Analytical and Numerical Solutions for Nonlinear Equations
©Available online at https://ansne.du.ac.ir/
Online ISSN: 3060–785X
2027, Volume 12, Issue 2, pp. xx–xx

Research article

The Connected Domatic Number of Fullerene Graphs Is at Most Two: A Reformulation Via Induced Paths and Cycles

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Received: 07/10/2026 **Revised:** 01/11/2026 **Accepted:** 09/11/2026 **Published:** xx/xx/2026 10.22128/ansne.2026.3506.1250

Abstract

The connected domatic number $d_c(G)$ of a graph G is the largest number of pairwise disjoint connected dominating sets into which $V(G)$ can be partitioned. Connected dominating sets model backbones in communication networks, so d_c counts how many disjoint backbones a network can carry. We show that a connected cubic graph has $d_c = 4$ only for K_4, $d_c = 3$ only on six vertices, and $d_c \leq 2$ otherwise; hence every fullerene graph satisfies $d_c \leq 2$. For cubic graphs of order at least 8, $d_c = 2$ holds exactly when the vertex set splits into two sets inducing paths or cycles, and these sets differ in size by at most two. Using this characterization, we give explicit splittings for the dodecahedron, which has exactly 90 of them, for the truncated icosahedron C_{60}, and for the infinite family of $(5,0)$ nanotube fullerenes. An exhaustive search covers all fullerenes on at most 36 vertices. Whether $d_c = 2$ for every fullerene remains a conjecture.

Keywords: Connected domatic number, Fullerene graphs, Cubic graphs, Connected dominating set, Induced paths and cycles

Mathematics Subject Classification (2020): 05C69, 05C10, 92E10

1 Introduction and Literature Review

A set D of vertices of a graph G is *dominating* if every vertex outside D has a neighbour in D. Partitioning $V(G)$ into dominating sets gives the *domatic number*, introduced by Cockayne and Hedetniemi [3]; the standard reference for the whole theory is the monograph of Haynes, Hedetniemi and Slater [9]. If one also asks every class to induce a connected subgraph, one obtains the *connected domatic number* $d_c(G)$, studied by Hedetniemi and Laskar [10] and by Zelinka [13]. Connected dominating sets are the natural model for a backbone in a communication network, so d_c measures how many disjoint backbones a network can carry.

Hartnell and Rall investigated d_c for planar graphs [8]. They proved that $d_c(G) \leq 4$ for planar G, that K_4 is the only planar graph attaining the value 4, and they characterized the planar graphs with $d_c = 3$; they also recall the general bound $d_c(G) \leq \kappa(G)$, where κ is the vertex connectivity. Since a fullerene graph is cubic and 3-connected, these results leave open the two values 2 and 3 for fullerenes, and a natural question is which of them occurs. Fullerene graphs themselves, the cubic planar graphs with only pentagonal and hexagonal faces that model carbon cages [7, 11], have been studied in chemical graph theory from many angles.

Matchings enter the picture in two ways. Fullerene graphs are bridgeless cubic graphs and therefore have perfect matchings (Petersen's

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theorem); and, as we shall see, the only cubic graphs with $d_c = 3$ are those whose three classes are the edges of a perfect matching, each class inducing a single edge. Matchings and their algebraic counterparts have been a recurring theme in the author's own work: a Laplacian-spread inequality based on perfect matchings [1], the vertex matching polynomial [5], and the connection between the characteristic and matching polynomials of regular graphs [6].

We stress at the outset that d_c is a graph invariant: its value 2 is neither the number of vertex orbits nor the number of face orbits of the fullerene (see Remark 3), and d_c by itself says nothing about the physical properties of the corresponding molecules. Section 6 gives a chemical reading of the invariant and an exploratory look at a related counting descriptor.

In this paper we answer the question above. The value 3 never occurs: every fullerene graph has $d_c \leq 2$ (Theorem 1). What remains is to decide between $d_c = 2$ and $d_c = 1$, and we show that this is equivalent to a neat partition problem (Theorem 2).

2 Preliminaries

All graphs are finite, simple and connected. We write $N(v)$ and $N[v]$ for the open and closed neighbourhoods and $d_X(v) = |N(v) \cap X|$ for the number of neighbours of v in a set X. A set D is dominating if $N[D] = V(G)$, and *connected dominating* if moreover $G[D]$ is connected.

Definition 1. *The* connected domatic number $d_c(G)$ *is the largest k for which $V(G)$ can be partitioned into k connected dominating sets. We call such a partition a* connected domatic partition.

Since $V(G)$ itself is connected dominating, $d_c(G) \geq 1$. A *fullerene graph* is a 3-connected, cubic, planar graph all of whose faces have size 5 or 6. By Euler's formula it has exactly twelve pentagonal faces, and its order is 20 or an even number at least 24.

Lemma 1. *For every graph G, $d_c(G) \leq \delta(G) + 1$.*

Proof. Let $D_1, \ldots, D_k$ be a connected domatic partition and $v \in D_i$. For each $j \neq i$ the set D_j is dominating and $v \notin D_j$, so v has a neighbour in D_j. Hence $d(v) \geq k - 1$, and taking v of minimum degree gives $k \leq \delta(G) + 1$. □

3 Cubic Graphs and Fullerenes

The following theorem is the heart of the paper. The key observation is that in a cubic graph a vertex has only three neighbours to spend, and a connected domatic partition demands all of them.

Theorem 1. *Let G be a connected cubic graph of order n.*

(a) $d_c(G) = 4$ if and only if $G = K_4$.

(b) If $n = 6$, then $d_c(G) = 3$ (for both cubic graphs of order six, $K_{3,3}$ and the prism).

(c) If $n \geq 8$, then $d_c(G) \leq 2$.

Proof. Let $D_1, \ldots, D_k$ be a connected domatic partition. By Lemma 1, $k \leq 4$.

Suppose $k = 4$. Each vertex $v \in D_i$ has a neighbour in each of the three other classes, so all three neighbours of v lie outside D_i. Thus $G[D_i]$ has no edges, and being connected it is a single vertex u. As $\{u\}$ is dominating, u is adjacent to every other vertex, so $n = 4$ and $G = K_4$. Conversely K_4 has the partition into four singletons.

Suppose $k = 3$ and $n \geq 5$. No class can be a singleton, because a singleton dominating set forces $n = 4$. So each $G[D_i]$ is connected with at least two vertices, and every vertex $v \in D_i$ has at least one neighbour in D_i and at least one in each of the other two classes. Since $d(v) = 3$, the triple $(d_{D_1}(v), d_{D_2}(v), d_{D_3}(v))$ is a permutation of $(1,1,1)$, with the entry for D_i equal to 1. Hence $G[D_i]$ is 1-regular and connected, i.e. a single edge, so $|D_i| = 2$ and $n = 6$.

This proves (c) (a partition into 3 or 4 classes needs $n \leq 6$) and the "only if" part of (a). For (b), take $K_{3,3}$ with parts $\{a_1, a_2, a_3\}$, $\{b_1, b_2, b_3\}$ and classes $\{a_i, b_i\}$; and for the prism with triangles $x_1x_2x_3$, $y_1y_2y_3$ and edges x_iy_i, take the classes $\{x_i, y_i\}$. In both cases each vertex has exactly one neighbour in each class, so each class is connected and dominating. Finally $d_c \leq 3$ for $n = 6$ by the case $k = 4$. □

Corollary 1. Every fullerene graph F satisfies $d_c(F) \leq 2$.

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Proof. Fullerene graphs are connected, cubic and have at least 20 vertices. □

Remark 1. It is worth stressing what this changes. A fullerene graph never has a connected domatic partition into three classes, because such a partition would force each class to be a single edge and the graph to have six vertices. The local pattern $(2,1,0)$, which one might at first allow for a vertex with two neighbours in its own class, is excluded: the zero entry would mean that some class fails to dominate the vertex. Consequently any "structural characterization of fullerene graphs with $d_c = 3$" is vacuous.

4 Two Classes: a Reformulation

By Corollary 1 the real question for a fullerene is whether $d_c = 2$ or $d_c = 1$. The condition turns out to be purely a partition problem.

Theorem 2. *Let G be a connected cubic graph of order $n \geq 8$. Then $d_c(G) = 2$ if and only if $V(G)$ can be partitioned into two sets A, B such that $G[A]$ and $G[B]$ are paths or cycles.*

Proof. ($\Rightarrow$) Let A, B be connected dominating sets partitioning $V(G)$. Every vertex of A has a neighbour in B, since B is dominating, so every vertex of A has at most two neighbours in A. Thus $G[A]$ is a connected graph of maximum degree at most 2, i.e. a path or a cycle. The same holds for B.

($\Leftarrow$) Suppose $G[A]$ and $G[B]$ are connected with maximum degree at most 2. Then every vertex of A has at most two neighbours in A, hence at least one in B; so B dominates A and, symmetrically, A dominates B. Both sets are connected, so they form a connected domatic partition of size two. By Theorem 1(c), $d_c(G) = 2$. □

The cut between the two classes gives a counting condition. For $X \subseteq V(G)$ let ∂X be the set of edges between X and its complement. Counting degrees in the cubic graph G gives

$$|\partial X| = 3|X| - 2|E(G[X])|. \tag{1}$$

Proposition 1. *If A, B is a partition as in Theorem 2, then $\big||A| - |B|\big| \in \{0, 2\}$. More precisely, if $a = |A|$ and $b = |B|$:*

(i) if both parts are paths or both are cycles, then $a = b = n/2$;

(ii) if one part is a cycle and the other a path, then the cycle has exactly two fewer vertices than the path.

Proof. A path on a vertices has $a-1$ edges and a cycle has a. By (1) the cut has size $a+2$ if $G[A]$ is a path and a if it is a cycle, and likewise for B. Since $|\partial A| = |\partial B|$, we get $a + 2\varepsilon_A = b + 2\varepsilon_B$ where $\varepsilon = 1$ for a path and 0 for a cycle. So $a - b = 2(\varepsilon_B - \varepsilon_A) \in \{0, \pm 2\}$. □

Theorem 2 turns the question for fullerenes into a purely combinatorial one, and the evidence collected in Section 5 points in a single direction. We therefore state the main open problem here, so that it can be referred to throughout the paper.

Conjecture 1. Every fullerene graph F satisfies $d_c(F) = 2$; equivalently, the vertex set of every fullerene graph splits into two induced paths or cycles.

5 Examples

5.1 The Dodecahedron

Let F_{20} be the dodecahedral fullerene. We describe it in LCF notation (named after Lederberg, Coxeter and Frucht), which encodes a cubic Hamiltonian graph by a Hamiltonian cycle together with one chord at every vertex: take the Hamiltonian cycle $0, 1, \ldots, 19$ and join vertex i to $i + s_i \pmod{20}$, where $(s_0, \ldots, s_9) = (10, 7, 4, -4, -7, 10, -4, 7, -7, 4)$ repeated twice.

Proposition 2. $d_c(F_{20}) = 2$.

Proof. By Corollary 1, $d_c(F_{20}) \leq 2$. For the reverse inequality take

$$A = \{19, 3, 4, 5, 6, 7, 8, 9, 13, 12\}, \qquad B = \{2, 1, 0, 10, 11, 18, 17, 16, 15, 14\}.$$

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The listed order of A is an induced path: consecutive vertices are adjacent (note $19 \sim 3$, $9 \sim 13$ via chords, the others via the cycle), and a check of the remaining pairs shows that no other edge of F_{20} joins two vertices of A. The same verification works for B, where the chords used are $0 \sim 10$ and $11 \sim 18$. Thus $G[A]$ and $G[B]$ are induced paths on ten vertices each, and Theorem 2 gives $d_c(F_{20}) \geq 2$. □

Figure 1 shows this partition.

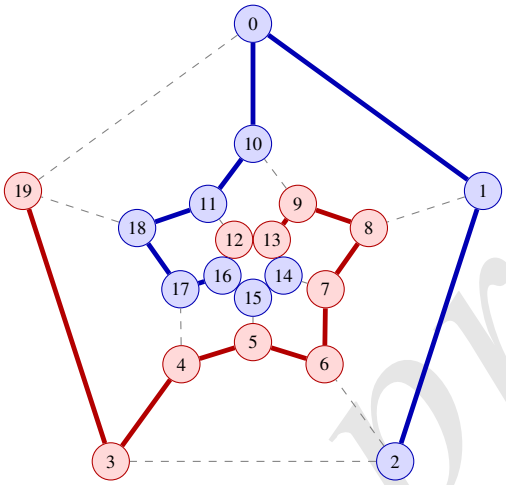


Figure 1. The dodecahedral fullerene C_{20} drawn as a Schlegel diagram (labels follow the LCF numbering of Section 5.1). The set A (red) and the set B (blue) are disjoint connected dominating sets; each induces an induced path on ten vertices (bold edges), and the dashed edges join the two sets. Hence $d_c(C_{20}) = 2$.

Remark 2. An exhaustive computer search over all 2^{19} splittings (vertex 0 fixed in the first class) shows that F_{20} has exactly 90 unordered partitions into two connected dominating sets, and every one of them consists of two induced paths of ten vertices. In particular no partition into a cycle and a path (nor into two cycles) occurs.

5.2 The Truncated Icosahedron

Let C_{60} be the truncated icosahedron, with twelve pentagonal and twenty hexagonal faces. We label its vertices $0, 1, \ldots, 59$ along a Hamiltonian cycle and, as in the LCF notation used for F_{20}, join vertex i to $i + s_i \pmod{60}$, where the offsets s_i are given in Table 1. (One checks that $s_{i+s_i} \equiv -s_i \pmod{60}$, that the resulting graph is cubic, planar and 3-connected with twelve pentagonal and twenty hexagonal faces, and that it is isomorphic to the truncated icosahedron.)

Table 1. Chord offsets s_i of the Hamiltonian-cycle labelling of C_{60}.

$s_0, \ldots, s_9$:	5, 30, 27, 23, 20, -5, 16, -8, 12, -12
$s_{10}, \ldots, s_{19}$:	9, -16, 5, -19, -23, -26, 30, -5, 27, -9
$s_{20}, \ldots, s_{29}$:	-12, 23, -16, 20, -20, 16, -23, 12, 9, -27
$s_{30}, \ldots, s_{39}$:	5, 30, 26, 23, 19, -5, 16, -9, 12, -12
$s_{40}, \ldots, s_{49}$:	8, -16, 5, -20, -23, -27, 30, -5, -8, 26
$s_{50}, \ldots, s_{59}$:	-12, 23, -16, -19, 19, 16, -23, 12, -26, 8

Proposition 3. $d_c(C_{60}) = 2$.

Proof. By Corollary 1, $d_c(C_{60}) \leq 2$. Let

$$A = (0, 5, 4, 24, 23, 43, 44, 45, 18, 17, 12, 13, 14, 51, 50, 49, 48, 40, 39, 27, 28, 29, 30, 35, 34, 33, 56, 57, 9, 8),$$

$$B = (15, 16, 46, 47, 42, 41, 25, 26, 3, 2, 1, 31, 32, 58, 59, 7, 6, 22, 21, 20, 19, 10, 11, 55, 54, 53, 52, 36, 37, 38),$$

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each list being given in path order. Consecutive entries of each list are adjacent, each list contains 30 distinct vertices, $A \cup B = V(C_{60})$, and a direct check of the $60 \cdot 3/2 = 90$ edges shows that A and B each span exactly 29 edges, so $G[A]$ and $G[B]$ are induced paths on thirty vertices. By Theorem 2, $d_c(C_{60}) \geq 2$. □

This certificate was found by computer search and then verified independently by a separate program, which tested connectivity, maximum degree at most 2 inside each class, and that every vertex has a neighbour in the other class.

5.3 An Infinite Family: the $(5,0)$ Nanotube Fullerenes

We now treat an infinite family. For $k \geq 1$ let T_k be the graph with vertex set $\{(l,i) : 0 \leq l \leq 2k+1,\ i \in \mathbb{Z}_5\}$ (the *layers* $V_l = \{(l,i)\}$ have five vertices each) and the following edges, where $L = 2k+1$:

(a) the two end cycles $(0,i)(0,i+1)$ and $(L,i)(L,i+1)$;

(b) the *rungs* $(l,i)(l+1,i)$ for all even l, $0 \leq l \leq L-1$;

(c) the *zigzag edges* $(l,i)(l+1,i)$ and $(l,i)(l+1,i+1)$ for all odd l, $1 \leq l \leq L-2$.

Every vertex has degree three, so T_k is a cubic graph on $10(k+1)$ vertices. The map $(l,i) \mapsto (L-l,-i)$ is an automorphism of T_k.

Lemma 2. *T_k is a fullerene graph for every $k \geq 1$. The graph T_1 is the dodecahedron, T_2 is the D_{5h} fullerene C_{30}, and T_5 is the D_{5d} isomer of C_{60} (not the icosahedral one).*

Proof. Consider the following cycles: the two end cycles (pentagons); the ten pentagons $(0,i),(0,i+1),(1,i+1),(2,i+1),(1,i)$, $i \in \mathbb{Z}_5$, and their images under $(l,i) \mapsto (L-l,-i)$; and the $5(k-1)$ hexagons

$$(l,i),\ (l+1,i+1),\ (l+2,i+1),\ (l+3,i+1),\ (l+2,i),\ (l+1,i),$$
$$l \text{ odd},\ 1 \leq l \leq 2k-3,\ i \in \mathbb{Z}_5.$$

One checks directly that every edge of T_k lies in exactly two of these $5k+7$ cycles. Hence they are the faces of an embedding of the connected graph T_k in a closed surface, and since $n - e + f = 10(k+1) - 15(k+1) + (5k+7) = 2$ the surface is the sphere. All faces are pentagons (twelve of them) or hexagons, so T_k is a cubic plane graph with faces of size 5 and 6. It remains to see that T_k is 3-connected. Since T_k is cubic, $\kappa(T_k) = \kappa'(T_k)$ (vertex and edge connectivity coincide for cubic graphs; see Whitney [12] for $\kappa \leq \kappa' \leq \delta$ and, e.g., Bondy and Murty [2] for the cubic case), so it suffices to exclude bridges and 2-edge cuts. By the cut–cycle duality for plane graphs (see Section 4.6 of Diestel [4]), a bridge of T_k would be a face lying on both sides of an edge, and a minimal 2-edge cut would be a pair of faces having two edges in common. Every edge of T_k lies in two *different* faces, as shown above, so there is no bridge. Two faces share an edge only when they lie in a window of at most four consecutive layers, and the pattern of rungs and zigzag edges has period two in the layer index, so every such pair already occurs in T_4 or in the two ends of T_k; for these we list the faces explicitly and see that no two of them share more than one edge (this was also checked by computer for all $k \leq 12$). Hence T_k is 3-connected, and therefore a fullerene graph. For $k = 1$ there are no hexagons, and T_1 is the dodecahedron; for $k = 5$ one gets a 60-vertex fullerene with twenty hexagons and a five-fold axis, which is not the truncated icosahedron (its automorphism group has order 20 rather than 120). □

Theorem 3. *$d_c(T_k) = 2$ for every $k \geq 1$. Consequently Conjecture 1 holds for the infinite family $\{T_k\}_{k \geq 1}$ of fullerene graphs $C_{10(k+1)}$.*

Proof. By Theorem 2 (note $|V(T_k)| \geq 20$) it suffices to split $V(T_k)$ into two sets each inducing a path. Let $L = 2k+1$ and put $\varphi = 0$ if k is odd and $\varphi = 2$ if k is even. For a layer index l let $\rho(l) \in \{0,1,2,3\}$ with $\rho(l) \equiv l + \varphi \pmod 4$. Then $\rho(l) \equiv l \pmod 2$, $\rho(0) \in \{0,2\}$, and $\rho(L) = 3$. Define

$$S_0 = \{0,1,2,3\},\ S_1 = \{3\},\ S_2 = \{4\},\ S_3 = \{0,1,2,4\} \subseteq \mathbb{Z}_5,$$
$$A = \{(l,i) : i \in S_{\rho(l)}\}, \qquad B = V(T_k) \setminus A.$$

Thus the layers have the pattern $\rho = 0,1,2,3,0,1,2,3,\ldots$ if k is odd, and $\rho = 2,3,0,1,2,3,0,1,\ldots$ if k is even, always ending with $\rho = 3$.

Step 1: the edges inside A and inside B. Reading the sets S_ρ one obtains the following list; every other edge of T_k joins A to B.

- *Rung between layers $l, l+1$ (l even).* If $\rho(l) = 0$: the A-edge $(l,3)(l+1,3)$ and the B-edge $(l,4)(l+1,4)$. If $\rho(l) = 2$: the A-edge $(l,4)(l+1,4)$ and the B-edge $(l,3)(l+1,3)$.

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- *Zigzag between layers $l, l+1$ (l odd).* If $\rho(l)=1$: the A-edge $(l,3)(l+1,4)$, and the B-edges $(l,4)(l+1,0)$, $(l,j)(l+1,j)$, $(l,j)(l+1,j+1)$ for $j=0,1,2$. If $\rho(l)=3$: the A-edges $(l,4)(l+1,0)$, $(l,j)(l+1,j)$, $(l,j)(l+1,j+1)$ for $j=0,1,2$, and the B-edge $(l,3)(l+1,4)$.
- *End cycles.* If $\rho(0)=0$ the layer 0 contributes the A-edges $(0,j)(0,j+1)$, $j=0,1,2$, and no B-edge; if $\rho(0)=2$ it contributes the same three edges as B-edges and no A-edge. Layer L contributes the A-edges $(L,4)(L,0)$, $(L,0)(L,1)$, $(L,1)(L,2)$ and no B-edge.

Step 2: two paths. For l with $\rho(l)=3$, $l<L$, let

$$W_l = (l,4),(l{+}1,0),(l,0),(l{+}1,1),(l,1),(l{+}1,2),(l,2),\\ (l{+}1,3),(l{+}2,3),(l{+}3,4),$$

and for l with $\rho(l)=0$, $l+3\le L$, let

$$Y_l = (l,4),(l{+}1,4),(l{+}2,0),(l{+}1,0),(l{+}2,1),(l{+}1,1),\\ (l{+}2,2),(l{+}1,2),(l{+}2,3),(l{+}3,3).$$

By Step 1, consecutive entries of W_l are adjacent inside A (they use the seven zigzag A-edges, then the rung $(l{+}1,3)(l{+}2,3)$ with $\rho(l{+}1)=0$, and the zigzag edge $(l{+}2,3)(l{+}3,4)$ with $\rho(l{+}2)=1$), and consecutive entries of Y_l are adjacent inside B (the rung $(l,4)(l{+}1,4)$, the seven zigzag B-edges, and the rung $(l{+}2,3)(l{+}3,3)$ with $\rho(l{+}2)=2$). Moreover the last vertex $(l{+}3,4)$ of W_l is adjacent in A to the first vertex $(l{+}4,4)$ of W_{l+4} (a rung with $\rho(l{+}3)=2$), and the last vertex $(l{+}3,3)$ of Y_l is adjacent in B to the first vertex $(l{+}4,4)$ of Y_{l+4} (a zigzag edge with $\rho(l{+}3)=3$).

Case k odd. Here $L\equiv 3 \pmod 4$. Let

$$\begin{aligned} A:\ & (0,0),(0,1),(0,2),(0,3),(1,3),(2,4),\ W_3,W_7,\dots,W_{L-4},\\ & (L,4),(L,0),(L,1),(L,2),\\ B:\ & Y_0,Y_4,\dots,Y_{L-3}. \end{aligned}$$

(For $k=1$ the list of W's is empty.) The first six entries of A are adjacent in turn by the end-cycle edges of layer 0, the rung $(0,3)(1,3)$ with $\rho(0)=0$, and the zigzag edge $(1,3)(2,4)$ with $\rho(1)=1$; the last entry $(2,4)$ is adjacent to the start $(3,4)$ of W_3 by a rung ($\rho(2)=2$). The last vertex $(L-1,4)$ of W_{L-4} is adjacent to $(L,4)$ by a rung ($\rho(L-1)=2$), and the last four entries are joined by the end-cycle edges of layer L.

Case k even. Here $L\equiv 1 \pmod 4$ and

$$\begin{aligned} A:\ & (0,4),\ W_1,W_5,\dots,W_{L-4},\ (L,4),(L,0),(L,1),(L,2),\\ B:\ & (0,0),(0,1),(0,2),(0,3),(1,3),(2,4),\ Y_2,Y_6,\dots,Y_{L-3}. \end{aligned}$$

Here $(0,4)(1,4)$ is a rung with $\rho(0)=2$, the first four entries of B are adjacent by the end-cycle edges of layer 0, $(0,3)(1,3)$ is a rung with $\rho(0)=2$, and $(1,3)(2,4)$ is a zigzag edge with $\rho(1)=3$, ending at the start of Y_2.

Step 3: these are induced paths partitioning the vertex set. In each case, consecutive entries are adjacent in A (resp. B) by Step 2. Every vertex of A occurs exactly once: the vertices $(l,0),\dots,(l,3)$ of a layer with $\rho(l)=0$, and $(l,4)$ of a layer with $\rho(l)=3$, $l<L$, occur in the segment W_l or W_{l-1} as displayed; the vertex $(l,3)$ of a layer with $\rho=1$ and $(l,4)$ of a layer with $\rho=2$ occur in W_{l-2}, W_{l-3} respectively, or in the initial piece, and the vertices of layer L in the final piece. The same inspection shows that B is covered exactly once by the Y_l and the initial piece. Finally, every A-edge and every B-edge listed in Step 1 joins two consecutive entries of the corresponding list (for instance the seven zigzag A-edges for $\rho(l)=3$ are the consecutive pairs of W_l inside layers $l, l{+}1$). Hence $G[A]$ and $G[B]$ are induced paths, and $|A|=|B|=5(k+1)$. By Theorem 2, $d_c(T_k)=2$. □

As a safeguard, we also checked the sets A,B of the proof by computer for all $k\le 40$ (connectivity of both classes and maximum degree at most two in each class). The pattern of A has period four in the layer index, and this periodicity is what makes the argument work for all k at once, without induction. For $k=1$ we recover a splitting of the dodecahedron, and for $k=5$ one of a second C_{60} isomer.

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5.4 Symmetry and the Number of Orbits

The truncated icosahedron is vertex-transitive: it has a single orbit of vertices under its automorphism group (of order 120), and its dual has two orbits of faces. One might ask whether the value $d_c = 2$ reflects either number. It does not.

Remark 3. The bound $d_c \leq 2$ comes from the local structure of cubic graphs (Theorem 1), and the value 2 is attained exactly when a splitting as in Theorem 2 exists. A splitting is not required to be invariant under any automorphism: the two paths of Proposition 3 are not invariant under the full symmetry group of C_{60} (a path on thirty vertices cannot be), so the existence of a splitting is compatible with vertex-transitivity. Neither orbit count explains the value: the dodecahedron has one vertex orbit and one face orbit, yet $d_c = 2$, and the fullerenes in Table 2 have up to 36 vertex orbits, again with $d_c = 2$.

To test whether low symmetry can destroy the splitting, we generated all fullerene graphs on at most 36 vertices with a spiral algorithm (our counts $1,1,1,2,3,6,6,15$ for $n = 20,24,26,28,30,32,34,36$ agree with the known numbers of isomers) and tested each for a splitting of the vertex set into two induced paths or cycles. Every graph admits one, and in every case the two classes are paths (for $n \leq 32$ we counted all splittings and found no path–cycle or cycle–cycle splitting).

Table 2. Exhaustive survey of fullerene graphs with at most 36 vertices. |Aut| is the order of the automorphism group of the graph (including reflections). The isomer with trivial automorphism group has 36 vertex orbits.

n	isomers	with $d_c = 2$	|Aut| (range)	vertex orbits (range)
20	1	1	120	1
24	1	1	24	2
26	1	1	12	4
28	2	2	4–24	3–7
30	3	3	4–20	3–10
32	6	6	2–12	4–16
34	6	6	2–6	8–20
36	15	15	1–24	3–36

The conjecture holds for every fullerene graph with at most 36 vertices, for C_{60} (Proposition 3), and for the infinite family T_k of Theorem 3. The survey of Table 2 includes graphs of trivial symmetry, so it is not a symmetry artefact, but it is of course limited to small order. An exhaustive study of all 1812 isomers of C_{60}, and its relation to orbit numbers, has not yet been carried out. The lower bound $d_c(F) \geq 2$ for general fullerenes is not established by any argument we know; the connectivity bound $d_c \leq \kappa$ gives no obstruction since $\kappa(F) = 3$.

6 A Chemical Reading, and a Counting Descriptor (Exploratory)

This section is exploratory. Its observations rest on a small sample and are offered as hypotheses for future work, not as conclusions; nothing in the rest of the paper depends on them.

A fullerene is a carbon cage, and its graph records which atoms are bonded. In that language a connected dominating set is a chain of bonded atoms with the property that every other atom of the cage is bonded to some atom of the chain. A connected domatic partition of size two is therefore a way of cutting the cage into two vertex-disjoint carbon chains, each of which touches every atom. By Theorem 2 the two chains can be taken to be linear (induced paths), the two strands being tied together by the remaining bonds. This is a purely structural picture, a statement about the connectivity of the skeleton, and nothing in it depends on bond lengths, energies or electrons.

There is a catch that we should say plainly. If Conjecture 1 is true, then $d_c = 2$ for every fullerene, and a number that is the same for every isomer cannot tell two isomers apart. As a descriptor, d_c itself is useless. What can vary from one isomer to the next is the number of ways the cage can be cut in two. For a fullerene graph F let $\sigma(F)$ denote the number of unordered partitions of $V(F)$ into two induced paths or cycles. We computed σ for every fullerene on at most 34 vertices; in all cases the two classes are paths. The values are in Table 3, together with the number $p(F)$ of pairs of adjacent pentagons and two quantities from simple Hückel theory: the total π-energy per atom

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E_π/n and the HOMO–LUMO gap, both in units of $|\beta|$. Here $E_\pi = 2\sum_{i\le n/2}\lambda_i$ and the gap is $\lambda_{n/2} - \lambda_{n/2+1}$, where $\lambda_1 \ge \cdots \ge \lambda_n$ are the eigenvalues of the adjacency matrix.

Table 3. Number σ of splittings into two induced paths, number p of pairs of adjacent pentagons, and Hückel descriptors for all fullerenes with $20 \le n \le 34$. The isomer number is just the order in which our generator produced the graphs; it is not a standard numbering.

n	isomer	|Aut|	σ	p	E_π/n	gap
20	1	120	90	30	1.471	0.000
24	1	24	126	24	1.476	0.000
26	1	12	138	21	1.475	0.067
28	1	4	146	20	1.497	0.093
28	2	24	162	18	1.480	0.000
30	1	20	60	20	1.496	0.000
30	2	4	146	18	1.511	0.404
30	3	4	164	17	1.504	0.058
32	1	2	145	17	1.507	0.012
32	2	4	151	18	1.507	0.000
32	3	12	150	18	1.505	0.000
32	4	2	171	16	1.516	0.253
32	5	12	174	18	1.514	0.394
32	6	6	177	15	1.520	0.364
34	1	2	144	17	1.507	0.023
34	2	2	138	15	1.511	0.040
34	3	2	190	15	1.518	0.122
34	4	2	152	15	1.516	0.114
34	5	2	175	14	1.517	0.002
34	6	6	186	15	1.514	0.000

The question is whether σ carries any chemical signal at all. Since σ grows with n, we compared isomers of the same size only: for each n with at least two isomers ($n = 28, 30, 32, 34$, seventeen graphs in total) we standardised σ and each descriptor within its size class and computed the Spearman rank correlation over the pooled data. We found $\rho = -0.62$ between σ and p ($P = 0.008$), $\rho = +0.51$ between σ and E_π/n ($P = 0.04$), and $\rho = +0.18$ between σ and the gap ($P = 0.50$). In words: among cages of equal size, those with fewer adjacent pentagons and higher Hückel π-energy tended to admit more splittings, while there is no visible relation with the gap.

We want to be careful about what this does and does not show. All three correlations, and in particular the one with the HOMO–LUMO gap, which is statistically indistinguishable from zero here, are exploratory and preliminary. The sample is small (17 graphs with $28 \le n \le 34$) and consists of the smallest fullerenes only, the P-values are not corrected for the three comparisons, and Hückel theory is a crude model. The two correlations are also not independent of each other, because adjacent pentagons are well known to lower the π-energy, so the data may simply say that σ responds to pentagon adjacency. The observation is therefore a hypothesis for future work, not a firm conclusion. A real test needs a larger sample, such as all 1812 isomers of C_{60}, and computed energies in place of Hückel ones, and it would have to ask whether σ adds anything beyond p. We have not done this.

7 Conclusion

For connected cubic graphs the connected domatic number takes the value 4 only for K_4 and the value 3 only on six vertices; in particular, every fullerene graph has $d_c \le 2$. For cubic graphs of order at least eight, $d_c = 2$ is equivalent to a splitting of the vertex set into two induced paths or cycles whose sizes differ by at most two. We verified this for the dodecahedron, for the truncated icosahedron (with an explicit certificate), by exhaustive search for all fullerenes on at most 36 vertices, including graphs with trivial symmetry, and by a proof for the infinite family of $(5,0)$ nanotube fullerenes $C_{10(k+1)}$ (Theorem 3); we conjecture that $d_c = 2$ for all fullerene graphs. The invariant

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d_c is graph-theoretic; the counting descriptor σ of Section 6 shows a possible link with pentagon adjacency and Hückel energies, but this is only an exploratory, preliminary observation on a small sample, and it should be tested on larger data sets before any conclusion is drawn. Settling Conjecture 1, for instance by relating the splitting to Hamiltonian cycles or to cyclic edge cuts, is the natural next step, as is a survey of all 1812 isomers of C_{60}.

Authors' Contributions

The author is solely responsible for the conception, results, computations and writing of this paper.

Data Availability

All vertex sets and chord offsets needed to verify the computational statements (the splittings of F_{20} and C_{60}, and the sets A, B of Theorem 3) are given in the paper. Further data are available from the author upon reasonable request.

Code Availability

The code used to generate the results in this study is available from the corresponding author upon reasonable request.

Conflicts of Interest

The author declares that there is no conflict of interest.

Ethical Considerations

Not applicable.

Funding

This research received no specific funding.

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