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Topological Chirality of Minimally Colored Kuratowski Graphs

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We prove that topological chirality in a $K_{3,3}$ graph requires a minimum of two non-adjacent colored edges, while topological chirality in a K_5 graph requires a minimum of three colored edges that form an open path.

INTRODUCTION

In conjunction with a study of protein topology, we recently noted that topological chirality in a $K_{3,3}$ graph requires a minimum of two non-adjacent colored edges, while topological chirality in a K_5 graph requires a minimum of three colored edges that form an open path.[1] In the present paper we supply the proof for this observation. To provide the necessary background, we begin by introducing some preliminary concepts.

A graph is a set of vertices together with a set of edges that connect some or all of the vertices. Of particular interest in the present context are the two Kuratowski graphs, $K_{3,3}$ and K_5, shown in Figure 1. $K_{3,3}$ is a bipartite graph consisting of two disjoint sets of three vertices each, with each vertex of one set adjacent to all three of the other, while K_5 is a complete graph comprised of five vertices that are all adjacent to one another.[2] Because the crossings of edges in the abstract or standard projections of Figure 1 are single points, instead of transverse double points, the associated topological chirality or achirality remains undefined. That is, in order to determine whether or not a graph is topologically chiral, all crossings of edges in the graph's projection must represent transverse double points, with over- and under-characteristics clearly marked. We refer to such graphs as »spatial graphs«. A spatial graph is a three-dimensional topological object that can be distorted in space without limit by continuous deformations (ambient iso-

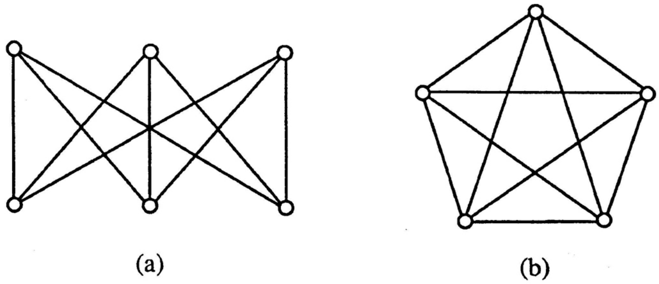


Figure 1. Abstract or standard presentations of (a) $K_{3,3}$ and (b) K_5 graphs, with vertices symbolized by open circles.

topy) such as bending, stretching, or twisting but not tearing, breaking, or rejoining of edges. Two spatial graphs are said to be isotopic if they can be converted into each other by ambient isotopy. A spatial graph is topologically achiral if and only if it is isotopic with its mirror image; otherwise it is topologically chiral. Molecular graphs, in which vertices symbolize atoms and edges symbolize chemical bonds, are examples of spatial graphs. Figures 2a and 2b represent the simplest spatial realizations of Figures 1a and 1b, respectively.[3,4] Both graphs are topologically achiral. In what follows, discussions in connection with topological chirality are limited to spatial graphs.

A graph is said to be planar if it can be embedded in the plane without the crossing of any edges; otherwise it is nonplanar. A graph is nonplanar if and only if it contains a subgraph that is homeomorphic[3] or contractible[4–6] to $K_{3,3}$ or K_5. Nonplanarity is a prerequisite for topological chirality, *i.e.*, a

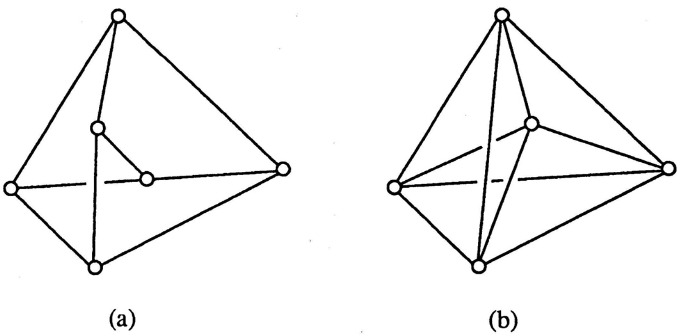
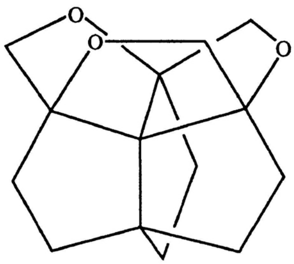


Figure 2. (a) $K_{3,3}$ and (b) K_5 graphs with vertices symbolized by open circles. The two graphs are K_b and K_a of Ref. 4, which correspond to Figure 1 and Figure 2 of Ref. 3, with subscripts *b* and *a* replaced by 3,3 and 5, respectively.

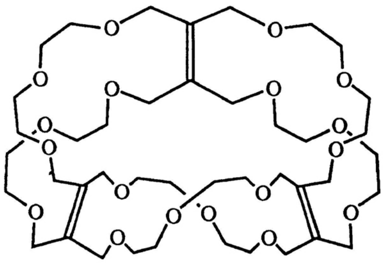
topologically chiral graph must contain a subgraph that is homeomorphic or contractible to $K_{3,3}$, to K_5, or to a nontrivial knot or link.

Nonplanarity and topological chirality of molecular graphs have proven to be a source of inspiration for the synthesis of novel chemical structures. In particular, »molecules with nonplanar graphs represent a novel, not to say exotic, structure type, and ... this topological perspective has sparked fruitful investigations in a previously unexplored area«.[7] Figure 3 depicts eight such molecules:[8–14] the graphs of the four molecules in Figures 3a-d are topologically chiral,[15,16] whereas the four molecules in Figures 3e-h are topologically achiral because each of them has an attainable achiral symmetry.

By means of branched coverings, Simon showed[15] that Figure 4a (the colored three-rung Möbius ladder graph M_3, an abstracted model of Figure 3b)



(a)



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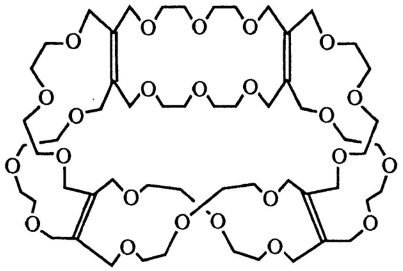
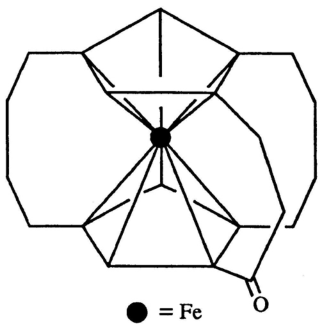


(c)



(d)

Figure 3. (a) The Simmons-Paquette molecule.[8,9] (b)-(c) The three-rung and four-rung Möbius ladder molecules.[10] (d) Molecule [4](1,1')[4](3,3')[3](4,4')-ferrocenophan-16-one.[11] (e)-(f) Centropentaindan and bridgehead-disubstituted derivatives.[12] (g) A cage complex $[Co(sep)]^{3+}$ (sep = sepulchrate).[13] (h) The ansa icosahedron: $(1,7\text{-}C_2B_{10}H_{10}\text{-}1',3'\text{-}C_6H_4)_3$.[14] In all molecular graphs shown on this and the following page, unlabeled vertices represent carbon atoms, and hydrogen atoms are suppressed for clarity.

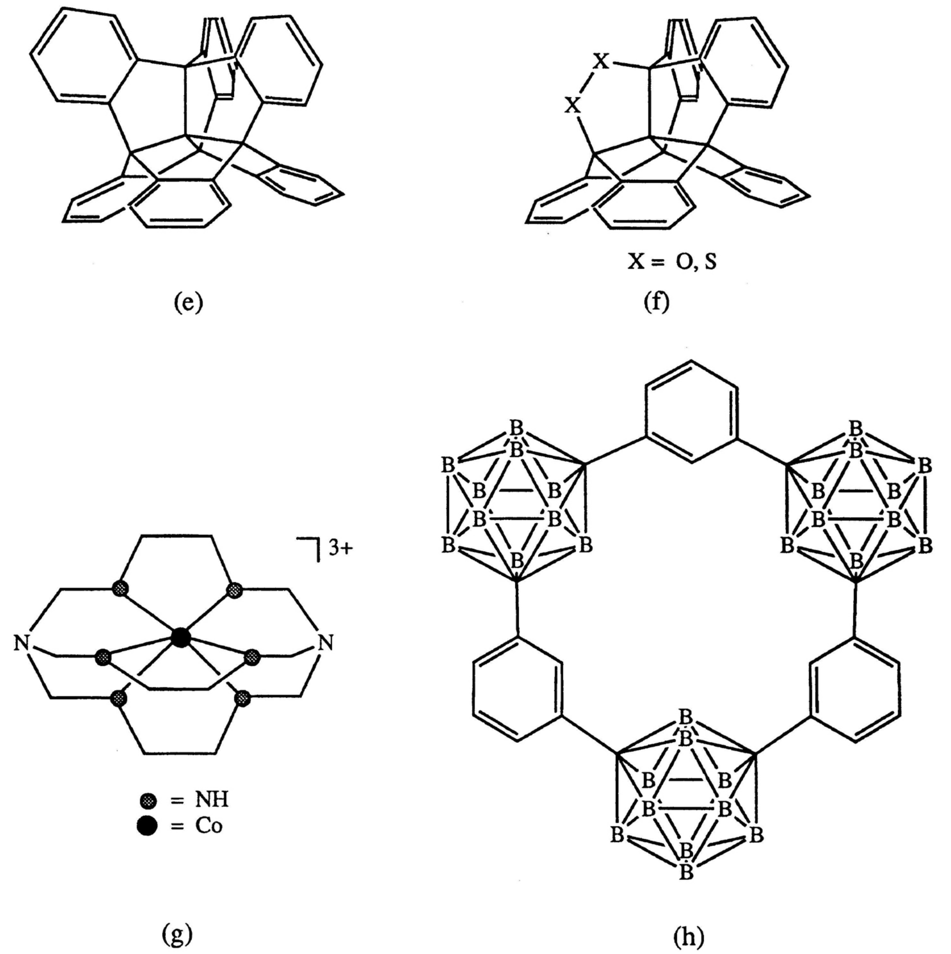


Figure 3. Cont.

and Figure 4b (M_3*, the mirror image of M_3) are not isotopic. Thus the three-rung Möbius ladder molecule shown in Figure 3b is topologically chiral. Similarly, Simon proved[15] that the molecular graphs in Figures 3a and 3c are both topologically chiral.

In proving the topological chirality of the molecular graph in Figure 3d, Wolcott[16] showed that (i) a one-to-one mapping can be uniquely defined between the mirror images of the graph, and (ii) the graph contains a subgraph that is homeomorphic to M_3 or to M_3*. In the present paper we show that M_3 (or M_3*) is not the simplest topologically chiral graph. The application of Wolcott proofs is therefore limited. For example, the graph of the hy-

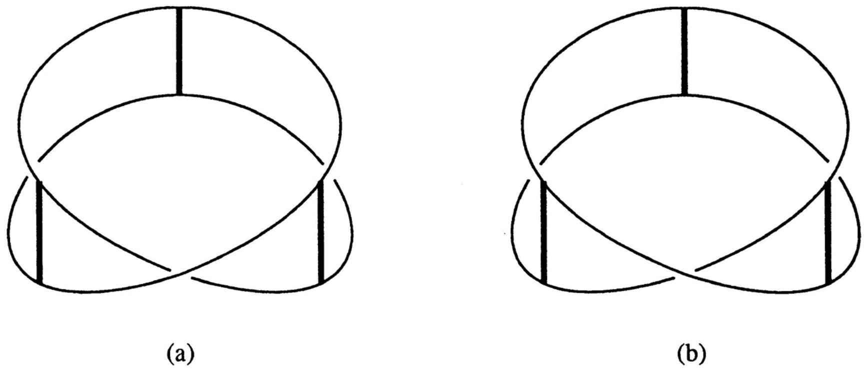


Figure 4. (a) M_3, the colored three-rung Möbius ladder graph abstracted from Figure 3b. The three colored edges (rungs) are symbolized by heavy lines. (b) M_3*, the mirror image of M_3.

pothetical molecule in Figure 5 satisfies the above condition (i) but does not contain any subgraph that is homeomorphic to M_3 or to M_3*, yet the molecule is topologically chiral (see below). Obviously, the simplest topologically chiral graphs can be derived from the simplest nonplanar graphs themselves. As shown below, this end can be achieved by selective coloring of $K_{3,3}$ and K_5.

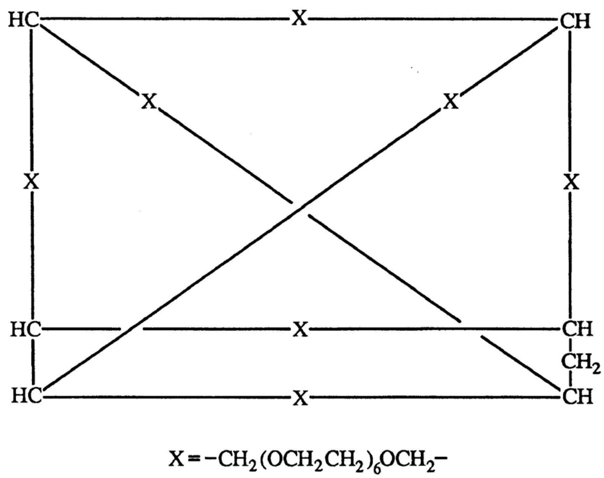
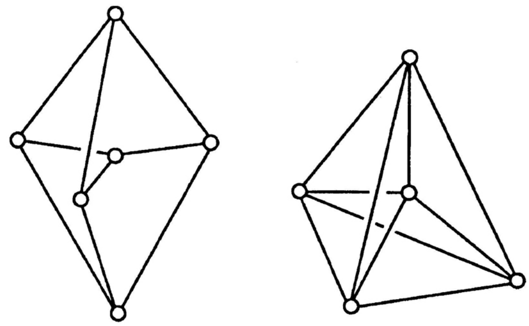


Figure 5. A hypothetical molecule that can be abstracted as a $K_{3,3}$ graph with two differently colored non-adjacent edges.

PROOFS FOR THE TOPOLOGICAL CHIRALITY OF MINIMALLY COLORED KURATOWSKI GRAPHS

As noted above, $K_{3,3}$ and K_5 are topologically achiral graphs because they can assume achiral symmetries in space. The highest attainable achiral symmetries for $K_{3,3}$ and K_5 are D_{3h} (Figure 6a) and T_d (Figure 6b), respec-



(a) (b)

Figure 6. The highest attainable achiral symmetry of the Kuratowski graphs. (a) $K_{3,3}$ graph (D_{3h}). (b) K_5 graph (T_d).

tively. To achieve topological chirality, the two graphs must therefore be selectively colored. In what follows we prove two theorems regarding the minimal edge-coloring of $K_{3,3}$ and K_5 graphs that is necessary to attain topological chirality.

THEOREM 1. A $K_{3,3}$ graph with any two non-adjacent colored edges is topologically chiral.

Proof:

The D_{3h} presentation of a $K_{3,3}$ graph shows that coloration of any single edge or of any two adjacent edges results in achiral symmetry (C_s or C_{2v}). It is easily shown that all colorations of two non-adjacent edges give rise to four and only four distinct (not properly congruent) patterns: P_1, P_2, P_1*, and P_2* (Figure 7). P_1 and P_1* are geometrical enantiomorphs, and so are P_2 and P_2*.

In pattern P_1 there are four classes of edges: (i) colored edges with colored end-vertices; (ii) uncolored edges with colored end-vertices; (iii) uncolored edges with one colored and one uncolored end-vertex; and (iv) uncolored edges with two uncolored end-vertices. Class (iv) contains only a single

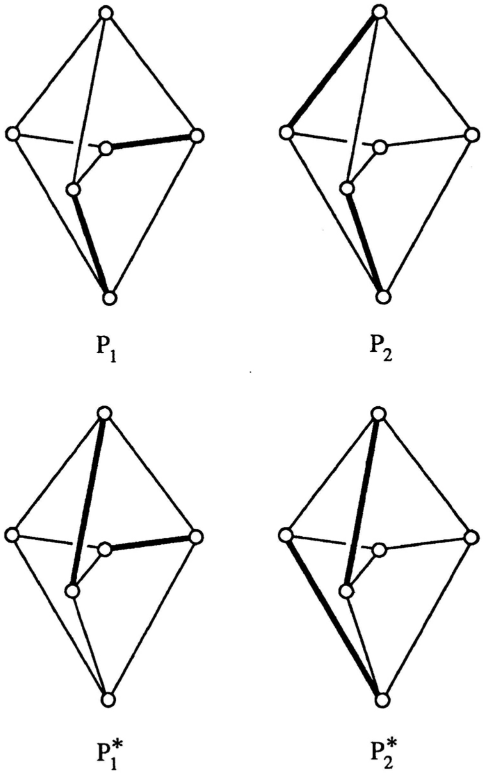


Figure 7. Two pairs of enantiomorphous $K_{3,3}$ graphs, $P_1 - P_1{}^*$ and $P_2 - P_2{}^*$, derived from the D_{3h} presentation by coloration of two non-adjacent edges. Colored edges are shown by heavy lines.

member which is unique in P_1. P_1 is therefore isotopic to the colored three-rung Möbius ladder graph M_3, in the sense that the two colored edges of P_1 are isotoped onto any two colored edges of M_3, and the unique edge of P_1 is mapped onto the only remaining colored edge of M_3. Since it has been proven[15] that M_3 is topologically chiral, it follows that P_1 is topologically chiral, and P_1 and $P_1{}^*$ are presentations of topological enantiomorphs.

Pattern P_2 is isotopic to P_1, and so is $P_2{}^*$ to $P_1{}^*$. That is, P_2 ($P_2{}^*$) can be converted into P_1 ($P_1{}^*$) by continuous deformations in space. Thus there are only two non-isotopic and enantiomorphous $K_{3,3}$ graphs with two non-adjacent colored edges. It follows that a $K_{3,3}$ graph with any two colored non-adjacent edges is topologically chiral. □

THEOREM 2. A K_5 graph with any three colored edges that form an open path is topologically chiral.

Proof:

The T_d presentation of a K_5 graph shows that the coloration of any two edges or of any three edges that do not form an open path yields an achiral symmetry (C_s, C_{2v}, C_{3v}, or D_{2d}). Coloration of three edges that form an open path gives rise to three and only three enantiomorphous pairs, Q_1-Q_1*, Q_2-Q_2*, and Q_3-Q_3*, which are depicted in Figure 8.

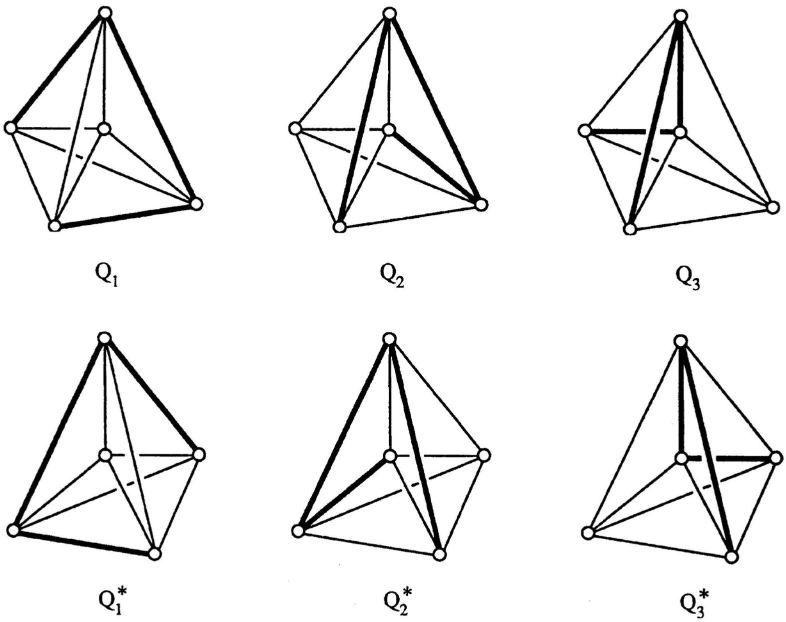


Figure 8. Three pairs of enantiomorphous K_5 graphs, Q_1–Q_1*, Q_2–Q_2*, and Q_3–Q_3*, derived from the T_d presentation by coloration of three edges that form an open path. Colored edges are shown by heavy lines.

However, Q_1, Q_2, and Q_3 (Q_1*, Q_2*, and Q_3*) are isotopic to one another. That is, Q_1 (Q_1*) can be transformed into Q_2 (Q_2*) or Q_3 (Q_3*) by continuous deformations in space. We can therefore choose Q_1 as a general presentation of a K_5 graph with three colored edges that form an open path. For purposes of the following discussion, we show Q_1 and Q_1* with labeled vertices in Figure 9.

Let us initially assume that there exists an orientation-preserving homeomorphism h of three-dimensional space onto itself such that $h(Q_1) = Q_1^*$.

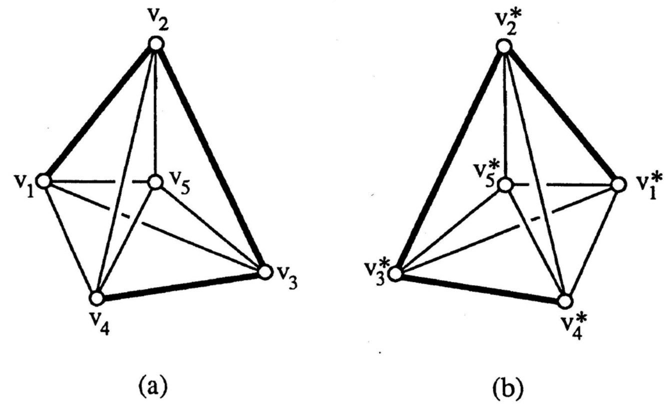


Figure 9. (a) Q_1 with labeled vertices. (b) Q_1*, the mirror image of Q_1, with labeled vertices.

Because v_5 is the only uncolored vertex, it immediately follows that $h(v_5) = v_5{}^*$. Vertices v_1 and v_4 are the only vertices incident to one colored edge, hence either $h(v_1) = v_1{}^*$ and $h(v_4) = v_4{}^*$, or $h(v_1) = v_4{}^*$ and $h(v_4) = v_1{}^*$. Similarly, either $h(v_2) = v_2{}^*$ and $h(v_3) = v_3{}^*$, or $h(v_2) = v_3{}^*$ and $h(v_3) = v_2{}^*$. If $h(v_1) = v_1{}^*$ and $h(v_4) = v_4{}^*$, then there is only one vertex, v_2 (say), that is joined to vertices v_4 and v_5 through uncolored edges, thus $h(v_2) = v_2{}^*$ and $h(v_3) = v_3{}^*$. Consequently, if $h(v_1) = v_4{}^*$ and $h(v_4) = v_1{}^*$, then $h(v_2) = v_3{}^*$ and $h(v_3) = v_2{}^*$. We thus have only two types of vertex-mapping under h: (i) $h(v_1) = v_1{}^*$, $h(v_2) = v_2{}^*$, $h(v_3) = v_3{}^*$, $h(v_4) = v_4{}^*$, $h(v_5) = v_5{}^*$; and (ii) $h(v_1) = v_4{}^*$, $h(v_4) = v_1{}^*$, $h(v_2) = v_3{}^*$, $h(v_3) = v_2{}^*$, $h(v_5) = v_5{}^*$. An isotopy, consisting of a rotation about the line passing through vertex v_5 and the midpoints of edges v_2v_3 and v_1v_4, demonstrates that the above two types of vertex-mapping are equivalent. We can therefore conclude that h sends each vertex v_i into its own mirror image $v_i{}^*$, *i.e.*, all the vertices of Q_1 can be considered differently labeled as shown. But it has been proven[15] that no h can convert a K_5 graph whose vertices are differently labeled into its mirror image, contrary to our initial assumption. Hence Q_1 and Q_1* are presentations of topological enantiomorphs, and it follows that a K_5 graph with any three colored edges that form an open path is topologically chiral. □

The molecular graph in Figure 5 is asymmetric; thus there is a one-to-one mapping between the graph and its mirror image. In addition, the graph contains a subgraph that is homeomorphic to $K_{3,3}$ with two differently colored non-adjacent edges. The hypothetical molecule in Figure 5 is therefore topologically chiral.

In conclusion, based on Wolcott's proof and the present work, the general conditions for topological chirality in graphs are as follows: (i) a one-to-one mapping can be uniquely defined between the graph and its mirror image, and (ii) the graph contains a subgraph that is homeomorphic to a $K_{3,3}$ graph with two non-adjacent colored edges, or to a K_5 graph with three colored edges that form an open path, or to any other derived topologically chiral graphs (*e.g.*, M_3 or M_3*).

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SAŽETAK

Topološka kiralnost minimalno obojenih grafova Kuratowskog

Chengzhi Liang i Kurt Mislow

Dokazano je da topološka kiralnost grafa $K_{3,3}$ zahtijeva najmanje dvije susjedne obojene grane, dok topološka kiralnost grafa K_5 zahtijeva najmanje tri obojene grane povezane u otvorenu stazu.