Counting Chemical Reactions and Simplexes in R^4

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Chemical reactions as $2H_2$+2CO =CH_4+CO_2 or mechanisms of consequtive reactions can be considered as linear combination of some vectors in $\mathbf{R}^n$ resulting $\underline{0}$. When considering *minimal* reactions, we are not allowed to delete any vector from them so that the remaining vectors still form a reaction / mechanism.

Mathematically speaking: a subset $S\subset\mathbf{R}^n$ is called an **(algebraic) simplex** iff it is minimal dependent, i.e. *S* itself is linearly dependent but all proper subsets of *S* is linearly independent.

Our starting **question** is the following:
How many simplexes *S* can be in a given set *H* of $\mathbf{R}^n$ of fixed size $|H|=m$?
In which cases is the number of simplexes is minimal or maximal?

The number of simplexes, contained in *H* is denoted by ***simp(H)*** .

Theorem (1991): If *H* spans $\mathbf{R}^n$ and $|H|=m$ then

$$n\cdot\binom{m/n}{2}\le simp(H)\le\binom{m}{n+1}$$

and we described the minimal and maximal situations as well**.**
The lower bound occurs when *H* may contain parallel vectors (isomer molecules).

Next question is: what is the lower bound when *H* does **not** contain parallel vectors?
The exact **answer** is known ony in the case ***n*=3** and (=number of atoms) **(1998):**

$$\binom{m-2}{3}+1+\binom{m-3}{2}\le simp(H)$$

and for ***n*=4** (**2010**):

$$\binom{\lfloor m/2\rfloor}{3}+1+\binom{\lceil m/2\rceil}{3}\le simp(H)$$

and we have conjectures for higher dimensions.

In the cases *n =3* és *n =4* the problem can be formulated in elementary way about points, lines and planes in the **Eucledian space** R^2 and in R^3 . For example
Definition: *A set of points* $S\subset R^3$ *is an* **affine**

- **3 -element simplex** *iff* S *is three colinear points,*
- **4 -element simplex** *iff* S *is any four coplanar points* but *none three of them are colinear,*
- **5 -element simplex** *iff* S *is any five points* but none four are coplanar (and thus none three of them are colinear) **.**

The general problem about **matroids** (hypergraphs) was answered in **(2006)**: *What is the minimal and maximal number of cycles and bases in a matroid of given rank?*

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