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Complete polyhedral description of chemical graphs of maximum degree at most 3

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Abstract : Chemical graphs are simple undirected connected graphs, where vertices represent atoms in a molecule and edges represent chemical bonds. A degree-based topological index is a molecular descriptor used to study specific physicochemical properties of molecules. Such an index is computed from the sum of the weights of the edges of a chemical graph, each edge having a weight defined by a formula that depends only on the degrees of its endpoints. Given any degree-based topological index and given two integers n and m, we are interested in determining chemical graphs of order n and size m that maximize or minimize the index. Focusing on chemical graphs with maximum degree at most 3, we show that this reduces to determining the extreme points of a polytope that contains at most 10 facets. We also show that the number of extreme points is at most 16, which means that for any given n and m, there are very few different classes of extremal graphs, independently of the chosen degree-based topological index.

Keywords : Chemical graphs, degree-based topological index, extremal graphs

1 Introduction

Graph-theoretic descriptors, known as topological indices, play a fundamental role in mathematical chemistry by capturing structural properties of molecules and predicting their physicochemical behaviors [12, 22, 23, 32, 38–40]. As their name suggests, these indices depend on the structure of the molecules when modeled as a connected simple undirected graph, with the vertices representing the atoms and edges representing the chemical bonds. A common class of topological indices, called *degree-based topological indices* are computed as the sum of the weights of the edges of a graph, each edge having a weight defined by a formula that depends only on the degrees of its endpoints. As a consequence, considering the partition of the set of edges where each block consists of edges having the same two endpoints degrees, a degree-based topological index can be viewed as a linear combination of the block sizes of this partition.

One of the first and most popular degree-based topological indices is the Randić connectivity index [48], introduced in 1975. Since then, numerous such indices have been defined. They were categorized for the first time as degree-based in 2013 in [29], where the author describes and compares the most important of them, in particular regarding their correlations with physico-chemical parameters. As he claims, "To use a mild expression, today we have far too many such descriptors, and there seems to lack a firm criterion to stop or slow down their proliferation." In light of their links with physico-chemical properties, it is a natural question to ask what are the minimal or maximal values these indices can take. These questions have given rise to a large number of publications [2–6, 9–11, 13–17, 19–21, 24, 25, 27, 28, 30, 31, 34–37, 42–45, 47, 49, 50, 53–57]. In some of these papers, the index is optimized over the set of all graphs or all connected graphs. However, since degree-based topological indices concern physico-chemical properties of molecules, it is natural to narrow their study to chemical graphs that we now define.

As pointed out by Patrick Fowler [26], and as mentioned in [7], two definitions of chemical graphs appropriate to different kinds of carbon framework can be found in the literature. Chemical graphs can be regarded as the skeletons of saturated hydrocarbons (such as alkanes), which implies that the maximum degree in such graphs is at most 4. If instead the interest is in (unsaturated) conjugated systems, such as alkenes, polyenes, benzenoids [41], and fullerenes [51, 52], then the chemical graphs that model such compounds have maximum degree at most 3, since a conjugated carbon atom participates in at most three single bonds.

In this paper, we restrict our attention to chemical graphs with maximum degree at most 3. The main practical outcome of this paper, is that for any degree-based topological index and any given values n and m, we are able to give the maximum and the minimum values that the index can take over the set of all chemical graphs with n vertices and m edges (provided that such graphs exist), together with a characterization of the set of graphs reaching these optimum values.

1.1 Our approach

For a graph G and two integers i, j with $1 \leq i \leq j$, an ij-edge in G is an edge with endpoints of degree i and j, and we denote m_{ij} the number of ij-edges in G. A degree-based topological index is a linear function of the form $\sum_{i\leq j} c_{ij} m_{ij}$, where c_{ij} is any real number. For example, the Randić index has $c_{ij} = \frac{1}{\sqrt{ij}}$. Assuming that G is connected, of order at least 3, and of maximum degree at most 3, only 5 of the m_{ij} values can be strictly positive, namely m_{12}, m_{13}, m_{22}, m_{23}, and m_{33}. Moreover, as will be explained in Section 2, fixing n and m reduces the degrees of freedom by 2 and we therefore work in a 3-dimensional space spanned by three of the five variables of interest. We have chosen m_{12}, m_{13} and m_{33}, and we say that a triplet (m_{12}, m_{13}, m_{33}) is realizable for (n, m) if there is at least one connected graph of order n, size m, maximum degree at most 3, and with exactly m_{12} 12-edges, m_{13} 13-edges, and m_{33} 33-edges.

The linearity property of degree-based topological indices together with the aim of finding extremal values for them hinted us to carry out a polyhedral study of chemical graphs of maximum degree at most 3. Indeed, once we know how a polyhedron looks like, it is a trivial task to optimize a linear function of the underlying variables over that polyhedron. In our analysis, we partition the set of all possible combinations of n and m into 96 cases. In each of these cases, we explicitly describe the polytope $\mathcal{P}_{n,m}$ given by the convex hull of all points (m_{12}, m_{13}, m_{33}) that are realizable for the corresponding pair (n, m).

As will be shown all these polytopes contain at most 10 facets and at most 16 vertices. Concretely, this means that for any given n and m, there are very few different classes of extremal graphs, independently of the chosen degree-based topological index. This provides insight into why only a few graph families are sufficient to characterize the extremal graphs of many different degree-based topological indices, as was observed in [7].

1.2 Structure of the paper

Our paper is organized as follows. In Section 2, we introduce some basic definitions and notations. In Section 3, we explicit all cases where the polytopes $\mathcal{P}_{n,m}$ are degenerated, i.e. not 3-dimensional. In Section 4, we give a list of 21 inequalities on m_{12}, m_{13} and m_{33}, each with associated conditions on n and m. For each of these inequalities we show that they are valid for all chemical graphs of maximum degree at most 3 with n vertices and m edges, such that n and m satisfy the associated conditions. In Section 5, we give a list of 23 points (m_{12}, m_{13}, m_{33}), each with its associated condition on n and m to be realizable for (n, m). In Section 6, we show that the inequalities introduced in Section 4, subject to their respective conditions on n and m, are actually facet defining and induce bounded polyhedrons. In Section 7, we partition the set of all possible combinations of n and m into 96 cases, and for each case, we explicitly give the set of facets and the set of extreme points that define the associated polytope $\mathcal{P}_{n,m}$. In Section 8, we illustrate by an example how to apply our characterizations to find the optimal value of a degree-based topological index. Finally, we discuss in Section 9 how to extend our results to chemical graphs of maximum degree at most 4.

2 Basics and notations

As mentioned in the previous section, we denote m_{ij} the number of ij-edges in G. Let n_i be the number of vertices in G of degree i. A *chemical graph* of order n and size m is a connected graph with maximum degree at most 3. If $n \leq 2$ then the cliques of order 1 and 2 are the only chemical graphs of that order. Thus, in the following, we only consider chemical graphs with at least 3 vertices, which gives

$$2 \leq n - 1 \leq m \leq \min\left\{\left\lfloor \frac{3n}{2} \right\rfloor, \frac{n(n-1)}{2}\right\}. \tag{1}$$

Since chemical graphs are connected, Inequations (1) imply $m_{11} = 0$. Hence, a chemical graph can have at most 5 nonzero m_{ij} values, namely $m_{12}, m_{13}, m_{22}, m_{23}$ and m_{33}. We therefore have:

$$n_1 = m_{12} + m_{13} \tag{2}$$
$$n_2 = \frac{m_{12} + 2m_{22} + m_{23}}{2} \tag{3}$$
$$n_3 = \frac{m_{13} + m_{23} + 2m_{33}}{3} \tag{4}$$
$$n = n_1 + n_2 + n_3 = \frac{3}{2}m_{12} + \frac{4}{3}m_{13} + m_{22} + \frac{5}{6}m_{23} + \frac{2}{3}m_{33} \tag{5}$$
$$m = m_{12} + m_{13} + m_{22} + m_{23} + m_{33}. \tag{6}$$

Note that knowing n, m and three of the five m_{ij} values, we can deduce the other two. We have chosen to describe each chemical graph using m_{12}, m_{13} and m_{33}. It follows from Equations (5) and (6) that the other two values are obtained as follows:

$$m_{22} = 6n - 5m - 4m_{12} - 3m_{13} + m_{33} \quad (7)$$
$$m_{23} = 6m - 6n + 3m_{12} + 2m_{13} - 2m_{33}. \quad (8)$$

This leads to the following definitions.

Definition 1. A point (m_{12}, m_{13}, m_{33}) is *realizable* for a pair (n, m) if there exists a graph of order n and size m with m_{12} 12-edges, m_{13} 13-edges and m_{33} 33-edges.

Definition 2. Let n and m be two integers satisfying (1). The associated polytope $\mathcal{P}_{n,m}$ is the convex hull of all points (m_{12}, m_{13}, m_{33}) that are realizable for (n, m).

Note that a point of $\mathcal{P}_{n,m}$ possibly corresponds to several chemical graphs. For example, the two non-isomorphic chemical graphs of Figure 1 both correspond to point $(1, 0, 0)$ in $\mathcal{P}_{6,6}$.

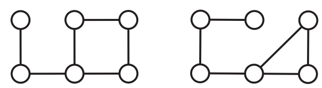


Figure 1: Two non-isomorphic chemical graphs with coordinates $(1, 0, 0)$ in $\mathcal{P}_{6,6}$

In view of Definition 2, we consider that a full-dimensional polytope $\mathcal{P}_{n,m}$ is of dimension 3. Note that given a degree-based topological index f with c_{ij} values, we have:

$$\begin{aligned} f(G) =& c_{12}m_{12} + c_{13}m_{13} + c_{22}m_{22} + c_{23}m_{23} + c_{33}m_{33} \\ =& c_{12}m_{12} + c_{13}m_{13} + c_{22}(6n - 5m - 4m_{12} - 3m_{13} + m_{33}) \\ &+ c_{23}(6m - 6n + 3m_{12} + 2m_{13} - 2m_{33}) + c_{33}m_{33} \\ =& (c_{12} - 4c_{22} + 3c_{23})m_{12} + (c_{13} - 3c_{22} + 2c_{23})m_{13} + (c_{22} - 2c_{23} + c_{33})m_{33} \\ &+ (6n - 5m)c_{22} + (6m - 6n)c_{23}. \end{aligned}$$

Hence, maximizing or minimizing $f(G)$ over all chemical graphs of order n and size m is equivalent to maximizing or minimizing the linear function $c'_{12}m_{12} + c'_{13}m_{13} + c'_{33}m_{33}$ in $\mathcal{P}_{n,m}$, where

- $c'_{12} = c_{12} - 4c_{22} + 3c_{23}$,
- $c'_{13} = c_{13} - 3c_{22} + 2c_{23}$,
- $c'_{33} = c_{22} - 2c_{23} + c_{33}$.

3 Degenerated polytopes

In this section, we describe degenerated polytopes, i.e., all polytopes of dimension < 3. As shown in Section 7, the other polytopes are full-dimensional. Some graphs mentioned in this section are shown in Figure 2.

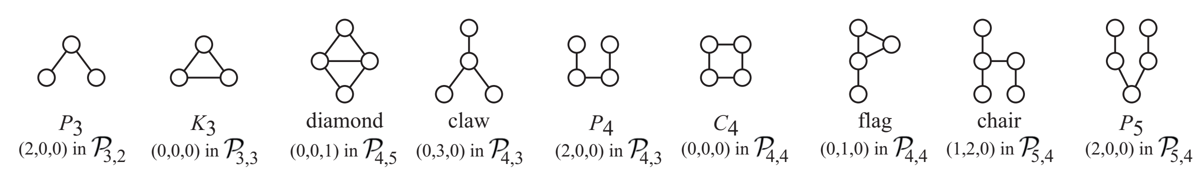


Figure 2: Some special graphs with their coordinates in a degenerated polytopes

3.1 0-dimensional polytopes

$\mathcal{P}_{n,m}$ is a 0-dimensional polytope, if it contains only one point. This is the case for $(n,m) = (3,2), (3,3)$ and $(4,5)$. Indeed, P_3 is the only point with coordinates $(2,0,0)$ in $\mathcal{P}_{3,2}$, K_3 is the only point with coordinates $(0,0,0)$ in $\mathcal{P}_{3,3}$, and the diamond is the only point with coordinates $(0,0,1)$ in $\mathcal{P}_{4,5}$. Other 0-dimensional polytopes appear when $m = \lfloor \frac{3n}{2} \rfloor$:

- if n is even, then the only point in $\mathcal{P}_{n,m}$ is $(0,0,\frac{3n}{2})$, and all connected cubic graphs of order n have these coordinates.
- if n is odd, then the only point in $\mathcal{P}_{n,m}$ is $(0,0,\frac{3n-5}{2})$, and all connected graphs of order n with one vertex of degree 2 and $n-1$ vertices of degree 3 have these coordinates. They can be obtained from a cubic graph with $n-1$ vertices by subdividing one of its edges into two edges.

3.2 1-dimensional polytopes

The polytope $\mathcal{P}_{n,m}$ has dimension 1, if all its realizable points are aligned. In our case, all such polytopes contain exactly two realizable points. This happens when $(n,m) = (4,3), (4,4)$ or $(5,4)$. More precisely,

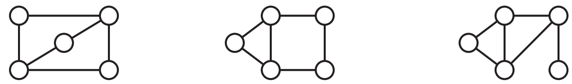
- if $(n,m) = (4,3)$, then
  - $(0,3,0)$ and $(2,0,0)$ are the only points in $\mathcal{P}_{4,3}$, and the only chemical graphs with these coordinates are the claw and P_4, respectively;
  - $\mathcal{P}_{4,3}$ can be defined with the two equalities $m_{33} = 0$ and $3m_{12} + 2m_{13} = 6$, and the inequalities $0 \leq m_{12} \leq 2$;
- if $(n,m) = (4,4)$, then
  - $(0,1,0)$ and $(0,0,0)$ are the only points in $\mathcal{P}_{4,4}$, and the only chemical graphs with these coordinates are the flag and C_4, respectively;
  - $\mathcal{P}_{4,4}$ can be defined with the two equalities $m_{12} = 0$ and $m_{33} = 0$, and the inequalities $0 \leq m_{13} \leq 1$;
- if $(n,m) = (5,4)$, then
  - $(1,2,0)$ and $(2,0,0)$ are the only points in $\mathcal{P}_{5,4}$, and the only chemical graphs with these coordinates are the chair and P_5, respectively;
  - $\mathcal{P}_{5,4}$ can be defined with the two equalities $m_{33} = 0$ and $2m_{12}+m_{13} = 4$, and the inequalities $0 \leq m_{13} \leq 2$.

3.3 2-dimensional polytopes

If $\mathcal{P}_{n,m}$ is a 2-dimensional polytope, it can be described as the intersection of a plane with at least 3 facets defined by inequalities. This happens when $(n,m) = (5,6)$ or when $n \geq 6$ is even and $m = \frac{3n-2}{2}$. The three points in $\mathcal{P}_{5,6}$ are shown in Figure 3, while when $n \geq 6$ is even and $m = \frac{3n-2}{2}$, the three points are:

- $(0,1,m-1)$, when we have one vertex of degree 1 and all others of degree 3. Such a graph is obtained from a cubic graph with $n-2$ vertices by subdividing an edge in two, and adding a pendant vertex to the newly created vertex;
- $(0,0,m-3)$, when we have 2 adjacent vertices of degree 2 and $n-2$ vertices of degree 3. Such a graph is obtained from a cubic graph with $n-2$ vertices by subdividing an edge in three;
- $(0,0,m-4)$, when we have 2 non-adjacent vertices of degree 2 and $n-2$ vertices of degree 3. Such a graph is obtained from a cubic graph with $n-2$ vertices by subdividing two edges in two.

These 2-dimensional polytopes $\mathcal{P}_{n,m}$ are triangles defined by the equality $m_{12} = 0$ and by the three inequalities $m_{13} \geq 0$, $-3m_{13} + m_{33} \geq 5m - 6n$, and $2m_{13} - m_{33} \geq 6n - 5m - 1$. It is not difficult to check that the ends of the triangle are the points defined above, and are the only realizable points of $\mathcal{P}_{n,m}$.



(0,0,0) (0,0,1) (0,1,3)

Figure 3: The three chemical graphs of order 5 and size 6, with their coordinates in $\mathcal{P}_{5,6}$

4 Twenty-one valid inequalities

In view of the previous section, full-dimensional polytopes appear when $(n, m) = (5, 5)$ and when $n \geq 6$ and $m \leq \lfloor \frac{3n-3}{2} \rfloor$. We will analyze the full-dimensional polytopes with $m < 12$ in Section 7, and we therefore assume here that

$$\max\{12, n-1\} \leq m \leq \left\lfloor \frac{3n-3}{2} \right\rfloor. \tag{9}$$

Note that this implies $n \geq 9$. In this section we give 21 constraints that all have the form of an inequality that is imposed when certain conditions (in addition to condition (9)) on the order n and the size m of a chemical graph G are satisfied. These constraints are shown in Table 1. The first column indicates the Id of the constraint, the second column gives the inequalities, and the third one gives conditions on n and m (which have to be satisfied in addition to (9)). Note that inequality F16 uses m_{23} instead of m_{33}. This is because it is easier to read (there is no quadratic term) when compared to the inequality we would have by using m_{12}, m_{13} and m_{33} which is:

$$6m^2 + 9n^2 - 15nm - 2m + 3n \leq (3n - 2m)(2m_{12} + m_{13} - m_{33}) + 2m_{13}. \tag{10}$$

Table 1: Twenty-one constraints for chemical graphs satisfying (9)

Id	Inequalities	Conditions on n and m
F1	$0 \leq m_{12}$	no condition
F2	$0 \leq m_{13}$	no condition
F3	$0 \leq m_{33}$	$m \leq \frac{6n-4}{5}$
F4	$2m-3n+2 \leq -3m_{12}$	$(m \bmod 3)=2$
F5	$4m-6n+2 \leq -6m_{12}-3m_{13}$	$(m \bmod 3)=1$
F6	$5m-6n \leq -4m_{12}-3m_{13}+m_{33}$	no condition
F7	$5m-6n+2 \leq -3m_{12}-3m_{13}+3m_{33}$	$(m \leq \frac{6n-5}{5}) \wedge (m \bmod 3)=2$
F8	$5m-6n+2 \leq -4m_{12}-2m_{13}+2m_{33}$	$(m \leq \frac{6n-2}{5}) \wedge (m-2n \bmod 4)=2$
F9	$5m-6n+3 \leq -4m_{12}+4m_{33}$	$(m \leq \frac{6n-3}{5}) \wedge (m-2n \bmod 4)=1$
F10	$15m-18n+3 \leq -12m_{12}-8m_{13}+4m_{33}$	$(m \leq \frac{6n-1}{5}) \wedge (m-2n \bmod 4)=3$
F11	$10m-12n+2 \leq -6m_{12}-6m_{13}+3m_{33}$	$(m \leq \frac{6n-4}{5}) \wedge (m \bmod 3)=1$
F12	$3n-3m \leq m_{12}+m_{13}-m_{33}$	$n \leq m \leq \frac{3n-6}{2}$
F13	$3n-3m+1 \leq 2m_{12}+m_{13}-m_{33}$	$(m \neq n) \wedge (n \bmod 2)=1$
F14	$0 \leq 2(n-2)m_{12}+(n-3)m_{13}-(n-1)m_{33}$	$(m=n) \wedge (n \bmod 2)=1$
F15	$-2n+10 \leq 2(n-4)m_{12}+(n-2)m_{13}-(n-4)m_{33}$	$(m=n+1) \wedge (n \bmod 2)=0$
F16	$6n-4m \leq (3n-2m)(m_{12}+m_{23})+4m_{13}$	$(m \geq n+2) \wedge (n \bmod 2)=0$
F17	$4n-16 \leq 2(n-4)m_{12}+(n-4)m_{13}-(n-6)m_{33}$	$(m=n-1) \wedge (n \bmod 2)=0$
F18	$2n-18 \leq (n-9)m_{12}+(n-6)m_{13}-(n-6)m_{33}$	$(m=n-1) \wedge (n \bmod 3)=0$
F19	$4n-32 \leq (2n-16)m_{12}+(2n-13)m_{13}-(2n-10)m_{33}$	$(m=n-1) \wedge (n \bmod 3) = 2$
F20	$2n-14 \leq (n-7)m_{12}+(n-6)m_{13}-(n-4)m_{33}$	$m=n-1$
F21	$-1 \leq 2m_{12}+2m_{13}-m_{33}$	$m=n+1$

The inequalities in Table 1 are named Fi ($i = 1, \ldots, 21$), the reason for choosing the letter 'F' being that, as we will see in Section 6, these inequalities are facet defining. In this section, we only prove that they are all valid. In other words, a chemical graph of order n and size m necessarily satisfies inequality Fi if n and m satisfy the conditions associated with Fi. Note that the inequalities Fi are possibly valid for other values of n and m but, as we will see in Section 6, the inequalities are then not facet defining.

The following theorem gives a proof that the 21 inequalities in Table 1 are valid. Before we give this proof, it is useful to note that Equations (2), (4), (5) and (6) imply

$$n_1 = n_3 + 2(n - m). \tag{11}$$

Also, given any two integers a and b, it directly follows from (5) and (6) that

$$am + bn = (a + \frac{3b}{2})m_{12} + (a + \frac{4b}{3})m_{13} + (a + b)m_{22} + (a + \frac{5b}{6})m_{23} + (a + \frac{2b}{3})m_{33}. \tag{12}$$

Note finally that $2m = 3n - 2n_1 - n_2 = 3n - 2m_{12} - 2m_{13} - n_2$. Hence,

$$m \equiv 2m_{13} + (n_2 - m_{12})(\text{mod}3). \tag{13}$$

Theorem 1. If n and m satisfy condition (9) as well as the conditions associated with a Fi ($1 \le i \le 21$), then all chemical graphs of order n and size m satisfy inequality Fi.

Proof. Let n and m be two integers satisfying condition (9), and let G be a chemical graph of order n and size m, with m_{ij} ij-edges.

- F1, F2 and F3 are clearly valid (even if $m > \frac{6n-4}{5}$ for F3).
- If m mod $3 = 2$, we know from (13) that $(2m_{13} + (n_2 - m_{12}))$ mod $3 = 2$. Hence, $2m_{13} + (n_2 - m_{12}) \ge 2$ and F4 is valid since

$$2m = 3n - 3m_{12} - (2m_{13} + (n_2 - m_{12})) \le 3n - 3m_{12} - 2.$$

- If m mod $3 = 1$, we know from (13) that $m_{13}+2(n_2-m_{12})$ mod $3 = 2$. Hence, $m_{13}+2(n_2-m_{12}) \ge 2$ and F5 is valid since (12) gives

$$\begin{aligned} 6n - 4m &= 5m_{12} + 4m_{13} + 2m_{22} + m_{23} \\ &= 6m_{12} + 3m_{13} + (m_{13} + 2m_{22} + m_{23} - m_{12}) \\ &= 6m_{12} + 3m_{13} + (m_{13} + 2(n_2 - m_{12})) \\ &\ge 6m_{12} + 3m_{13} + 2. \end{aligned}$$

- F6 is valid since (12) gives

$$5m - 6n = -4m_{12} - 3m_{13} - m_{22} + m_{33} \le -4m_{12} - 3m_{13} + m_{33}.$$

- If m mod $3 = 2$ then $m_{12} + m_{22} + 2m_{33} \ge 2$. Indeed, this is obvious if $m_{33} \ge 1$ while for $m_{33} = 0$, we have $m_{12} + m_{22} \ge 2$ since (7) gives $m_{13} = \frac{6n-5m-(4m_{12}+m_{22})}{3}$, which implies m mod $3 = (m_{12} + m_{22})$ mod $3 = 2$. Hence, F7 is valid since (12) gives

$$\begin{aligned} 5m - 6n &= -4m_{12} - 3m_{13} + m_{33} - m_{22} \\ &= -3m_{12} - 3m_{13} + 3m_{33} - (m_{12} + m_{22} + 2m_{33}) \\ &\le -3m_{12} - 3m_{13} + 3m_{33} - 2. \end{aligned}$$

- If $(m - 2n)$ mod $4 = 2$ then $m_{13} + m_{22} + m_{33} \ge 2$. Indeed, 3 times (7) plus 4 times (8) gives $m_{23} = \frac{9m-6n-(m_{13}+3m_{22}+5m_{33})}{4}$, which implies $(m-2n)$ mod $4 = (m_{13}+3m_{22}+m_{33})$ mod $4 = 2$. Hence, F8 is valid since (12) gives

$$\begin{aligned} 5m - 6n &= -4m_{12} - 3m_{13} + m_{33} - m_{22} \\ &= -4m_{12} - 2m_{13} + 2m_{33} - (m_{13} + m_{22} + m_{33}) \\ &\le -4m_{12} - 2m_{13} + 2m_{33} - 2. \end{aligned}$$

- If $(m-2n) \bmod 4 = 1$ then $3m_{13}+3m_{33}+m_{22} \geq 3$. Indeed, this is obvious if $m_{13}+m_{33} \geq 1$ while for $m_{13}=m_{33}=0$ we have $m_{22} \geq 3$ since, as in the previous case, we deduce from (7) and (8) that $m_{23} = \frac{9m-6n-3m_{22}}{4}$, which implies $(m-2n) \bmod 4 = 3m_{22} \bmod 4 = 1$. Hence, F9 is valid since (12) gives

$$\begin{aligned}5m-6n &= -4m_{12}-3m_{13}+m_{33}-m_{22}\\ &= -4m_{12}+4m_{33}-(3m_{13}+3m_{33}+m_{22})\\ &\leq -4m_{12}+4m_{33}-3.\end{aligned}$$

- If $(m-2n) \bmod 4 = 3$ then $m_{13}+m_{33}+3m_{22} \geq 3$. Indeed, this is obvious if $m_{22} \geq 1$ while for $m_{22}=0$ we have $m_{13}+m_{33} \geq 3$ since we deduce from (7) and (8) that $m_{23} = \frac{9m-6n-(m_{13}+5m_{33})}{4}$, which implies $(m-2n) \bmod 4 = (m_{13}+m_{33}) \bmod 4 = 3$. Hence, F10 is valid since (12) gives

$$\begin{aligned}15m-18n &= -12m_{12}-9m_{13}+3m_{33}-3m_{22}\\ &= -12m_{12}-8m_{13}+4m_{33}-(m_{13}+m_{33}+3m_{22})\\ &\leq -12m_{12}-8m_{13}+4m_{33}-3.\end{aligned}$$

- If $m \bmod 3 = 1$ then $2m_{12}+2m_{22}+m_{33} \geq 2$. Indeed, this is obvious if $m_{12}+m_{22} \geq 1$ while for $m_{12}=m_{22}=0$ we must have $m_{33} \geq 2$ since (7) gives $m_{13} = \frac{6n-5m+m_{33}}{3}$, which implies $(m+m_{33}) \bmod 3 = (1+m_{33}) \bmod 3 = 0$. Hence, F11 is valid since (12) gives

$$\begin{aligned}10m-12n &= -8m_{12}-6m_{13}-2m_{22}+2m_{33}\\ &= -6m_{12}-6m_{13}+3m_{33}-(2m_{12}+2m_{22}+m_{33})\\ &\leq -6m_{12}-6m_{13}+3m_{33}-2.\end{aligned}$$

- F12 is valid since $m > n-1$ implies that G is not a path and we therefore have $m_{12} \leq m_{23}$, and (12) then gives

$$3n-3m = \frac{3}{2}m_{12}+m_{13}-\frac{1}{2}m_{23}-m_{33} = m_{12}+m_{13}-m_{33}+\frac{m_{12}-m_{23}}{2} \leq m_{12}+m_{13}-m_{33}.$$

- If n is odd, then G has at least one vertex of degree 2 and if in addition $m \neq n$, $m_{12}+m_{23} \geq 2$ else G is a cycle with $m=n$. This last inequality is equivalent to $\frac{m_{12}-m_{23}}{2} \leq m_{12}-1$. Hence, F13 is valid since (12) gives

$$3n-3m = \frac{3}{2}m_{12}+m_{13}-\frac{1}{2}m_{23}-m_{33} = m_{12}+m_{13}-m_{33}+\frac{m_{12}-m_{23}}{2} \leq 2m_{12}+m_{13}-m_{33}-1.$$

- If $n=m$, then we can assume that G is not a cycle since F14 is clearly valid when $m_{12}=m_{13}=m_{33}=0$. Equation (11) gives $n_1=n_3$, which is equivalent to $m_{13} = \frac{n-n_2-2m_{12}}{2}$. We know from (12) that $3n-3m = 0 = \frac{3m_{12}-m_{23}}{2}+m_{13}-m_{33}$, which is equivalent to $2m_{12}+m_{13}-m_{33} = \frac{m_{12}+m_{23}}{2}$ and $m_{12}-m_{33} = \frac{m_{23}-m_{12}}{2}-m_{13} = \frac{m_{12}+m_{23}+n_2-n}{2}$. Hence, proving F14 is equivalent to proving

$$\begin{aligned}0 &\leq \frac{n-3}{2}(2m_{12}+m_{13}-m_{33})+m_{12}-m_{33}\\ &= \frac{n-3}{2}\left(\frac{m_{12}+m_{23}}{2}\right)+\frac{m_{23}+m_{12}+n_2-n}{2}.\end{aligned}$$

  If $n=m$ is an odd number, then $n_2 \geq 1$, which implies $m_{12}+m_{23} \geq 2$. Hence, $\frac{n-3}{2}\left(\frac{m_{12}+m_{23}}{2}\right)+\frac{m_{23}+m_{12}+n_2-n}{2} \geq \frac{n-3}{2}-\frac{n-3}{2}=0$, and F14 is therefore valid.
- If $m=n+1$, we know from (12) that $3n-3m = -3 = \frac{3m_{12}-m_{23}}{2}+m_{13}-m_{33}$, which is equivalent to $2m_{12}+m_{13}-m_{33}+2 = \frac{m_{12}+m_{23}}{2}-1$. Proving the validity of F15 is therefore equivalent to proving

$$1 \leq \frac{n-4}{2}(2m_{12}+m_{13}-m_{33}+2)+m_{13}$$

$$= \frac{n-4}{2}\left(\frac{m_{12}+m_{23}}{2}-1\right)+m_{13}.$$

Note that $m_{12}+m_{23}$ is an even number. Hence, we have one of the five following cases:

- if $m_{12}+m_{23}\geq 4$, then the inequality is clearly satisfied.
- if $m_{12}=m_{23}=1$, then $m_{13}\geq 1$, else $m_{33}=4$ and $n_3=3$ (by Equation 4), which is impossible. Hence $\frac{n-4}{2}\left(\frac{m_{12}+m_{23}}{2}-1\right)+m_{13}=m_{13}\geq 1$.
- if $m_{12}=0$ and $m_{23}=2$, then $m_{13}\geq 1$, else $m_{33}=2$ and $n_3=2$, which is impossible. Hence $\frac{n-4}{2}\left(\frac{m_{12}+m_{23}}{2}-1\right)+m_{13}=m_{13}\geq 1$.
- if $m_{12}=2$ and $m_{23}=0$, then G is a path, a contradiction with $m=n+1$.
- if $m_{12}=m_{23}=0$, then $n_2=0$ and Equation (11) implies $m_{13}=\frac{n-2}{2}$. Hence $\frac{n-4}{2}\left(\frac{m_{12}+m_{23}}{2}-1\right)+m_{13}=-\frac{n-4}{2}+\frac{n-2}{2}=1$.

- To prove F16 we analyze the possible values of $m_{12}+m_{23}$ which is an even number.
  - If $m_{12}+m_{23}\geq 2$ then $(3n-2m)(m_{12}+m_{23})+4m_{13}\geq 2(3n-2m)=6n-4m$.
  - If $m_{12}+m_{23}=0$ then $m_{22}=0$ (since $m\neq n$). Hence $n_2=0$, which implies $m_{13}=\frac{3n-2m}{2}$. Therefore, $(3n-2m)(m_{12}+m_{23})+4m_{13}=2(3n-2m)=6n-4m$.

- If $m{=}n{-}1$, then we know from (12) that $6n-6m=6=3m_{12}+2m_{13}-m_{23}-2m_{33}$, which is equivalent to $2m_{12}+m_{13}-m_{33}-4=\frac{m_{12}+m_{23}}{2}-1$. Hence, proving F17 is equivalent to proving

$$\begin{aligned}4 &\leq \frac{n-6}{2}(2m_{12}+m_{13}-m_{33}-4)+2m_{12}+m_{13}\\ &= \frac{n-6}{2}\left(\frac{m_{12}+m_{23}}{2}-1\right)+2m_{12}+m_{13}.\end{aligned}$$

  - if $m_{12}\geq 2$ then the inequality is clearly satisfied;
  - if $m_{12}=1$, then G is not a chain, which means that $m_{23}\geq 1$ and $n_1\geq 3$, which implies $m_{13}\geq 2$. Hence, $\frac{n-6}{2}\left(\frac{m_{12}+m_{23}}{2}-1\right)+2m_{12}+m_{13}\geq 4$;
  - if $m_{12}=0$ then m_{23} is even and $m_{13}\geq 4$ (since $n>4$). Hence, the inequality is clearly satisfied if $m_{23}\geq 2$, while for $m_{23}{=}0$, we have $n_2{=}0$ and Equation (11) implies $m_{13}=\frac{n+2}{2}$, which gives $\frac{n-6}{2}\left(\frac{m_{12}+m_{23}}{2}-1\right)+2m_{12}+m_{13}=-\frac{n-6}{2}+\frac{n+2}{2}=4$.

- If $m=n-1$, then we can assume $n_3>0$, else $m_{12}=2$ and $m_{13}=m_{33}=0$, which implies that inequality F18 is valid. We know from (12) that $3n-3m=3=\frac{3m_{12}-m_{23}}{2}+m_{13}-m_{33}$. Hence, $m_{12}+m_{13}-m_{33}=3+\frac{m_{23}-m_{12}}{2}$ which implies that $m_{33}\leq m_{12}+m_{13}-3$. Therefore, proving F18 is equivalent to proving

$$\begin{aligned}0 &\leq (n-9)(m_{12}+m_{13}-m_{33}-2)+3(m_{13}-m_{33})\\ &= (n-9)\left(\frac{m_{23}-m_{12}}{2}+1\right)+3(m_{13}-m_{33}).\end{aligned}$$

  We know from Equation (11) that $n_1{=}n_3{+}2$, which implies $\frac{3}{2}m_{12}{=}\frac{n+2-(n_2-m_{12})}{2}{-}m_{13}{\leq}\frac{n+2}{2}$. Hence, $m_{12}{\leq}\frac{n+2}{3}$, and assuming n mod 3=0 implies $m_{12}\leq\frac{n}{3}$. Since $m_{23}\geq m_{12}$ and $m_{13}-m_{33}\geq 3-m_{12}$, we have

$$\begin{aligned}(n-9)\left(\frac{m_{23}-m_{12}}{2}+1\right)+3(m_{13}-m_{33}) &\geq (n-9)+3(3-m_{12})\\ &\geq (n-9)+3(3-\frac{n}{3})=0.\end{aligned}$$

- If $m=n-1$, then as in the previous case, we know that $m_{12}+m_{13}-m_{33}=3+\frac{m_{23}-m_{12}}{2}$. Hence, proving F19 is equivalent to proving

$$\begin{aligned}0 &\leq (2n-16)(m_{12}+m_{13}-m_{33}-2)+3(m_{13}-2m_{33})\\ &= (2n-16)\left(\frac{m_{23}-m_{12}}{2}+1\right)+3m_{13}-6m_{33}.\end{aligned}$$

Let $f(G) = (2n-16)\left(\frac{m_{23}-m_{12}}{2}+1\right) + 3(m_{13}-2m_{33})$. We have to prove that if G is a tree of order n with $(n \bmod 3) = 2$, then $f(G) \geq 0$. We may assume $m_{33} > 0$ and $n_3 > 0$ since $f(G) \geq 0$ when $n_3 = 0$ or $m_{33} = 0$. So assume G minimizes f over all trees of order n with $(n \bmod 3) = 2$, $n_3 > 0$ and $m_{33} > 0$. It remains to prove that $f(G) \geq 0$.

Note first that G does not contain a chain $[v_1, v_2, \ldots, v_p]$ $(p \geq 3)$ with v_1 and v_p of degree 3 and the other vertices of degree 2. Indeed if such a chain exists then let uw be an edge in G with u of degree 1 and let G' be the tree obtained from G by removing uw, v_1v_2, $v_{p-1}v_p$ and adding uv_2, wv_{p-1}, v_1v_p. Then $f(G') = f(G) - (2n-16) - 6 < f(G)$ if w has degree 2, and $f(G') = f(G) - (2n-16) - 9 < f(G)$ if w has degree 3. Both cases contradict the fact that G minimizes f.

So $m_{12} = m_{23}$, which implies $n_1 = m_{12} + m_{13} = m_{33} + 3$. Hence, $m_{22} = m - (m_{12} + m_{13}) - m_{23} - m_{33} = m - 6 - 3m_{33} + m_{13}$, which implies $3m_{33} = n - 7 - m_{22} + m_{13}$. Note also that since $n = 3m_{33} + 7 + m_{22} - m_{13}$ and $n \bmod 3 = 2$, we have $(m_{22} - m_{13}) \bmod 3 = 1$. Hence, $m_{13}+2m_{22} \geq 2$. Indeed, this is clearly true if $m_{22} \geq 1$, while $m_{22} = 0$ implies $m_{13} \geq 2$. Therefore

$$\begin{aligned} f(G) &= 2n - 16 + 3m_{13} - 2(n - 7 - m_{22} + m_{13}) \\ &= m_{13} + 2m_{22} - 2 \geq 0. \end{aligned}$$

- Let $f(G) = (n-7)(m_{12}+m_{13}-m_{33}-2)+m_{13}-3m_{33}$. Proving the validity of F20 is equivalent to proving that $f(G) \geq 0$ for all trees G. If G is a path, then $f(G) = 0$. So let G be a tree with $n_3 > 0$ and assume that G has minimum value among all trees having at least one vertex of degree 3.

  We first prove that G does not contain any chain $[v_1, v_2, \ldots, v_p]$ with v_1 and v_p of degree 3 and all other vertices of degree 2. Consider any vertex u of degree 1, let w be its neighbor, and let G' be the tree obtained from G by removing the edges uw, v_1v_2, $v_{p-1}v_p$ and adding the edges uv_2, wv_{p-1}, v_1v_p. Then $f(G')=f(G)-(n-7)-4$ if w has degree 3, while $f(G')=f(G)-(n-7)-3$ if w has degree 2. Hence, $f(G')<f(G)$, which contradicts the fact that G minimizes f.

  So $m_{12} = m_{23}$ which, as shown in the previous case, implies $m_{33}=m_{12}+m_{13}-3$ and $3m_{33} = n-7-m_{22}+m_{13}$. It follows that $f(G)=(n-7)+m_{13}-(n-7-m_{22}+m_{13})=m_{22}\geq 0$.
- Let $f(G) = 2m_{12} + 2m_{13} - m_{33}$. To prove F21, we have to prove that $f(G) \geq -1$. Let $\mathcal{G}$ be the set of graphs that minimize $f(G)$ among all graphs of size $m = n+1$ that satisfy condition (9) and let G be a graph in $\mathcal{G}$ having the smallest number of vertices of degree 1. Since $m = n+1$, G has a least one vertex of degree 3.

  If G has at least one vertex of degree 1, then let $[v_1, v_2, \ldots, v_p]$ $(p \geq 2)$ be a chain in G with v_1 of degree 1, v_p of degree 3 and all other vertices of degree 2. Let $u \neq v_{p-1}$ be a second neighbor of v_p and let G' be the graph obtained from G by replacing uv_p by uv_1. Then G' is still connected, has $m_{12}+m_{13}-1$ vertices of degree 1 and at least $m_{33}-2$ 33-edges. Hence, G' has less vertices of degree 1 than G and $f(G')\leq f(G)$, a contradiction.

  So $n_1=0$, and it follows from Equation (11) that $n_3=2$. Therefore, $f(G)=-m_{33}\geq -1$. □

5 Twenty-three realizable points

In this section, we give 23 points (m_{12}, m_{13}, m_{33}) and conditions on n and m so that they are realizable for (n, m). These points appear in Table 2, where the first column indicates the Id of the point and the last three columns give the 3 components m_{12}, m_{13} and m_{33}.

The conditions on n and m for realizability are given in the second column of Table 3. As we will see in Section 7, given any two integers n and m that satisfy condition (9), the set of extreme points of the polytope $\mathcal{P}_{n,m}$ is a subset of these 23 points. It may happen that a Vi is realizable for (n, m) but not an extreme point of $\mathcal{P}_{n,m}$. The analysis in Section 7 will show that the conditions on n and m for Vi to be an extreme point of $\mathcal{P}_{n,m}$ are those shown in the third column of Table 3. So, for example, V21 is realizable for (n, m) with $m \leq n$, while it is an extreme point of $\mathcal{P}_{n,m}$ only if $m = n-1$.

Table 2: Twenty-three realizable points

Id	m_{12}	m_{13}	m_{33}
V1	0	0	0
V2	2	0	0
V3	0	0	1
V4	0	0	$5m-6n$
V5	$\frac{6n-5m-3((m-2n) \bmod 4)}{4}$	$(m-2n) \bmod 4$	0
V6	$\frac{6n-5m+(m-2n) \bmod 4}{4}$	0	$(m-2n) \bmod 4$
V7	$\frac{6n-5m-(2n-m) \bmod 4}{4}$	0	0
V8	1	$\frac{3n-2m-n \bmod 2-4}{2}$	$\frac{4m-3n-n \bmod 2-2}{2}$
V9	2	$\frac{3n-2m-n \bmod 2-6}{2}$	$\frac{4m-3n-n \bmod 2-2}{2}$
V10	0	$\frac{3n-2m-n \bmod 2}{2}$	$\frac{4m-3n-3(n \bmod 2)}{2}$
V11	1	$\frac{3n-2m-3}{2}$	$\frac{4m-3n-1}{2}$
V12	$3m-3n-2$	$3m-3n-2$	$6m-6n-1$
V13	$3m-3n-1$	0	$6m-6n-1$
V14	0	$3m-3n-2$	$6m-6n-3$
V15	0	$\frac{6n-5m-m \bmod 3}{3}$	0
V16	$m \bmod 3$	$\frac{6n-5m-4(m \bmod 3)}{3}$	0
V17	0	$\frac{6n-5m+(2m) \bmod 3}{3}$	$(2m) \bmod 3$
V18	$\frac{3n-2m-m \bmod 3}{3}$	0	$\frac{7m-6n-4(m \bmod 3)}{3}$
V19	$\frac{3n-2m-2((2m) \bmod 3)}{3}$	$(2m) \bmod 3$	$\frac{7m-6n+(2m) \bmod 3}{3}$
V20	$\frac{3n-2m-m \bmod 3}{3}$	0	$\frac{7m-6n-m \bmod 3}{3}$
V21	0	$3n-3m+1$	0
V22	0	0	$3m-3n-1$
V23	1	0	$3m-3n+1$

Table 3: Conditions on n and m for the realizability of each Vi of Table 2 and for them to be an extreme point of $\mathcal{P}_{n,m}$ (in addition to condition (9))

Id	Conditions for realizability	Conditions for being an extreme point of $\mathcal{P}_{n,m}$
V1	$n \le m \le \lfloor \frac{6n}{5} \rfloor$	$n \le m \le \lfloor \frac{6n}{5} \rfloor$
V2	$m \le \lfloor \frac{6n-8}{5} \rfloor$	$n-1=m$ or ($m=\lfloor \frac{6n-8}{5} \rfloor$ and $m \bmod 6 \neq 0$)
V3	$n+1 \le m \le \lfloor \frac{6n+1}{5} \rfloor$	$m=n+1$ or ($m=\lfloor \frac{6n+1}{5} \rfloor$ and $m \bmod 6 = 5$)
V4	$\lfloor \frac{6n+4}{5} \rfloor \le m$	$\lfloor \frac{6n+4}{5} \rfloor \le m$
V5	$m \le \frac{6n-3((m-2n) \bmod 4)}{5}$	$m \le \frac{6n-3((m-2n) \bmod 4)}{5}$
V6	$m \le \lfloor \frac{6n+3}{5} \rfloor$	$m \le \lfloor \frac{6n+3}{5} \rfloor$
V7	$m \le \lfloor \frac{6n}{5} \rfloor$	$m \le \lfloor \frac{6n}{5} \rfloor$
V8	$m \le \lfloor \frac{3n-4}{2} \rfloor$	$m = \lfloor \frac{3n-4}{2} \rfloor$
V9	$m \le \lfloor \frac{3n-6}{2} \rfloor$	$m \in \{\frac{3n-10}{2}, \frac{3n-8}{2}, \frac{3n-7}{2}, \frac{3n-6}{2}\}$
V10	no condition	no condition
V11	$n \bmod 2 = 1$	$n \bmod 2 = 1$
V12	$n+1 \le m \le \lfloor \frac{21n+13}{20} \rfloor$	$m=n+1$
V13	$n+1 \le m \le \lfloor \frac{12n+3}{11} \rfloor$	$n+1=m$ or ($m=\lfloor \frac{12n+3}{11} \rfloor$ and $m \bmod 12 \in \{9,10,11\}$)
V14	$n+1 \le m \le \lfloor \frac{9n+3}{8} \rfloor$	$n+1=m$ or ($m=\lfloor \frac{9n+3}{8} \rfloor$ and $m \bmod 9 = 6$)
V15	$m \le \lfloor \frac{6n}{5} \rfloor$	$m \le \lfloor \frac{6n}{5} \rfloor$
V16	$m \le \frac{6n-3((m-2n) \bmod 4)}{5}$	$m \le \frac{6n-3((m-2n) \bmod 4)}{5}$
V17	$m \le \lfloor \frac{6n+2}{5} \rfloor$	$m \le \lfloor \frac{6n+2}{5} \rfloor$
V18	no condition	no condition
V19	no condition	no condition
V20	no condition	no condition
V21	$m \le n$	$m = n-1$
V22	$n+2 \le m$	$n+2 \le m$
V23	$n+2 \le m$	$n+2 \le m$

Given n, m and a point $V=(a,b,c)$ with three non-negative components, it is shown in [33] that a necessary and sufficient condition for V to be realizable for (n,m) is that the following inequalities are valid

$$m_{33} \le \frac{n_3(n_3-1)}{2} \qquad \text{if } n_3 = 1, 2 \text{ or } 3, \tag{14}$$

$$m_{22} \le \frac{n_2(n_2-1)}{2} \quad \text{if } n_2 = 1 \text{ or } 2, \tag{15}$$
$$m_{23} \le n_2 n_3 \quad \text{if } n_2 = 1 \text{ or } 2 \text{ and } n_3 = 1, \tag{16}$$
$$m_{23} \ge \delta(n_2) + \delta(n_3) - 1, \tag{17}$$
$$m_{23} + m_{33} \ge n_3 + \delta(n_2) - 1, \tag{18}$$
$$m_{22} + m_{23} \ge n_2 + \delta(n_3) - 1, \tag{19}$$
$$m_{22} + m_{23} + m_{33} \ge n_2 + n_3 - 1. \tag{20}$$

where $m_{12} = a$, $m_{13} = b$, $m_{33} = c$, $n_1, n_2, n_3, n, m, m_{22}$ and m_{23} are derived from m_{12}, m_{13}, m_{33} from Equations (2)–(8) of Section 2, and where

$$\delta(x) = \begin{cases} 1 & \text{if } x \ge 1, \\ 0 & \text{otherwise.} \end{cases}$$

Condition (20) is equivalent to $m - m_{12} - m_{13} \ge n - m_{12} - m_{13} - 1$, which is equivalent to $m \ge n - 1$. Hence, given a point $Vi = (m_{12}, m_{13}, m_{33})$ in Table 2, and given n and m that satisfy the conditions for Vi in the second column of Table 3, we can prove that Vi is realizable by showing that inequalities (14)–(19) are satisfied. Let us illustrate this with V1.

Lemma 2. Let n and m be integers satisfying $\max\{12, n\} \le m \le \lfloor \frac{6n}{5} \rfloor$. Then, the point V1=*(0,0,0)* is realizable for (n, m).

Proof. It follows from Equations (2)–(8) that $m_{22} = 6n - 5m$, $m_{23} = 6m - 6n$, $n_1 = 0$, $n_2 = 3n - 2m$ and $n_3 = 2m - 2n$. Hence, all m_{ij} and all n_i are non-negative and integers. Observe also that $m \ge 12$ implies $n \ge 10$ which implies $m \le \frac{6n}{5} \le \frac{3n-3}{2}$, and we thus have $n_2 = 3n - 2m \ge 3$.

- Inequality (14) is satisfied since $\frac{n_3(n_3-1)}{2} \ge 0 = m_{33}$.
- There is no need to check inequalities (15) and (16) since $n_2 > 2$.
- $n_3 > 0$ if and only if $m > n$. Hence, inequality (17) is satisfied since $m_{23} = 6(m - n) \ge \delta(n_3) = \delta(n_2) + \delta(n_3) - 1$.
- Inequality (18) is satisfied since $m_{23} + m_{33} = 6(m - n) \ge 2(m - n) = n_3 + \delta(n_2) - 1$.
- Inequality (19) is satisfied since $m_{22} + m_{23} = m \ge n \ge n_2 \ge n_2 + \delta(n_3) - 1$. □

As second illustration, we show that points V8, V9, V10 and V11 are realizable for (n, m) if the conditions of the second column of Table 3 are satisfied. For this purpose, we consider the point V which is defined as follows:

$$\text{V}=\left(a+2b+d, \frac{3n-2m-(4a+6b+3d)+(d-1)(n \bmod 2)}{2}, \frac{4m-3n-(2a+2b+d)+(d-2c-1)(n \bmod 2)}{2}\right)$$

where a, b, c, d are binary variables such that $a + b + c + d = 1$. Note that V is equal to V8 if $a = 1$, to V9 if $b = 1$, to V10 if $c = 1$, and to V11 if $d = 1$.

Lemma 3. Let n and m be two integers satisfying condition (9) and let a, b, c, d be binary variables such that $a + b + c + d = 1$. Assume also that $m \le \lfloor \frac{3n-4}{2} \rfloor$ if $a = 1$, $m \le \lfloor \frac{3n-6}{2} \rfloor$ if $b = 1$, and $n \bmod 2 = 1$ if $d = 1$. Then, the point V is realizable for (n, m).

Proof. It follows from Equations (2)–(8) that

$$\begin{aligned} m_{22} &= (1 - c - d)(n \bmod 2) + a, \\ m_{23} &= a + 2b + 2c(n \bmod 2) + d, \\ n_1 &= \frac{3n - 2m - (2a + 2b + d) + (d - 1)(n \bmod 2)}{2}, \\ n_2 &= 2a + 2b + d - (d - 1)(n \bmod 2), \end{aligned}$$

$$n_3 = \frac{2m - n - (2a + 2b + d) + (d - 1)(n \bmod 2)}{2}.$$

Note that all m_{ij} are non-negative. Indeed,

- m_{12}, m_{22} and m_{23} are clearly non-negative;
- $\max\{12, n-1\} \leq m \leq \frac{3n-3}{2}$ implies $n \geq 9$ and $m_{33} \geq n - 7 \geq 2$;
- $m_{13} \geq 0$ since
  - $m \leq \lfloor \frac{3n-4}{2} \rfloor$ if $a = 1$, which is equivalent to $3n - 2m \geq 4 + n \bmod 2$;
  - $m \leq \lfloor \frac{3n-6}{2} \rfloor$ if $b = 1$, which is equivalent to $3n - 2m \geq 6 + n \bmod 2$;
  - $m \leq \lfloor \frac{3n-3}{2} \rfloor$ if $c + d = 1$, which implies $3n - 2m \geq 3 \geq 3d + (d - 1)n \bmod 2$.

Also, all m_{ij} and all n_i are integers since n mod 2=1 when d=1. Let's now look at inequalities (14)–(19):

- Since $m \geq 12$ and $m \geq n - 1$, we have $n_3 \geq \frac{2m-n-3}{2} \geq \frac{m-4}{2} \geq 4$, meaning that inequalities (14) and (16) do not need to be checked;
- inequality (15) is satisfied. Indeed, if $c + d = 1$ then $m_{22} = 0 \leq \frac{n_2(n_2-1)}{2}$ for $n_2 \in \{1, 2\}$. If $a + b = 1$, then $n_2 \geq 2$, ensuring that $m_{22} \leq 1 \leq \frac{n_2(n_2-1)}{2}$ in that case;
- inequality (19) is satisfied since $m_{22} + m_{23} - n_2 + 1 = 1 + c(n \bmod 2) \geq 1 \geq \delta(n_3)$;
- to show that inequalities (17) and (18) are satisfied, we consider two cases:
  - if $c = 0$, then
    - $m_{23} + 1 = a + 2b + d + 1 \geq 2 \geq \delta(n_2) + \delta(n_3)$;
    - $m_{23} + m_{33} - n_3 + 1 = m - n + a + 2b + d + 1 \geq 1 \geq \delta(n_2)$;
  - if $c = 1$, then $n_2 = \delta(n_2) = n \bmod 2$, which implies
    - $m_{23} + 1 = 2(n \bmod 2) + 1 \geq \delta(n_2) + \delta(n_3)$;
    - $m_{23} + m_{33} - n_3 + 1 = m - n + (n \bmod 2) + 1 \geq \delta(n_2)$. □

The two previous lemmas show that 5 of the 23 points of Table 2 are realizable. A similar proof can easily be obtained for the 18 other points. A simple way to get a proof that a Vi is realizable for (n, m) is to prove that it is impossible to satisfy the conditions of the second column of Table 3 for this Vi while violating at least one of the inequalities (14)–(19). This can be done using a Satisfiability Modulo Theories (SMT) solver like Z3 [18].

Note that another way of proving that a point (m_{12}, m_{13}, m_{33}) is realizable for (n, m) is to exhibit a chemical graph of order n, size m, and with m_{12} 12-edges, m_{13} 13-edges and m_{33} 33-edges. For example, we could have proved Lemma 2 by observing that the following graph shows that $(0, 0, 0)$ is realizable for (n, m) when $\max\{12, n\} \leq m \leq \lfloor \frac{6n}{5} \rfloor$: consider a cycle with vertices $v_1, \ldots, v_{2n-m}$ and edges $v_i v_{i+1}$ $(1 \leq i < 2n - m)$ and $v_1 v_{2n-m}$; for $j = 1, \ldots, m - n$, add a vertex w_j linked to v_{2j-1} and to $v_{2n-m-2j+1}$. For illustration, such a graph is shown in Figure 4 for $(n, m) = (20, 23)$.

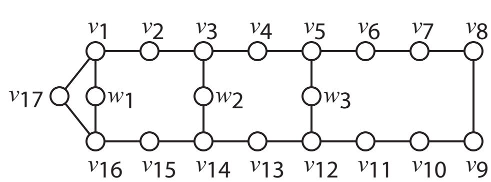


Figure 4: A chemical graph which shows that $(0, 0, 0)$ is realizable for $(n, m) = (20, 23)$

We want to mention here that we provide a webpage ChemicHull [8] which, given n, m and one of the 23 points V$i = (a, b, c)$, exhibits a chemical graph of order n, size m, with a 12-edges, b 13-edges, and with c 33-edges.

6 The inequalities of Table 1 are facet defining and induce bounded polyhedrons

We first prove that each Fi of Table 1 is facet defining. For this purpose, it is sufficient to give three affinely independent realizable points on the hyperplane defined by Fi. To prove that three points p_1, p_2, p_3 in $\mathbb{R}^3$ are affinely independent, it is sufficient to prove that $p_2 - p_1$ is not a multiple of $p_3 - p_1$. As we will see, the 23 points of the previous section are sufficient for this purpose.

We give in Table 4 three points of Table 2 for every possible case of each Fi. For example, F7 is defined when $m \le \frac{6n-5}{5}$ and $(m \bmod 3) = 2$. This is equivalent to say that either $m = \frac{6n-5}{5}$ or $m \le \frac{6n-8}{5}$ and $(m \bmod 3) = 2$. We show here how to prove that there are three affinely independent realizable points in each case for F7.

- if $m = \frac{6n-5}{5}$, then according to Table 3, V7=(1,0,0), V15=(0,1,0) and V17=(0,2,1) are realizable. Moreover, they belong to the hyperplane defined by F7 since $5m-6n+2 = -3m_{12}-3m_{13}+3m_{33} = -3$ for these three points. They are affinely independent since V15-V7=(-1,1,0) is not a multiple of V17-V7=(-1,2,1);
- if $m \le \frac{6n-8}{5}$ and $(m \bmod 3) = 2$, then according to Table 3, V15=$(0, \frac{6n-5m-2}{3}, 0)$, V16=$(2, \frac{6n-5m-8}{3}, 0)$ and V17=$(0, \frac{6n-5m+1}{3}, 1)$ are realizable. Moreover, they belong to the hyperplane defined by F7 since $-3m_{12}-3m_{13}+3m_{33} = 5m-6n+2$ for these three points. They are affinely independent since V16-V15=(2,-2,0) is not a multiple of V17-V15=(0,1,1).

It is an easy exercise to show that all triplets of points given in Table 4 are realizable, belong to the indicated hyperplane and are affinely independent.

In what follows, given n and m, we say that a facet Fi is *active* for (n,m) if the conditions associated with Fi in Table 1 are satisfied. Let $\mathcal{P}'_{n,m}$ be the polyhedron defined by the active facets Fi for (n,m). We now prove that $\mathcal{P}'_{n,m}$ is bounded for all pairs (n,m) satisfying condition (9).

Theorem 4. $\mathcal{P}'_{n,m}$ is bounded for all (n,m) with $\max\{12, n-1\} \le m \le \lfloor \frac{3n-3}{2} \rfloor$.

Proof. Note first that F1, F2 and F6 are active for all pairs (n,m) satisfying condition (9). Hence, $m_{12} \ge 0$, $m_{13} \ge 0$, and $m_{33} \ge 5m-6n$. It remains to prove that m_{12}, m_{13} and m_{33} are upper bounded. Consider F12, F13, F16 and F20. At least one of these four facets is active for (n,m). Indeed:

- if $n-1 = m$ then F20 is active;
- if $n \le m \le \frac{3n-6}{2}$, then F12 is active;
- if $m \ge \frac{3n-5}{2}$ and n is odd then F13 is active;
- if $m \ge \frac{3n-5}{2}$ and n is even then F16 is active.

We can rewrite each of the above four inequalities as follows:

$$p_{12}(n,m)m_{12} + p_{13}(n,m)m_{13} - p_{33}(n,m)m_{33} \ge b(n,m) \tag{21}$$

where $p_{12}(n,m)$, $p_{13}(n,m)$, $p_{33}(n,m)$ and $b(n,m)$ are polynomials in n and m. We now prove that if the pair (n,m) satisfies condition (9), then $-4p_{33}(n,m) + p_{12}(n,m) < 0$ and $-3p_{33}(n,m) + p_{13}(n,m) < 0$:

- for F12, we have $p_{12}(n,m) = p_{13}(n,m) = p_{33}(n,m) = 1$, which gives $-4p_{33}(n,m) + p_{12}(n,m) = -3$ and $-3p_{33}(n,m) + p_{13}(n,m) = -2$;
- for F13 we have $p_{12}(n,m) = 2$, $p_{13}(n,m) = p_{33}(n,m) = 1$, which gives $-4p_{33}(n,m)+p_{12}(n,m) = -3p_{33}(n,m) + p_{13}(n,m) = -2$;
- for F16, it follows from (10) that $p_{12}(n,m) = 2(3n-2m)$, $p_{13}(n,m) = 3n-2m+2$ and $p_{33}(n,m) = 3n-2m$, which gives $-4p_{33}(n,m)+p_{12}(n,m) = 2(2m-3n) \le -6$ and $-3p_{33}(n,m)+p_{13}(n,m) = 2(2m-3n+1) \le -4$;

- for F20 we have $p_{12}(n,m) = n-7$, $p_{13}(n,m) = n-6$ and $p_{33}(n,m) = n-4$, which gives $-4p_{33}(n,m)+p_{12}(n,m) = -3(n-3) < 0$ and $-3p_{33}(n,m)+p_{13}(n,m) = -2(n-3) < 0$.

Table 4: Three affinely independent points for every inequality Fi

Id	Three points			Conditions on n and m
F1	V4	V10	V22	$\frac{6n+1}{5} \le m$
	V1	V10	V17	$n \le m \le \frac{6n}{5}$
	V10	V15	V21	$n-1=m$
F2	V4	V18	V22	$\frac{6n+1}{5} \le m$
	V1	V18	V22	$\frac{6n-3}{5} \le m \le \frac{6n}{5}$
	V1	V7	V18	$n \le m \le \frac{6n-4}{5}$
	V2	V7	V20	$n-1=m$
F3	V1	V7	V15	$n \le m \le \frac{6n-4}{5}$
	V2	V7	V16	$n-1=m$
F4	V18	V19	V20	$(m \bmod 3) = 2$
F5	V18	V19	V20	$(m \bmod 3) = 1$
F6	V4	V10	V18	$\frac{6n+3}{5} \le m$
	V10	V17	V18	$m \le \frac{6n+2}{5}$
F7	V7	V15	V17	$m = \frac{6n-5}{5}$,
	V15	V16	V17	$(m \le \frac{6n-8}{5}) \wedge ((m \bmod 3) = 2)$
F8	V6	V15	V17	$m = \frac{6n-2}{5}$
	V5	V6	V7	$(m \le \frac{6n-6}{5}) \wedge ((m-2n) \bmod 4 = 2)$
F9	V5	V6	V7	$(m \le \frac{6n-3}{5}) \wedge ((m-2n) \bmod 4 = 1)$
F10	V6	V7	V17	$m \in \{\frac{6n-5}{5}, \frac{6n-1}{5}\}$
	V5	V6	V7	$(m \le \frac{6n-9}{5}) \wedge ((m-2n) \bmod 4 = 3)$
F11	V15	V16	V17	$(m \le \frac{6n-4}{5}) \wedge ((m \bmod 3) = 1)$
F12	V19	V20	V23	$(n+2 \le m \le \frac{3n-6}{2}) \wedge ((m \bmod 3) \neq 0)$
	V10	V18	V23	$(n+2 \le m \le \frac{3n-6}{2}) \wedge ((m \bmod 3) = 0) \wedge ((n \bmod 2) = 0)$
	V11	V18	V23	$(n+2 \le m \le \frac{3n-7}{2}) \wedge ((m \bmod 3) = 0) \wedge ((n \bmod 2) = 1)$
	V10	V12	V19	$(n+1=m) \wedge ((n \bmod 2) = 0)$
	V11	V12	V19	$(n+1=m) \wedge ((n \bmod 2) = 1)$
	V1	V19	V20	$(n=m) \wedge ((n \bmod 3) \neq 0)$
	V1	V10	V18	$(n=m) \wedge ((n \bmod 6) = 0)$
	V1	V11	V18	$(n=m) \wedge ((n \bmod 6) = 3)$
F13	V10	V11	V22	$(n+2 \le m \le \frac{3n-3}{2}) \wedge ((n \bmod 2) = 1)$
	V10	V11	V14	$(n+1=m) \wedge ((n \bmod 2) = 1)$
	V2	V10	V11	$(n-1=m) \wedge ((n \bmod 2) = 1)$
F14	V1	V10	V11	$(n=m) \wedge ((n \bmod 2) = 1)$
F15	V10	V12	V14	$(n+1=m) \wedge ((n \bmod 2) = 0)$
F16	V10	V22	V23	$(n+2 \le m) \wedge ((n \bmod 2) = 0)$
F17	V2	V10	V21	$(n-1=m) \wedge ((n \bmod 2) = 0)$
F18	V2	V19	V20	$(n-1=m) \wedge ((n \bmod 3) = 0)$
F19	V2	V19	V20	$(n-1=m) \wedge ((n \bmod 3) = 2)$
F20	V2	V11	V19	$(n-1=m) \wedge ((n \bmod 2) = 1)$
	V2	V10	V19	$(n-1=m) \wedge ((n \bmod 2) = 0)$
F21	V12	V13	V14	$n+1=m$

Hence, by adding $p_{33}(n,m)$ times inequality F6 to (21) we get

$$\big(-4p_{33}(n,m)+p_{12}(n,m)\big)m_{12} + \big(-3p_{33}(n,m)+p_{13}(n,m)\big)m_{13} \ge p_{33}(n,m)(5m-6n)+b(n,m),$$

which implies that m_{12} and m_{13} are upper bounded by a polynomial that depends on n and m (since F1 and F2 forbid negative values for these two variables). But (21) is equivalent to

$$p_{33}(n,m)m_{33} \leq p_{12}(n,m)m_{12} + p_{13}(n,m)m_{13} - b(n,m),$$

which implies that m_{33} is also upper bounded by a polyomial that depends on n and m. □

7 Extreme points of $\mathcal{P}_{n,m}$

As proved in Sections 4 and 6, the 21 inequalities of Table 1 are valid and facet defining. They are defined with constraints on n and m. Hence, depending on n and m, not all of facets are active for (n,m). The set of integer pairs (n,m) that satisfy condition (9) can be partitioned into 75 subsets, each one having a different set of active facets for (n,m). Hence, there are 75 polytope types, each one having its subset of active facets. These polytope types are listed in Table 5. We indicate in the first column the Id of each polytope type, we then give the set of active facets, and we finally indicate the constraints on n and m.

Table 5: Polytopes with their facets and their conditions on n and m (in addition to condition (9))

$m = n - 1$

Id	facets	n mod 12
P1	F1, F2, F3, F4, F6, F7, F10, F17, F18, F20	0
P2	F1, F2, F3, F6, F8, F13, F20	1
P3	F1, F2, F3, F5, F6, F9, F11, F17, F19, F20	2
P4	F1, F2, F3, F4, F6, F7, F13, F18, F20	3
P5	F1, F2, F3, F6, F10, F17, F20	4
P6	F1, F2, F3, F5, F6, F8, F11, F13, F19, F20	5
P7	F1, F2, F3, F4, F6, F7, F9, F17, F18, F20	6
P8	F1, F2, F3, F6, F13, F20	7
P9	F1, F2, F3, F5, F6, F10, F11, F17, F19, F20	8
P10	F1, F2, F3, F4, F6, F7, F8, F13, F18, F20	9
P11	F1, F2, F3, F6, F9, F17, F20	10
P12	F1, F2, F3, F5, F6, F11, F13, F19, F20	11

$m = n$

Id	facets	n mod 12
P13	F1, F2, F3, F6, F12	0
P14	F1, F2, F3, F5, F6, F10, F11, F12, F14	1
P15	F1, F2, F3, F4, F6, F7, F8, F12	2
P16	F1, F2, F3, F6, F9, F12, F14	3
P17	F1, F2, F3, F5, F6, F11, F12	4
P18	F1, F2, F3, F4, F6, F7, F10, F12, F14	5
P19	F1, F2, F3, F6, F8, F12	6
P20	F1, F2, F3, F5, F6, F9, F11, F12, F14	7
P21	F1, F2, F3, F4, F6, F7, F12	8
P22	F1, F2, F3, F6, F10, F12, F14	9
P23	F1, F2, F3, F5, F6, F8, F11, F12	10
P24	F1, F2, F3, F4, F6, F7, F9, F12, F14	11

$m = n + 1$

Id	facets	n mod 12
P25	F1, F2, F3, F5, F6, F9, F11, F12, F15, F21	0
P26	F1, F2, F3, F4, F6, F7, F12, F13, F21	1
P27	F1, F2, F3, F6, F10, F12, F15, F21	2
P28	F1, F2, F3, F5, F6, F8, F11, F12, F13, F21	3
P29	F1, F2, F3, F4, F6, F7, F9, F12, F15, F21	4
P30	F1, F2, F3, F6, F12, F13, F21	5
P31	F1, F2, F3, F5, F6, F10, F11, F12, F15, F21	6
P32	F1, F2, F3, F4, F6, F7, F8, F12, F13, F21	7
P33	F1, F2, F3, F6, F9, F12, F15, F21	8
P34	F1, F2, F3, F5, F6, F11, F12, F13, F21	9

(Table 5 continued)

P35	F1, F2, F3, F4, F6, F7, F10, F12, F15, F21	10
P36	F1, F2, F3, F6, F8, F12, F13, F21	11

$n+1 < m < \frac{6n-3}{5}$

Id	facets	n mod 2	m mod 3	$(m-2n)$mod4
P37	F1, F2, F3, F6, F12, F16	0	0	0
P38	F1, F2, F3, F6, F9, F12, F16	0	0	1
P39	F1, F2, F3, F6, F8, F12, F16	0	0	2
P40	F1, F2, F3, F6, F10, F12, F16	0	0	3
P41	F1, F2, F3, F5, F6, F11, F12, F16	0	1	0
P42	F1, F2, F3, F5, F6, F9, F11, F12, F16	0	1	1
P43	F1, F2, F3, F5, F6, F8, F11, F12, F16	0	1	2
P44	F1, F2, F3, F5, F6, F10, F11, F12, F16	0	1	3
P45	F1, F2, F3, F4, F6, F7, F12, F16	0	2	0
P46	F1, F2, F3, F4, F6, F7, F9, F12, F16	0	2	1
P47	F1, F2, F3, F4, F6, F7, F8, F12, F16	0	2	2
P48	F1, F2, F3, F4, F6, F7, F10, F12, F16	0	2	3
P49	F1, F2, F3, F6, F12, F13	1	0	0
P50	F1, F2, F3, F6, F9, F12, F13	1	0	1
P51	F1, F2, F3, F6, F8, F12, F13	1	0	2
P52	F1, F2, F3, F6, F10, F12, F13	1	0	3
P53	F1, F2, F3, F5, F6, F11, F12, F13	1	1	0
P54	F1, F2, F3, F5, F6, F9, F11, F12, F13	1	1	1
P55	F1, F2, F3, F5, F6, F8, F11, F12, F13	1	1	2
P56	F1, F2, F3, F5, F6, F10, F11, F12, F13	1	1	3
P57	F1, F2, F3, F4, F6, F7, F12, F13	1	2	0
P58	F1, F2, F3, F4, F6, F7, F9, F12, F13	1	2	1
P59	F1, F2, F3, F4, F6, F7, F8, F12, F13	1	2	2
P60	F1, F2, F3, F4, F6, F7, F10, F12, F13	1	2	3

$\frac{6n-3}{5} \leq m < \frac{6n}{5}$

Id	facets	n mod 2	m mod 3
P61	F1, F2, F6, F9, F12, F16	0	0
P62	F1, F2, F5, F6, F10, F12, F16	0	1
P63	F1, F2, F4, F6, F8, F12, F16	0	2
P64	F1, F2, F6, F9, F12, F13	1	0
P65	F1, F2, F5, F6, F10, F12, F13	1	1
P66	F1, F2, F4, F6, F8, F12, F13	1	2

$\frac{6n}{5} \leq m < \lfloor \frac{3n}{2} \rfloor - 2$

Id	facets	n mod 2	m mod 3
P67	F1, F2, F6, F12, F16	0	0
P68	F1, F2, F5, F6, F12, F16	0	1
P69	F1, F2, F4, F6, F12, F16	0	2
P70	F1, F2, F6, F12, F13	1	0
P71	F1, F2, F5, F6, F12, F13	1	1
P72	F1, F2, F4, F6, F12, F13	1	2

$\lfloor \frac{3n}{2} \rfloor - 2 \leq m$

Id	facets	m mod 3
P73	F1, F2, F6, F13	0
P74	F1, F2, F5, F6, F16	1
P75	F1, F2, F4, F6, F13	2

Note that we do not indicate redundant constraints on n and m. For example, if $\frac{6n-3}{5} \leq m < \frac{6n}{5}$ and $m \bmod 3 = 0$, then $m = \frac{6n-3}{5}$ and, whatever the parity of n, we necessarily have $1 = (-3) \bmod 4 = (5m - 6n) \bmod 4 = (m - 2n) \bmod 4$. This explains the existence of facet F9 for polytope types P61 and P64, even if it is not explicitly mentioned that $(m - 2n) \bmod 4 = 1$.

As a reminder, given two integers n and m that satisfy condition (9), $\mathcal{P}'_{n,m}$ is the polytope defined by all active facets for (n,m). We now prove that the set of extreme points of $\mathcal{P}'_{n,m}$ is a subset of the 23 points described in Section 5. We therefore have $\mathcal{P}'_{n,m} = \mathcal{P}_{n,m}$.

It is proved in Section 6 that $\mathcal{P}'_{n,m}$ is bounded for all n and m that satisfy condition (9). So, let I be the set of indices i such that Fi is active for (n,m). It is sufficient to prove that given any subset of three distinct indices i_1, i_2, i_3 in I, the point at the intersection of the hyperplanes defined by Fi_1, Fi_2 and Fi_3 (if it exists) is either outside $\mathcal{P}'_{n,m}$, or it is one of the 23 points of Table 2 which is realizable for (n,m) according to Table 3. Let's illustrate this process with an example.

Lemma 5. *If $n \bmod 2 = 1, m \bmod 3 = 0$ and $\frac{6n}{5} \leq m \leq \frac{3n-5}{2}$, then the extreme points of $\mathcal{P}'_{n,m}$ are V4, V10, V11, V18=V19=V20, V22 and V23.*

Proof. Note first that Table 3 shows that V4, V10, V11, V18 = V19 = V20, V22 and V23 are realizable for (n,m). As shown in Table 5, the conditions on n and m are associated with P70 which has F1, F2, F6, F12 and F13 as active facets. Hence, $I = \{1,2,6,12,13\}$. Let's consider all triplets (i_1,i_2,i_3) of indices in I.

- $(i_1,i_2,i_3) = (1,2,6)$. The intersection point of the hyperplanes defined by F1, F2, F6, is V4 $= (0,0,5m-6n)$. Inequalities F12 and F13 are satisfied since $m_{12}+m_{13}-m_{33} = 2m_{12}+m_{13}-m_{33} = 6n-5m > 3n-3m+1$. Hence, V4 is an extreme point.
- $(i_1,i_2,i_3) = (1,2,12)$. The intersection point of the hyperplanes defined by F1, F2, F12 is $(0,0,3m-3n)$. Inequality F13 is violated since $2m_{12}+m_{13}-m_{33} = 3n-3m < 3n-3m+1$. Hence, this point is outside the polytope.
- $(i_1,i_2,i_3) = (1,2,13)$. The intersection point of the hyperplanes defined by F1, F2, F13 is V22 $= (0,0,3m-3n-1)$. Inequalities F6 and F12 are satisfied since $-4m_{12}-3m_{13}+m_{33} = 3m-3n-1 > 5m-6n$ and $m_{12}+m_{13}-m_{33} = 3n-3m+1 > 3n-3m$. Hence, V22 is an extreme point.
- $(i_1,i_2,i_3) = (1,6,12)$.The intersection point of the hyperplanes defined by F1, F6, F12 is $(0, \frac{3n-2m}{2}, \frac{4m-3n}{2})$. Inequality F13 is violated since $2m_{12}+m_{13}-m_{33} = 3n-3m < 3n-3m+1$. Hence, this point is outside the polytope.
- $(i_1,i_2,i_3) = (1,6,13)$. The intersection point of the hyperplanes defined by F1, F6, F13 is V10 $= (0, \frac{3n-2m-1}{2}, \frac{4m-3n-3}{2})$. Inequalities F2 and F12 are satisfied since $3n-2m-1 > 0$ and $m_{12}+m_{13}-m_{33} = 3n-3m+1 > 3n-3m$. Hence, V10 is an extreme point.
- $(i_1,i_2,i_3) = (1,12,13)$. There is no intersection point for the hyperplanes defined by F1, F12, F13 since F1 implies $m_{12} = 0$, while F13-F12 implies $m_{12} = 1$.
- $(i_1,i_2,i_3) = (2,6,12)$. The intersection point of the hyperplanes defined by F2, F6, F12 is V18 = V19 = V20 $= (\frac{3n-2m}{3}, 0, \frac{7m-6n}{3})$. Inequalities F1 and F13 are satisfied since $3n-2m > 0$ and $2m_{12}+m_{13}-m_{33} = 3n-3m+\frac{3n-2m}{3} > 3n-3m+1$. Hence, V18=V19=V20 is an extreme point.
- $(i_1,i_2,i_3) = (2,6,13)$. The intersection point of the hyperplanes defined by F2, F6, F13 is $(\frac{3n-2m-1}{2}, 0, m-2)$. Inequality F12 is violated since $m_{12}+m_{13}-m_{33} = 3n-3m+\frac{2m-3n+3}{2} \leq 3n-3m-1$. Hence, this point is outside the polytope.
- $(i_1,i_2,i_3) = (2,12,13)$. The intersection point of inequalities F2, F12, F13 is V23 $= (1,0,3m-3n+1)$. Inequalities F1 and F6 are satisfied since $1 > 0$ and $-4m_{12}-3m_{13}+m_{33} = 3m-3n-3 > 5m-6n$. Hence, V23 is an extreme point.
- $(i_1,i_2,i_3) = (6,12,13)$. The intersection point of the hyperplanes defined by F6, F12, F13 is V11 $= (1, \frac{3n-2m-3}{2}, \frac{4m-3n-1}{2})$. Inequalities F1 and F2 are satisfied since $1 > 0$ and $3n-2m-3 > 0$. Hence, V11 is an extreme point. □

Table 6: Extreme points for the 75 polytopes of Table 5 when (n, m) satisfies condition (9)

Polytopes	Extreme points	
P1	V2, V5, V6, V7, V10, V15, V16, V17, V18, V19, V20, V21	
P2	V2, V5, V6, V7, V10, V11, V15=V16=V17, V18=V19=V20, V21	
P3	V2, V5, V6, V7, V10, V15, V16, V17, V18, V19, V20, V21	
P4	V2, V5=V6=V7, V10, V11, V15, V16, V17, V18, V19, V20, V21	
P5	V2, V5, V6, V7, V10, V15=V16=V17, V18=V19=V20, V21	
P6	V2, V5, V6, V7, V10, V11, V15, V16, V17, V18, V19, V20, V21	
P7	V2, V5, V6, V7, V10, V15, V16, V17, V18, V19, V20, V21	
P8	V2, V5=V6=V7, V10, V11, V15=V16=V17, V18=V19=V20, V21	
P9	V2, V5, V6, V7, V10, V15, V16, V17, V18, V19, V20, V21	
P10	V2, V5, V6, V7, V10, V11, V15, V16, V17, V18, V19, V20, V21	
P11	V2, V5, V6, V7, V10, V15=V16=V17, V18=V19=V20, V21	
P12	V2, V5=V6=V7, V10, V11, V15, V16, V17, V18, V19, V20, V21	
P13	V1, V5=V6=V7, V10, V15=V16=V17, V18=V19=V20	
P14	V1, V5, V6, V7, V10, V11, V15, V16, V17, V18, V19, V20	
P15	V1, V5, V6, V7, V10, V15, V16, V17, V18, V19, V20	
P16	V1, V5, V6, V7, V10, V11, V15=V16=V17, V18=V19=V20	
P17	V1, V5=V6=V7, V10, V15, V16, V17, V18, V19, V20	
P18	V1, V5, V6, V7, V10, V11, V15, V16, V17, V18, V19, V20	
P19	V1, V5, V6, V7, V10, V15=V16=V17, V18=V19=V20	
P20	V1, V5, V6, V7, V10, V11, V15, V16, V17, V18, V19, V20	
P21	V1, V5=V6=V7, V10, V15, V16, V17, V18, V19, V20	
P22	V1, V5, V6, V7, V10, V11, V15=V16=V17, V18=V19=V20	
P23	V1, V5, V6, V7, V10, V15, V16, V17, V18, V19, V20	
P24	V1, V5, V6, V7, V10, V11, V15, V16, V17, V18, V19, V20	
P25	V1, V3, V5, V6, V7, V10, V12, V13, V14, V15, V16, V17, V18, V19, V20	
P26	V1, V3, V5=V6=V7, V10, V11, V12, V13, V14, V15, V16, V17, V18, V19, V20	
P27	V1, V3, V5, V6, V7, V10, V12, V13, V14, V15=V16=V17, V18=V19=V20	
P28	V1, V3, V5, V6, V7, V10, V11, V12, V13, V14, V15, V16, V17, V18, V19, V20	
P29	V1, V3, V5, V6, V7, V10, V12, V13, V14, V15, V16, V17, V18, V19, V20	
P30	V1, V3, V5=V6=V7, V10, V11, V12, V13, V14, V15=V16=V17, V18=V19=V20	
P31	V1, V3, V5, V6, V7, V10, V12, V13, V14, V15, V16, V17, V18, V19, V20	
P32	V1, V3, V5, V6, V7, V10, V11, V12, V13, V14, V15, V16, V17, V18, V19, V20	
P33	V1, V3, V5, V6, V7, V10, V12, V13, V14, V15=V16=V17, V18=V19=V20	
P34	V1, V3, V5=V6=V7, V10, V11, V12, V13, V14, V15, V16, V17, V18, V19, V20	
P35	V1, V3, V5, V6, V7, V10, V12, V13, V14, V15, V16, V17, V18, V19, V20	
P36	V1, V3, V5, V6, V7, V10, V11, V12, V13, V14, V15=V16=V17, V18=V19=V20	
P37	V1, V5=V6=V7, V10, V15=V16=V17, V18=V19=V20, V22, V23	
P38	V1, V5, V6, V7, V10, V15=V16=V17, V18=V19=V20, V22, V23	
P39	V1, V5, V6, V7, V10, V15=V16=V17, V18=V19=V20, V22, V23	
P40	V1, V5, V6, V7, V10, V15=V16=V17, V18=V19=V20, V22, V23	
P41	V1, V5=V6=V7, V10, V15, V16, V17, V18, V19, V20, V22, V23	
P42	V1, V5, V6, V7, V10, V15, V16, V17, V18, V19, V20, V22, V23	
P43	V1, V5, V6, V7, V10, V15, V16, V17, V18, V19, V20, V22, V23	
P44	V1, V5, V6, V7, V10, V15, V16, V17, V18, V19, V20, V22, V23	
P45	V1, V5=V6=V7, V10, V15, V16, V17, V18, V19, V20, V22, V23	
P46	V1, V5, V6, V7, V10, V15, V16, V17, V18, V19, V20, V22, V23	
P47	V1, V5, V6, V7, V10, V15, V16, V17, V18, V19, V20, V22, V23	
P48	{ V1, V6, V7, V10, V15, V17, V18, V19, V20, V22, V23	if $n \bmod 5 = 0$ and $m = \frac{6n-5}{5}$
	V1, V5, V6, V7, V10, V15, V16, V17, V18, V19, V20, V22, V23	otherwise
P49	V1, V5=V6=V7, V10, V11, V15=V16=V17, V18=V19=V20, V22, V23	
P50	V1, V5, V6, V7, V10, V11, V15=V16=V17, V18=V19=V20, V22, V23	
P51	V1, V5, V6, V7, V10, V11, V15=V16=V17, V18=V19=V20, V22, V23	
P52	V1, V5, V6, V7, V10, V11, V15=V16=V17, V18=V19=V20, V22, V23	
P53	V1, V5=V6=V7, V10, V11, V15, V16, V17, V18, V19, V20, V22, V23	
P54	V1, V5, V6, V7, V10, V11, V15, V16, V17, V18, V19, V20, V22, V23	
P55	V1, V5, V6, V7, V10, V11, V15, V16, V17, V18, V19, V20, V22, V23	
P56	V1, V5, V6, V7, V10, V11, V15, V16, V17, V18, V19, V20, V22, V23	
P57	V1, V5=V6=V7, V10, V11, V15, V16, V17, V18, V19, V20, V22, V23	
P58	V1, V5, V6, V7, V10, V11, V15, V16, V17, V18, V19, V20, V22, V23	
P59	V1, V5, V6, V7, V10, V11, V15, V16, V17, V18, V19, V20, V22, V23	
P60	{ V1, V6, V7, V10, V11, V15, V17, V18, V19, V20, V22, V23	if $n \bmod 5 = 0$ and $m = \frac{6n-5}{5}$
	V1, V5, V6, V7, V10, V11, V15, V16, V17, V18, V19, V20, V22, V23	otherwise
P61	V1=V7, V5=V15=V16=V17, V6, V10, V18=V19=V20, V22, V23	
P62	V1=V7=V15, V6, V10, V17, V18, V19, V20, V22, V23	
P63	V1=V7=V15, V6, V10, V17, V18, V19, V20, V22, V23	
P64	V1=V7, V5=V15=V16=V17, V6, V10, V11, V18=V19=V20, V22, V23	
P65	V1=V7=V15, V6, V10, V11, V17, V18, V19, V20, V22, V23	
P66	V1=V7=V15, V6, V10, V11, V17, V18, V19, V20, V22, V23	
P67	V4, V10, V18=V19=V20, V22, V23	
P68	V4, V10, V18, V19, V20, V22, V23	
P69	V4, V10, V18, V19, V20, V22, V23	
P70	V4, V10, V11, V18=V19=V20, V22, V23	
P71	V4, V10, V11, V18, V19, V20, V22, V23	
P72	V4, V10, V11, V18, V19, V20, V22, V23	
P73	V4, V10, V11=V18=V19=V20=V23, V22	
P74	V4, V8=V20=V23, V10=V19, V18, V22	
P75	V4, V8=V20=V23, V10, V11=V19, V18, V22	

The same analysis can be done for the 74 other polytope types. We give in Table 6 the set of extreme points for the 75 distinct polytopes.[1] For two extreme points Vi and Vj of a polytope, we write Vi=Vj only if the two points are always equal in the considered polytope. When Vi and Vj are not indicated as being equal, they may coincide for some pairs (n, m), but there is at least one pair (n, m) for which they are not equal. For example, for P2, we have V18=V19, meaning that these two points are always equal when n mod $12 = 1$. Still for P2, V6 and V18 are typically distinct, while V6=V18(=V19=V20)=(5,0,2) for $n = 13$.

Let's now analyze the pairs (n, m) that satisfy condition (1), but not condition (9). The cases where $n \geq 6$ and $m = \frac{3n-2}{2}$ or when $n \geq 4$ and $m = \lfloor \frac{3n}{2} \rfloor$ are treated in Section 3. The other cases which all have $m \leq 11$ can easily be analyzed by generating all chemical graphs of order n and size m, using for example *Nauty's geng* [46], and then building the polytope $\mathcal{P}_{n,m}$ for determining its extreme points. It is therefore not difficult to determine the extreme points for all these pairs (n, m). We list in Table 7 the extreme points for these 32 particular cases. The third column of the table indicates the dimension of $\mathcal{P}_{n,m}$. We observe that among these 32 polytopes, 5 are of dimension 0, 3 of dimension 1, 2 of dimension 2 and 22 of dimension 3. Among the 22 full-dimensional polytopes, 11 are special cases of the polytopes of Table 5. We indicate their Id in the last column of Table 7. The 11 new full-dimensional polytopes are named P76–P86, and their Id appears in italics in the last column of Table 7.

Table 7: Extreme points of $\mathcal{P}_{n,m}$ for pairs (n, m) satisfying (1) but not (9)

n	m	dim.	extreme points	Id
3	2	0	(2,0,0)	
3	3	0	(0,0,0)	
4	3	1	(0,3,0), (2,0,0)	
4	4	1	(0,0,0), (0,1,0)	
4	5	0	(0,0,1)	
5	4	1	(1,2,0), (2,0,0)	
5	5	3	(0,0,0), (0,1,0), (0,2,1), (1,0,0)	*P76*
5	6	2	(0,0,0), (0,0,1), (0,1,3)	
6	5	3	(0,4,1), (1,2,0), (2,0,0), (2,1,0)	*P77*
6	6	3	(0,0,0), (0,2,0), (0,3,3), (1,0,0), (1,1,1)	*P78*
6	7	3	(0,0,0), (0,0,1), (0,1,2), (0,2,5), (1,0,3)	*P79*
7	6	3	(0,4,0), (1,3,1), (2,0,0), (3,0,0)	*P80*
7	7	3	(0,0,0), (0,2,0), (0,3,2), (1,0,0), (1,1,0), (1,2,3), (2,0,1)	*P81*
7	8	3	(0,0,0), (0,0,1), (0,1,1), (0,1,3), (0,2,4), (1,0,2), (1,0,3), (1,1,5)	*P82*
7	9	3	(0,0,3), (0,0,5), (0,1,6), (1,0,7)	P73
8	7	3	(0,4,0), (0,5,2), (1,3,0), (2,0,0), (2,2,1), (3,0,0)	*P83*
8	8	3	(0,0,0), (0,2,0), (0,3,1), (0,4,4), (2,0,0), (2,0,1), (2,1,3)	*P84*
8	9	3	(0,0,0), (0,0,1), (0,1,0), (0,1,3), (0,3,6), (1,0,1), (1,1,5), (2,0,5)	*P85*
8	10	3	(0,0,2), (0,0,5), (0,2,8), (1,0,6), (1,0,7)	P74
9	8	3	(0,4,0), (0,5,1), (1,4,2), (2,0,0), (2,2,0), (3,0,0), (3,1,1)	*P86*
9	9	3	(0,0,0), (0,3,0), (0,4,3), (1,3,4), (2,0,0), (3,0,3)	P22
9	10	3	(0,0,0), (0,0,1), (0,1,0), (0,1,3), (0,2,2), (0,3,5), (1,0,0), (1,1,5), (1,2,6), (2,0,4), (2,0,5)	P34
9	11	3	(0,0,1), (0,0,5), (0,2,7), (1,0,5), (1,0,7), (1,1,8)	P75
10	9	3	(0,4,0), (0,5,0), (0,6,3), (2,0,0), (3,0,0), (3,1,0), (4,0,1)	P11
10	10	3	(0,0,0), (0,3,0), (0,4,2), (0,5,5), (1,2,0), (2,0,0), (2,2,4), (3,0,2), (3,0,3)	P23
10	11	3	(0,0,0), (0,0,1), (0,1,0), (0,1,3), (0,2,1), (0,4,7), (1,0,0), (1,1,5), (2,0,3), (2,0,5), (2,1,6)	P35
11	10	3	(0,4,0), (0,5,0), (0,6,2), (1,4,0), (1,5,3), (2,0,0), (3,2,2), (4,0,0), (4,0,1)	P12
11	11	3	(0,0,0), (0,3,0), (0,4,1), (0,5,4), (1,4,5), (2,0,0), (2,1,0), (3,0,1), (3,0,3), (3,1,4)	P24
12	11	3	(0,4,0), (0,5,0), (0,6,1), (0,7,4), (2,0,0), (2,3,0), (4,0,0), (4,0,1), (4,1,2)	P1
even ≥ 4	$\frac{3n}{2}$	0	(0,0,m)	
odd ≥ 5	$\frac{3n-1}{2}$	0	(0,0,$m-2$)	
even ≥ 6	$\frac{3n-2}{2}$	2	(0,0,$m-4$), (0,0,$m-3$), (0,1,$m-1$)	

In summary, our polyhedral description is based on a partition of the set of all possible combinations of n and m into 96 cases: 5 polytopes are of dimension 0, 3 of dimension 1, 2 of dimension 2 and 86

[1]These were obtained with the help of a dedicated procedure available at `https://github.com/umons-dept-comp-sci/chemichull-paper`.

of dimension 3. The facets of the degenerated polytopes are given in Section 3. For completeness, we give in Table 8 the facets of the 3-dimensional polytopes P76-P86, where F22, F23, F24 and F25 are new facets defined as follows:

- F22: $2m_{13} - 4m_{33} \geq 0$;
- F23: $4m_{13} - 4m_{33} \geq 0$;
- F24: $2m_{12} + 5m_{13} - 4m_{33} \geq 0$;
- F25: $2m_{12} + 8m_{13} - 4m_{33} \geq 0$.

Table 8: Facets of the full-dimensional polytopes P76-P86

Id	facets	Id	facets
P76	F1, F3, F7, F22	P82	F6, F1, F2, F13, F4, F8, F21
P77	F3, F7, F20, F17	P83	F6, F3, F11, F10, F20, F17, F19
P78	F6, F1, F3, F8, F23	P84	F6, F1, F2, F12, F3, F4, F7, F25
P79	F6, F1, F2, F15, F10	P85	F6, F1, F2, F12, F15, F9, F21
P80	F6, F3, F13, F20	P86	F6, F3, F13, F7, F8, F20, F18
P81	F6, F1, F2, F3, F11, F9, F14, F24		

8 Example of application

In this section, we illustrate how the results of this paper can be applied to determine chemical graphs that maximize or minimize a degree-based topological index.

Consider for example the problem of minimizing the Albertson topological index [1] with $c_{ij} = | i - j |$. As mentioned in Section 2, minimizing $c_{12}m_{12} + c_{13}m_{13} + c_{22}m_{22} + c_{23}m_{23} + c_{33}m_{33}$ is equivalent to minimizing $f(m_{12}, m_{13}, m_{33}) = c'_{12}m_{12} + c'_{13}m_{13} + c'_{33}m_{33}$, where $c'_{12} = c_{12} - 4c_{22} + 3c_{23}$, $c'_{13} = c_{13} - 3c_{22} + 2c_{23}$ and $c'_{33} = c_{22} - 2c_{23} + c_{33}$. For the Albertson index, this means that we have to minimize $f(m_{12}, m_{13}, m_{33}) = 4m_{12} + 4m_{13} - 2m_{33}$.

If we are interested, for example, in graphs of order $n = 13$ and size $m = 15$, then we have to consider P64, and as shown in Table 6, the set of extreme points is {V1=V7, V5=V15=V16=V17, V6, V10, V11, V18=V19=V20, V22, V23}. Since f(V1)=0, f(V5)=4, f(V6)=2, f(V10)=-2, f(V11)=-4, f(V18)=-6 and f(V22)=f(V23)=-10, we deduce that the points that minimize the Albertson index are V22=(0,0,5) and V23=(1,0,7). Examples of chemical graphs that minimize the Albertson index for (n, m)=(13, 15) are shown in Figure 5.

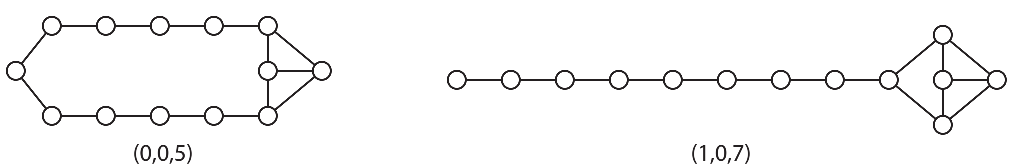


Figure 5: Two chemical graphs that minimize the Albertson index for $(n, m) = (13, 15)$

If we are interested in minimizing the Albertson index for all possible pairs (n, m) that satisfy condition (9), then we can compute the value $f(\mathrm{V}i)$ for all $i = 1, \ldots, 23$. These values are given in Table 9.

It is not difficult to check that the minimum value of $f(\mathrm{V}i)$ is $12n - 12m + 4$ for $m \geq n + 1$, but the unique point that reaches this value is V21 which is an extreme point only if $m = n - 1$, while for $m = n - 1$, a better value is obtained, for example by V1. The second best value is $6n - 6m + 2$ which is reached by V22 and V23 for $m \geq n+1$. Since V22 and V23 are extreme points only if $m \geq n+2$, we deduce that these two points minimize the Albertson index for $m \geq n + 2$. The third best value is -2 which is reached by V3, V12, V13 and V14 when $m = n+1$. The fourth best value is 0 and is reached

Table 9: $f(\mathbf{V}i)$ $(i = 1, \ldots, 23)$ for the Albertson index

Vi	f(Vi)	Vi	f(Vi)	Vi	f(Vi)
V1	0	V9	$9n - 8m - 2 - n \bmod 2$	V17	$\frac{4}{3}(6n - 5m - \frac{(2m) \bmod 3}{2})$
V2	8	V10	$9n - 8m + n \bmod 2$	V18	$\frac{2}{3}(12n - 11m + 2(m \bmod 3))$
V3	-2	V11	$9n - 8m - 1$	V19	$\frac{2}{3}(12n - 11m + m \bmod 3)$
V4	$12n - 10m$	V12	$12m - 12n - 14$	V20	$\frac{2}{3}(12n - 11m - m \bmod 3)$
V5	$6n - 5m + (m - 2n) \bmod 4$	V13	-2	V21	$12n - 12m + 4$
V6	$6n - 5m - (m - 2n) \bmod 4$	V14	-2	V22	$6n - 6m + 2$
V7	$6n - 5m - (2n - m) \bmod 4$	V15	$\frac{4}{3}(6n - 5m - m \bmod 3)$	V23	$6n - 6m + 2$
V8	$9n - 8m - 2 - n \bmod 2$	V16	$\frac{4}{3}(6n - 5m - m \bmod 3)$		

by V1 for $m = n$. The fifth best value is 8 which is reached by V2 for $m = n - 1$. Note that when there are more than one extreme point for a pair (n, m), then, according to Theorem 3.1 of [33], all integer convex combinations of extreme points are realizable and therefore also optimal. This occurs here when $m = n + 1$. Indeed, we have $(1, 0, 3) = \frac{1}{2}$(V3+V13). In summary, the best extreme points are those given in Table 10. This is exactly the same result as what is stated in [7]. Note that once we know the list of extreme points that minimize the Albertson index (i.e. the points in Table 10), it is very easy to determine which ones are optimal for a given pair (n, m). For the above example with $(n, m) = (13, 15)$, we have $m \geq n + 2$, which implies that V22=(0,0,5) and V23=(1,0,7) are the points we are interested in.

Table 10: Points that minimize the Albertson index for (n, m) satisfying condition (9)

	m_{12}	m_{13}	m_{33}	
V2	2	0	0	if $m = n - 1$
V1	0	0	0	if $m = n$
V3	0	0	1	
V12	1	1	5	
V13	2	0	5	if $m = n + 1$
V14	0	1	3	
$\frac{1}{2}$(V3+V13)	1	0	3	
V22	0	0	$3m - 3n - 1$	if $n + 2 \leq m \leq \frac{3n-3}{2}$
V23	1	0	$3m - 3n + 1$	

9 Concluding remarks and future work

We have given a complete polyhedral description of all chemical graphs of maximum degree at most 3. This allowed us to describe the convex hull associated with chemical graphs for any pair (n, m), and to observe that the maximum number of extreme points is 16. This is an important reinforcement of the formulation induced by Hansen et al. [33]. Indeed, as they mention in their paper, Equations (14)–(20) can be transformed into an integer linear program (IP) with $2^{\Delta-1} + \Delta(\Delta + 2) - 2$ variables and $2^{\Delta} + \frac{\Delta}{2}(\Delta^2 - \Delta + 6) - 4 + B_{\Delta}$ constraints, where Δ is an upper bound on the maximum degree and B_i is the i^{th} Bell number. For example, if $n = 14$, $m = 13$ and $\Delta = 3$, the IP induced by Equations (14)–(20) has 17 variables and 27 constraints. Its linear relaxation is very far from the convex hull defined in this paper (12 extreme points and 10 facets) since it contains 11 648 extreme points.

The same work could be done for a maximum degree at most 4. The work would be essentially the same. More precisely, a chemical graph would then be characterized using 9 variables instead of 5, since m_{14}, m_{24}, m_{34} and m_{44} are then potentially strictly positive. Here too, when the values of n and m are fixed, this reduces the degree of freedom by 2 and we can therefore work in a 7-dimensional space spanned by 7 of the 9 variables. To obtain a polyhedral description, it would be necessary, as we did for a maximum degree at most 3, to determine inequalities that are valid when conditions on

n and m are imposed, and to show that they are facet defining by exhibiting 7 affinely independent points of the hyperplane defined by each inequality. Subsequently, for a pair (n, m), by denoting $\mathcal{P}'_{n,m}$ the polytope defined by the set of active facets for (n, m), we could examine all the intersections of 7 facets and show that if the intersection exists and is in $\mathcal{P}'_{n,m}$, then it corresponds to a point that is realizable for (n, m).

The work to be done for a complete polyhedral description of chemical graphs of maximum degree at most 4 is however much more complex than it was for a maximum degree at most 3. Indeed, while the polytopes that we have described in this paper all have at most 10 facets and at most 16 extreme points, these numbers explode when the maximum degree can be equal to 4. For example, we generated all the chemical graphs of maximum degree at most 4 for $n = 21$ and $m = 23$ and we were thus able to observe that the associated polytope contains 761 facets and 402 extreme points. In summary, although this complete polyhedral description is possible, using the same tools as those described in this article, the number of cases to be considered is enormous and therefore requires considerable work that we nevertheless plan to carry out in the near future.

We conclude by pointing out that the ChemicHull website [8] mentioned in Section 5 allows, for any given pair (n, m), to list and visualize the associated polytope, its facets and its extreme points.

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