

On the Mathematical Foundation of Reaction Mechanisms

(manuscript in preparation, 130611)

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February 13, 2019

Abstract

We investigate stoichiometric reactions and mechanisms from abstract linear algebraic point of view.

Keywords stoichiometry, minimal reactions, linear algebra, simplexes, matroids, hypergraphs.

Foundation-1b-190213.tex, manuscript version 0.0

0 Introduction

Dozens of articles use graph theory and linear algebra for studying stoichiometric reactions and mechanisms, see eg. [83HS] through [13bSz] and the reference list in [13aSz]. However each of these works use the elements of linear algebra.

In this work we focus mainly on the theoretical mathematical aspects of stoichiometric reactions, mechanisms and systems of mechanisms, using higher algebra, too. The term *hierarchies* was invented by prof.Á.Pethő in [90P] and indicated in [13aSz]. The present paper is based on P.Sellers' private communications to the second author in 2002.

To avoid confusion, let us now fix some (possibly) nonstandard notations.

Definition 1 (i) \mathbb{N} denotes the set of natural numbers, including 0 .

(ii) For any functions (mappings) $f : A \rightarrow B$ and $g : B \rightarrow C$ the **composite** function $g \circ f : A \rightarrow C$ is defined as

$$(g \circ f)(a) := g(f(a)) \quad \text{for } a \in A . \quad (1)$$

(iii) $[z_{u,v}]_{U,V}$ denotes the **matrix** containing the elements $z_{u,v}$ for $1 \leq u \leq U$ and $1 \leq v \leq V$ in U rows and V columns. \square

In the present work we provide exhaustive explanations because of the abstract content.

1 The hierarchy

1.1 Definitions

A chemical (stoichiometric) system is made up of an infinite hierarchy of *disjoint finite sets*:

Definition 2 We introduce the (arbitrary) nonempty disjoint finite sets \mathcal{A}_x for $x = 0, 1, \dots \in \mathbb{N}$ as ($\mathcal{A}, \mathcal{M}, \mathcal{E}, \mathcal{C}$ are special notations for $\mathcal{A}_0, \dots, \mathcal{A}_3$):

o) $\mathcal{A} := \mathcal{A}_0 = \{A_1, \dots, A_a\}$ called **atoms**,

i) $\mathcal{M} := \mathcal{A}_1 = \{M_1, \dots, M_m\}$ called **molecules** or **species**,

ii) $\mathcal{E} := \mathcal{A}_2 = \{E_1, \dots, E_e\}$ called **elementary mechanistic steps** or **reactions**,

iii) $\mathcal{C} := \mathcal{A}_3 = \{C_1, \dots, C_c\}$ called (elementary) **mechanisms** or **catalizatinos**,

...

x) $\mathcal{A}_x = \{A_1^{(x)}, \dots, A_{d(x)}^{(x)}\}$ called the x -**th level of hierarchy**,

... . \square

This hierarchy must have *infinite many levels*, since in extremely compound cases systems of mechanisms can occur, and so on.

In case $0 < x$ every element $A_i^{(x)}$ of each one of these sets \mathcal{A}_x corresponds to a *unique* linear combination with integer coefficients of elements in the preceding set \mathcal{A}_{x-1} . However, we must not put equality between \mathcal{A}_x and this linear combination, since, for example many *different* molecules (e.g. isomers) possesses the same empirical formula (linear combination). Similarly, complicated mechanisms can be sensitive on the order of the reactions involved, while different mechanisms can result the same overall reactions, etc. This problem explains the role of the linear mappings $\Delta_x : \mathcal{A}_x \rightarrow L_x$ (see (3)) as

$$\Delta_x \left(A_i^{(x)} \right) = \sum_{j=1}^{d(x-1)} \alpha_{i,j} \cdot A_j^{(x-1)}, \quad \alpha_j \in \mathbb{Z}. \quad (2)$$

To be more precise, first we have to consider the **algebras** generated by the finite sets \mathcal{A}_x as bases and the linear mappings Δ_x after. The **algebras** below are, in fact finitely generated free Abelian groups, or simply linear (vector-) spaces with integer coefficients.

Definition 3 We define the **algebras** $\mathcal{L}_x := (L_x, +, \cdot)$ for $x = 0, 1, \dots \in \mathbb{N}$ as the ground sets

$$L_x := \left\{ \sum_{j=1}^{d(x)} \alpha_j \cdot A_j^{(x)} : \alpha_j \in \mathbb{Z} \right\}, \quad (3)$$

abbreviating $\sum_{j=1}^{d(x)} \alpha_j \cdot A_j^{(x)}$ as $[\alpha_1, \dots, \alpha_{d(x)}]$, equipped with the usual operations

$$[\alpha_1, \dots, \alpha_{d(x)}] + [\beta_1, \dots, \beta_{d(x)}] := [\alpha_1 + \beta_1, \dots, \alpha_{d(x)} + \beta_{d(x)}] \quad (4)$$

and

$$\lambda \cdot [\alpha_1, \dots, \alpha_{d(x)}] := [\lambda \cdot \alpha_1, \dots, \lambda \cdot \alpha_{d(x)}] \quad \text{for } \lambda \in \mathbb{Z}. \quad (5)$$

Clearly the **bases** of \mathcal{L}_x are the sets \mathcal{A}_x . \square

Since the sets L_x are linear combinations of the corresponding \mathcal{A}_x , for example we can interpret the arbitrary elements of L_0 as "combinations of atoms", of L_1 as "combinations of molecules", of L_2 as "combinations of elementary reactions", etc.

The coefficients α_j might be assumed to be non-negative *only* in the first level \mathcal{L}_0 ("images" of molecules), since, for example in reactions (elements of \mathcal{E}) we must distinguish the different sides. In our interpretation \mathcal{L}_1 contains the "images" of reactions.

Now we make more precise the *connections* between the levels of our hierarchy, started in (2).

Especially, for $x = 2$ the *law of mass-balance* requires, that the number of each kind of atoms taking part in each reaction - a linear combination of molecules - must be (finally) *zero*. This can be expressed using the special cases of (2)

$$\Delta_1(M_j) = \sum_{k=1}^a \alpha_{j,k} \cdot A_k, \quad \Delta_2(E_i) = \sum_{j=1}^m \mu_{i,j} \cdot M_j \quad (1 \leq i \leq e) \quad (6)$$

as

$$\sum_{j=1}^m \mu_{i,j} \cdot \alpha_{j,k} = 0 \quad \text{for } 1 \leq i \leq e, 1 \leq k \leq a. \quad (7)$$

Using matrices (7) can be written as

$$[\mu_{i,j}]_{e,m} \cdot [\alpha_{j,k}]_{m,a} = [0]_{e,a}, \quad (8)$$

or in the language of the linear mappings

$$\boxed{\Delta_1 \circ \Delta_2 = O \quad \text{i.e.} \quad \text{Im}(\Delta_2) \subseteq \text{Ker}(\Delta_1)} \quad (9)$$

where, of course

$$\Delta_2 : \mathcal{L}_2 \rightarrow \mathcal{L}_1 \quad \text{and} \quad \Delta_1 : \mathcal{L}_1 \rightarrow \mathcal{L}_0. \quad (10)$$

($[\mu_{i,j}]_{e,m}$ is called *stoichiometric* while $[\alpha_{j,k}]_{m,a}$ is the *composition matrix*.)

Now we are able to define the mappings Δ_x in general:

Definition 4 For $x \in \mathbb{N}$, $x \neq 0$ we call the linear mappings

$$\Delta_x : \mathcal{L}_x \rightarrow \mathcal{L}_{x-1} \quad (11)$$

stoichiometric connections between \mathcal{L}_x and \mathcal{L}_{x-1} if the requirements

$$\Delta_x \circ \Delta_{x+1} = O \quad \text{for } x = 1, 2, \dots \quad (12)$$

where $O = O_x : \mathcal{L}_{x+1} \rightarrow \mathcal{L}_{x-1}$ is the null-mapping. \square

We drop the adjective "stoichiometric" in what follows.

Though we are talking bases and matrices, we do not have to deal with base transformations since we fixed the bases we use in each \mathcal{L}_x .

Remark 5 *The requirement (12) can be written equivalently as*

$$\text{Im}(\Delta_{x+1}) \subseteq \text{Ker}(\Delta_x) \quad \text{for } x = 1, 2, \dots \quad (13)$$

Definition 6 *We call a system of algebras and mappings*

$$\mathcal{H} = (\mathcal{L}_x, \Delta_{x+1} : x \in \mathbb{N}) \quad (14)$$

(stoichiometric) hierarchy, if it satisfies Definitions 2 through 4. \square

1.2 Properties

Now let us have a closer look to some properties of the above hierarchy.

For $\underline{v} = \sum_{j=1}^{d(x)} \alpha_j \cdot A_j^{(x)} \in L_x$ ($0 < x$), $\underline{v} \in \text{Ker}(\Delta_x)$ we know that

$$\begin{aligned} \Delta_x(\underline{v}) &= \sum_{j=1}^{d(x)} \alpha_j \cdot \Delta_x(A_j^{(x)}) = \sum_{j=1}^{d(x)} \alpha_j \cdot \left(\sum_{i=1}^{d(x-1)} \beta_i^{(j)} \cdot A_i^{(x-1)} \right) = \\ &= \sum_{i=1}^{d(x-1)} \left(\sum_{j=1}^{d(x)} \alpha_j \beta_i^{(j)} \right) \cdot A_i^{(x-1)} = \underline{0} \quad \text{which includes} \end{aligned}$$

$$\sum_{j=1}^{d(x)} \alpha_j \beta_i^{(j)} = 0 \quad \text{for } i \leq d(x-1) \quad (15)$$

since $\{A_1^{(x)}, \dots, A_{d(x)}^{(x)}\}$ was assumed to be a base.

For example, for any *elementary* reaction $E \in \mathcal{E} = \mathcal{A}_2$ we have that $\Delta_2(E)$ is a linear combination of molecules (where different signs of molecules distinguish starting and final ones), and by (13) $\underline{v} := \Delta_2(E) \in \text{Ker}(\Delta_1)$, so (15) means that E must correspond (via Δ_2) to a *balanced* reaction. The linearity of Δ_2 implies that *any* (composite) reaction $E \in L_2$ also corresponds

to a balanced reaction. Since $\text{Im}(\Delta_2) \subset L_1$ and $\text{Im}(\Delta_2) \subset \text{Ker}(\Delta_1)$, the above implies

$$\boxed{\text{Im}(\Delta_2) = \text{the set of all balanced reactions.}} \quad (16)$$

Especially, for $E \in \text{Ker}(\Delta_2)$ we have $\Delta_2(E) = \underline{0}$ (-reaction) which means that E is a mechanism resulting the 0-reaction. In other words

$$\boxed{\text{Ker}(\Delta_2) = \text{the set of all cycle-mechanisms.}} \quad (17)$$

In general we say:

Definition 7 For $x > 0$ the elements of $\text{Ker}(\Delta_x)$ and $\text{Im}(\Delta_x)$ are called (generalized) **cycle-mechanisms** and **balanced mechanisms**, respectively. \square

Clearly, by (13) each balanced mechanisms must be cycles.

We did *not* prescribe $\text{Ker}(\Delta_x) = \emptyset$, so we may use the following terminology.

Definition 8 For $x > 0$ we call the vectors $\underline{w}_1, \underline{w}_2 \in L_x$ to be **equivalent modulo $\text{Ker}(\Delta_x)$** if and only if

$$\underline{w}_2 - \underline{w}_1 \in \text{Ker}(\Delta_x) . \quad (18)$$

We shorten (18) as

$$\underline{w}_1 \rightleftharpoons \underline{w}_2 . \quad (19)$$

\square

Clearly (18) can be written as

$$\underline{w}_2 = \underline{w}_1 + \underline{y} \quad \text{for some } \underline{y} \in \text{Ker}(\Delta_x) . \quad (20)$$

It is well known, that \rightleftharpoons is an *equivalence relation* and the *partition* L_x by \rightleftharpoons (the **factor** L_x / \rightleftharpoons) is isomorphic to $\text{Im}(\Delta_x) \subset L_{x-1}$:

$$\boxed{L_x / \rightleftharpoons \cong \text{Im}(\Delta_x) .} \quad (21)$$

For molecules $M_1, M_2 \in \mathcal{M}$ the relation $M_1 \rightleftharpoons M_2$ means that M_1 and M_2 contains the *same amount of atoms* but have different (graph-) structures.

For reactions $E_1, E_2 \in \mathcal{E}$ $E_1 \rightleftharpoons E_2$ means that E_1 and E_2 *differ only* in a balanced reaction, i.e. which results $\underline{0}$.

The *factorization* L_x/\simeq means that $\underline{w_1}$ and $\underline{w_2}$ in (20) represent the *same object* and \underline{y} represents the *null object* in L_x . The phrases "same" and "equivalent" express the requirement that $\underline{w_1}$ and $\underline{w_2}$ finally must end the *same* results. The equality $\Delta_x(\underline{w_2}) = \Delta_x(\underline{w_1})$ expresses this, too, which is clearly equivalent to (18) and (20).

That is (writing \underline{w} instead of $\underline{w_1}$)

$$\boxed{\underline{w} + Ker(\Delta_x) = \text{set of all objects equivalent to } \underline{w}}, \quad (22)$$

e.g. in case $x = 2$

$$E + Ker(\Delta_2) = \text{set of all mechanisms resulting the reaction } \Delta_2(E). \quad (23)$$

Mathematically, the term $\underline{w} + Ker(\Delta_x)$ is a **coset** (a subspace translated by a vector), the factor set L_x/\simeq is contained from all of these cosets, as elements of L_x/\simeq .

1.3 Dual mappings

Now we turn to the dual spaces and mappings

$$\Delta_x^* : \mathcal{L}_{x-1}^* \rightarrow \mathcal{L}_x^* \quad (1 \leq x). \quad (24)$$

Recall first the general mathematical definition of dual spaces and mappings.

Definition 9 *Let V and W be any linear spaces and denote Γ the set from scalar coefficients for the elements of V and W can be chosen (usually the set of real numbers, $\Gamma = \mathbb{R}$).*

*(i) The **dual space** V^* is defined as the set of linear mappings (functions) $f : V \rightarrow \Gamma$. The addition and scalar multiplication for $f_1, f_2, f \in V^*$ and $\lambda \in \Gamma$ are defined pointwise, i.e.*

$$\begin{aligned} (f_1 \oplus f_2)(v) & : = f_1(v) + f_2(v) \\ (\lambda \odot f)(v) & : = \lambda \cdot f(v) \quad (v \in V, \lambda \in \Gamma). \end{aligned} \quad (25)$$

*(ii) For any linear mapping $\mathcal{M} : V \rightarrow W$, the **dual mapping***

$$\mathcal{M}^* : W^* \rightarrow V^*, \quad g \longmapsto f \quad (26)$$

or $f := \mathcal{M}^*(g) \in V^*$ ($g \in W^*$) is defined as

$$\mathcal{M}^*(g) := \mathcal{M} \circ g \quad (27)$$

i.e.

$$f(v) := \mathcal{M}(g(v)) \quad (v \in V). \quad (28)$$

□

Note that \mathcal{M}^* is also linear since \mathcal{M} was linear itself.

The elements of V^* are called also *functionals* or *valuations*, their stoichiometric aspects, together some linear algebraic citations are discussed in detail in [00Sz].

It is well known that fixing any base $B = \{b_1, \dots, b_n\}$ of V , then the corresponding functions (dual vectors) $B^* = \{f_{b_1}, \dots, f_{b_n}\}$ where $f_{b_i}(b_j) = \delta_{i,j}$ ⁽¹⁾, form a base for V^* . This means, that the dimensions of V and V^* are the same, so V and V^* are, in fact, isomorphic. Moreover, the dual base $B^* = \{f_{b_1}, \dots, f_{b_n}\}$ implies the natural correspondance between V and V^* as follows.

Using the notations for $v, w \in V$

$$v = \sum_{j=1}^n \nu_j \cdot b_j, \quad w = \sum_{i=1}^n \chi_i \cdot b_i, \quad (29)$$

the functional $f_v = \sum_j \nu_j \cdot f_{b_j} \in V^*$, related to v , works for any w as

$$f_v(w) = \sum_{j=1}^n \nu_j \cdot f_{b_j}(\sum_{i=1}^n \chi_i \cdot b_i) = \sum_{j=1}^n \sum_{i=1}^n \nu_j \cdot \chi_i \cdot \delta_{i,j} = \sum_{i=1}^n \nu_j \cdot \chi_i \quad (30)$$

that is

$$f_v(w) = \langle v, w \rangle_B == \sum_{i=1}^n \nu_j \cdot \chi_i \quad (31)$$

where $\langle v, w \rangle_B$ is called the **Euclidean scalar product** over the base B . (Recall, that $\dim(V) = n$ is equivalent to that V is isomorphic to \mathbb{R}^n .)

By (11) and (24) the below definition is natural.

¹⁾ here $\delta_{i,j}$ denotes the **Kronecker-delta**, i.e. $\delta_{i,j} = 1$ for $i = j$ and $\delta_{i,j} = 0$ for $i \neq j$.

Definition 10 The dual mappings $\Delta_x^* : \mathcal{L}_{x-1}^* \rightarrow \mathcal{L}_x^*$ ($1 \leq x$) are called *dual stoichiometric connections*. \square

It is well known that the *matrices* of Δ_x^* are the **transposes** of the matrices of Δ_x .

The below connection among the dual mappings Δ_x^* is also an easy consequence of (12) and (13).

Lemma 11 For each $x = 1, 2, \dots$ the assumptions (12) and (13) are equivalent to

$$\Delta_{x+1}^* \circ \Delta_x^* = O^* \quad (32)$$

and

$$\text{Im}(\Delta_x^*) \subseteq \text{Ker}(\Delta_{x+1}^*) \quad (33)$$

where $O^* = O_x^* : \mathcal{L}_{x-1}^* \rightarrow \mathcal{L}_{x+1}^*$ is the null-functional. \square

Similarly to (16) and (17), $\text{Ker}(\Delta_x^*)$ and $\text{Im}(\Delta_x^*)$ could be meaningful for some $x > 0$. First we consider

$$\text{Ker}(\Delta_2^*) = \{g \in L_1 \rightarrow \mathbb{R} : g \circ \Delta_2 = \mathcal{O}\} \quad (34)$$

where $g \circ \Delta_2 = \mathcal{O}$ means

$$g(w) = g(\Delta_2(v)) = 0 \quad \text{for all } v \in L_1. \quad (35)$$

The latter equality means in our interpretation, that each "combination of molecules" (w) resulted from "combination of elementary reactions" (v) via Δ_2 must satisfy the condition $g(w) = 0$. Since we consider (managed) all *balanced* reactions as zero vectors (see the comment just before (6)), the requirement (35) explains $\text{Ker}(\Delta_2^*)$ as:

$$\boxed{\text{Ker}(\Delta_2^*) = \text{set of all conservation conditions}} \quad (36)$$

where, of course by "*conservation condition*" we mean the condition we require to preserve during each (combination of) reactions. As mentioned, each $g \in \text{Ker}(\Delta_2^*)$ is a functional, a valuation operator in other words.

Second we see

$$\text{Im}(\Delta_1^*) = \{f \circ \Delta_1 : f \in \mathcal{L}_1^*\} \quad (37)$$

where $f \circ \Delta_1 : L_2 \rightarrow \mathbb{R}$ is a linear functional, ordering a real number to each "combination" of molecules M . Since $\Delta_1(M)$ "counts" the atoms in M , and Δ_1 and f are linear, $(f \circ \Delta_1)(M)$ finally counts the weighted sum (according to f) of the atoms contained in M . By (31) and (37) $f = f_{\underline{\mathbf{a}}}$ for all possible $\underline{\mathbf{a}} \in \mathbb{R}^a$ (see Def.2), which explains the equality

$$(f \circ \Delta_1)(M) = c \tag{38}$$

as the weighted sum (by $\underline{\mathbf{a}}$) of atoms in M is required to be c . In short:

$$\boxed{\text{Im}(\Delta_1^*) = \text{set of all "mass-conservation" conditions}} \tag{39}$$

By (36) and (39) we are allowed to introduce the below general notions, which are in synchron with (33).

Definition 12 For $x > 0$ the elements of $\text{Ker}(\Delta_x^*)$ and $\text{Im}(\Delta_x^*)$ are called (generalized) **conservation- and mass-conservation conditions**, respectively. \square

In practice, the term "condition" would rather mean an equality than a functional. Fortunately (38) makes the bridge between practice and present theory.

In some chemical applications $\text{Im}(\Delta_{x+1}) = \text{Ker}(\Delta_x)$ is assumed instead of (13) for some $x \in \mathbb{N}$, e.g. for $x = 1$. This is equivalent to $\text{Im}(\Delta_x^*) \subseteq \text{Ker}(\Delta_{x+1}^*)$ by Lemma 11. In fact, from $\Delta_2 : \mathcal{E} \rightarrow \mathcal{M}$ one can guess $\Delta_1 : \mathcal{M} \rightarrow \mathcal{A}$ in the case $\text{Im}(\Delta_2) = \text{Ker}(\Delta_1)$, and similarly for Δ_1^* and Δ_2^* .

2 Combinatorial properties

definitions, reference to the results and open problem listed in [13aSz]

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