we were able to find all optimal graphs on even number of vertices up to $n = 22$, for those of degree 4 we succeeded up to $n = 17$. Perhaps one can go a little further with better software and hardware resources.

n	6	8	10	12	14	16	18	20	22
$w_{n,3}$	21	44	75	126	189	264	351	450	573
diameter	2	2	2	3	3	3	3	3	4
# of graphs	2	2	1	2	7	6	1	1	1
# of VT-graphs	2	1	1	0	1	0	0	0	0

Table 1. Small graphs for the case $k = 3$.

We start with the case $k = 3$. In Table 1, for all $n \in \{6, 8, \dots, 22\}$ we have the number of extremal graphs, their Wiener index and their diameter. We present also the number of vertex-transitive extremal graphs (VT-graphs for short). We remark that in all cases, $w_{n,k}$ reaches the bound presented in Corollary 8. The only exception is $n = 22$ where the exact value of $w_{3,22}$ exceeds the bound by 12.

In the list below we provide some additional information with emphasis to the vertex-transitive graphs. With a unique exception, all the vertex-transitive graphs are Cayley. Of course, the exception is the well-known Petersen graph.

$n = 6$**:** The two graphs are $\mathrm{Cay}(\mathbb{Z}_6, \langle 1, 3\rangle)$ and $\mathrm{Cay}(\mathbb{Z}_6, \langle 2, 3\rangle)$.

$n = 8$**:** The vertex-transitive graph is $\mathrm{Cay}(\mathbb{Z}_8, \langle 1, 4\rangle)$.

$n = 10$**:** The vertex-transitive graph is the well-known Petersen graph.

$n = 12$**:** Both graphs have distance sequences $N(1, 3, 6, 2)$ and they are depicted in Figure 1.

$n = 14$**:** The vertex-transitive graph is a Cayley graph on dihedral group D_{14}, that is $\mathrm{Cay}(D_{14}, \langle(1, 0),\ (1, 2), (1, 6)\rangle)$, where $D_{14} = \mathbb{Z}_2 \ltimes \mathbb{Z}_4$ and the multiplication is $(a, b)(c, d) = (a + c, b + (-1)^a d)$. It is the Heywood graph, known as the Cage$(3, 6)$, which means that it is the graph of degree 3 and girth 6 with the minimum number of vertices. The distance sequence of this graph is $N(1, 3, 6, 4)$.

$n = 16$**:** All these graphs have distance sequences $N(1, 3, 6, 6)$ and they are depicted in Figure 1.

$n = 18$**:** The distance sequence of this graph is $N(1, 3, 6, 8)$, see Figure 1.

$n = 20$**:** The graph is the well-known Flower snark J_5. Its distance sequence is $N(1, 3, 6, 10)$. Although it is not a Moore graph, it is the unique graph of degree 3 and diameter 3 on the maximum possible number of vertices, see [4].

$n = 22$: Six vertices of this graph have distance sequence $N(1, 3, 6, 12)$, eight have distance sequence $N(1, 3, 6, 11, 1)$ and eight have distance sequence $N(1, 3, 6, 10, 2)$, see Figure 1.

On Figure 1 we present all graphs from $\mathcal{G}(n, 3)$, where $n \in \{12, 16, 18, 22\}$, since in these classes there is no Cayley (or generally known) graph in $\mathcal{G}(n, 3)$. The graphs are depicted so that a reader can observe at least some automorphisms immediately. The vertices in different orbits are depicted differently.

Now we consider the case $k = 4$. In Table 2, for all $n \in \{6, 7, \ldots, 17\}$ we have the number of extremal graphs, their Wiener index and their diameter. We present also the number of vertex-transitive extremal graphs. In all cases, $w_{n,k}$ reaches the bound presented in Corollary 8. The only exceptions are $n = 16$ and $n = 17$, where the exact value of $w_{4,16}$ exceeds the bound by 2 and 9, respectively.

n	6	7	8	9	10	11	12	13	14	15	16	17
$w_{n,4}$	18	28	40	54	70	88	108	130	154	180	210	247
diameter	2	2	2	2	2	2	2	2	2	2	3	3
# of graphs	1	2	6	16	24	37	26	10	1	1	1	2
# of VT-graphs	1	1	3	3	1	1	2	1	0	0	0	0

Table 2. Small graphs for the case $k = 4$.

In the list below we provide some additional information with emphasis to the vertex-transitive graphs.

$n = 6$: The graph is $\mathrm{Cay}(\mathbb{Z}_6, \langle 1, 2\rangle)$.

$n = 7$: The vertex-transitive graph is $\mathrm{Cay}(\mathbb{Z}_7, \langle 1, 3\rangle)$.

$n = 8$: The vertex-transitive graphs are $\mathrm{Cay}(\mathbb{Z}_8, \langle 1, 3\rangle)$, $\mathrm{Cay}(\mathbb{Z}_8, \langle 1, 2\rangle)$ and $\mathrm{Cay}(D_8, \langle (0, 1), (0, 2), (1, 1)\rangle)$, where $D_8 = \mathbb{Z}_2 \ltimes \mathbb{Z}_4$ and the multiplication is defined by $(a, b)(c, d) = (a + c, b + (-1)^a d)$.

$n = 9$: The vertex-transitive graphs are $\mathrm{Cay}(\mathbb{Z}_9, \langle 1, 4\rangle)$, $\mathrm{Cay}(\mathbb{Z}_9, \langle 1, 3\rangle)$ and $\mathrm{Cay}(\mathbb{Z}_3 \times \mathbb{Z}_3, \langle (0, 1), (1, 0)\rangle)$.

$n = 10$: The vertex-transitive graph is $\mathrm{Cay}(\mathbb{Z}_{10}, \langle 1, 4\rangle)$.

$n = 11$: The vertex-transitive graph is $\mathrm{Cay}(\mathbb{Z}_{11}, \langle 1, 4\rangle)$.

$n = 12$**:** The two vertex-transitive graphs are $\mathrm{Cay}(\mathbb{Z}_{12}, \langle 2, 3\rangle)$ and $\mathrm{Cay}(A_4, \langle (12)(34), (13)(24), (123)\rangle)$, where A_4 is the alternating group, i.e. the group of even permutations of the set $\{1, 2, 3, 4\}$.

$n = 13$**:** The vertex-transitive graph is $\mathrm{Cay}(\mathbb{Z}_{13}, \langle 1, 5\rangle)$.

$n = 14$**:** The graph is depicted in Figure 2.

$n = 15$**:** The graph is depicted in Figure 2. Though it is not a Moore graph, it is the unique graph of degree 4 and diameter 2 on the maximum possible number of vertices, see [4].

$n = 16$**:** Twelve vertices of this graph have distance sequence $N(1, 4, 11)$ and four have distance sequence $N(1, 4, 10, 1)$, see Figure 2.

$n = 17$**:** There are more than 86 millions of 4-regular connected graphs on 17 vertices, but only two of them have Wiener index 247. These graphs are depicted in Figure 2. The first graph has two vertices with distance sequence $N(1, 4, 12)$, twelve vertices with distance sequence $N(1, 4, 11, 1)$ and three with distance sequence $N(1, 4, 10, 2)$. The second graph has eight vertices with distance sequence $N(1, 4, 12)$ and nine with distance sequence $N(1, 4, 10, 2)$. Both these graphs have triangles, see Figure 2.

On Figure 2 we present all graphs from $\mathcal{G}(n, 4)$, where $n \in \{14, 15, 16, 17\}$, since in these classes there is no Cayley graph in $\mathcal{G}(n, 4)$. As in Figure 1, vertices in different orbits are depicted differently.

It seems to be surprising that although for larger values of n there are more regular graphs, for $n \in \{18, 20, 22\}$ in the case $k = 3$, and for $n \in \{14, 15, 16\}$ in the case $k = 4$, the extremal graphs are unique.

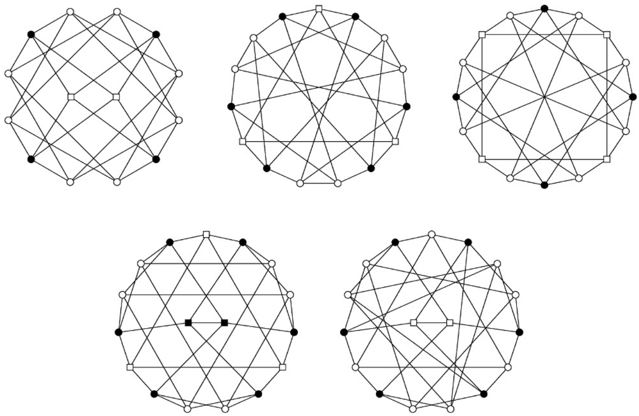

Figure 2. The graphs of $\mathcal{G}(14,4)$, $\mathcal{G}(15,4)$, $\mathcal{G}(16,4)$ and $\mathcal{G}(17,4)$.

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References

[1] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.

[2] R. Dougherty, V. Faber, The degree-diameter problem for several varieties of Cayley graphs, 1: the Abelian case, *SIAM J. Discr. Math.* **17** (2004) 478–519.

[3] R. C. Entringer, D. E. Jackson, D. A. Snyder, Distance in graphs, *Czech. Math. J.* **26** (1976) 283–296.

[4] B. Elspas, Topological constraints on interconnection-limited logic, *Proc. IEEE Fifth Symposium on Switching Circuit Theory and Logical Design, IEEE* **S-164** (1964) 133–147.

[5] G. Exoo, R. Jajcay, Dynamic cage survey, *El. J. Comb. Dyn. Survey DS16* (2013).

[6] I. Gutman, A property of the Wiener number and its modifications, *Indian J. Chem.* **36A** (1997) 128–132.

[7] I. Gutman, W. Linert, I. Lukovits, A. A. Dobrynin, Trees with extremal hyper-Wiener index: Mathematical basis and chemical applications, *J. Chem. Inf. Comput. Sci.* **37** (1997) 349–354.

[8] I. Gutman, Y.-N. Yeh, The sum of all distances in bipartite graphs, *Math. Slovaca* **45** (1995) 327–334.

[9] M. Knor, R. Škrekovski, Wiener index of line graphs, in: M. Dehmer, F. Emmert–Streib (Eds.), *Quantitative Graph Theory: Mathematical Foundations and Applications*, CRC Press, Boca Raton, 2014, pp. 279–301.

[10] M. Knor, R. Škrekovski, A. Tepeh, Mathematical aspects of Wiener index, *Ars Math. Contemp.* **11** (2016) 327–352.

[11] E. Loz, H. Péres-Rosés, G. Pineda-Villavicencio, The degree diameter problem for general graphs, *Combinatorics Wiki*, 24 May 2017, 15:30 UTC, ⟨http://combinatoricswiki.org/wiki/The_Degree_Diameter_Problem _for_General_Graphs⟩ [accessed 3 February 2018]

[12] M. Miller, J. Širáň, Moore graphs and beyond: A survey of the degree-diameter problem, *El. J. Comb. Dyn. Survey D14* (2005).

[13] H. Wang, The extremal values of the Wiener index of a tree with given degree sequence, *Discr. Appl. Math.* **156** (2009) 2647–2654.

[14] S. Wang, X. Guo, Trees with extremal Wiener indices, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 609–622.

[15] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[16] K. Xu, M. Liu, K. C. Das, I. Gutman, B. Furtula, A survey on graphs extremal with respect to distance-based topolgical indices, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 461–508.

[17] X. D. Zhang, Q. Y. Xing, L. Q. Xu and R. Y. Pang, The Wiener index of trees with given degree sequences, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 623–644.