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On valuation operators in stoichiometry and in reaction syntheses

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We investigate physical and chemical quantitative characteristics of species, reactions and mechanisms which are linear (additive and homogeneous) in general, using linear algebraic methods. We call such characteristics here as "*valuation operators*". After revealing the properties of these operators we reach to some practical consequences at the end of our paper which could be used either for calculating or forecasting the behaviour and the magnitude of these characteristics.

Though these results might have already been used by experts for a long time, the present paper could serve as a firm theoretical background for their computation methods.

KEY WORDS: stoichiometry, linear, valuation operator, additive quantities

1. Introduction and preliminaries

Using and extending the ideas of Pethö [1,2], of the present author [3] and independently Happel and Sellers [4,5] we can interpret the vectors of the n-dimensional Euclidean space $\mathbb{R}^n$ in several ways as species (groups of atoms), reactions, mechanisms, measure units, etc. (We give definitions below shortly, for details see our survey paper [6].) After then any linear (additive and homogeneous) quantity (we call them *valuation operators*) of any of these interpretations are, in fact, a linear functional $\mathcal{L}: \mathbb{R}^n \to \mathbb{R}$. Using the theory of linear functionals (especially the representation theorem of F. Riesz) we can investigate the structure of these linear functionals and may draw further conclusions. These conclusions are mentioned in each cases just after their theoretical background, but are also listed in the last section.

2. Vectors

The following examples of interpretations of vectors are separate ones though (linear) combinations of reactions are mechanisms, reactions are built up from species, etc. These and other connections of this "hierarchy" are extensively studied in our works [3,7–10] and are surveyed in [6].

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Example 2.1 (Species). If the species (either active or chemical or groups of atoms only) $A_1, \dots, A_n$ consist of the atoms $E_1, \dots, E_m$ as $A_j = \sum_{i=1}^m a_{i,j} E_i$, where $a_{i,j} \in \mathbb{N}$ for $j = 1, \dots, n$ and $i = 1, \dots, m$, and the set $\{E_1, \dots, E_m\}$ is fixed, we can assign the species A_j to the *vectors*[1]

$$\underline{A}_j := [a_{1,j}, a_{2,j}, \dots, a_{m,j}]^{\mathrm{T}} \in \mathbb{R}^m$$

or in other words, $\underline{A}_j = \sum_{i=1}^m a_{i,j} \underline{E}_i$ for $j = 1, \dots, n$ assuming that $\{\underline{E}_1, \dots, \underline{E}_m\} \subseteq \mathbb{R}^m$ is a (natural) base in $\mathbb{R}^m$.

We can use the same model when the components $E_1, \dots, E_m$ denote (functional) groups of atoms which is widely used in practice.

Example 2.2 (Reactions). If we are given the reactions $X_1, \dots, X_k$ which use the (fixed set of) species $A_1, \dots, A_n$ as $X_j = \sum_{i=1}^m b_{i,j} \cdot A_i$ then we can correspond these reactions to the vectors $\underline{X}_j := [b_{1,j}, \dots, b_{n,j}]^{\mathrm{T}} \in \mathbb{R}^n$, i.e., $\underline{X}_j = \sum_{i=1}^m b_{i,j}.\ \underline{A}_i$, where $b_{i,j} \in \mathbb{Z}$ for $j = 1, \dots, k$ and $i = 1, \dots, n$ if the base vectors were chosen $\underline{A}_1, \dots, \underline{A}_n \in \mathbb{R}^n$.[2]

Example 2.3 (Mechanisms). Any linear combinations of (the fixed set of) reactions $\{X_1, \dots, X_k\}$ are called mechanisms, and similarly we can assign these mechanisms $M_t = \sum_{j=1}^k \lambda_{t,j} \cdot X_j$ to the vectors $\underline{m}_t := [\lambda_{t,1}, \dots, \lambda_{t,k}]^{\mathrm{T}}$, i.e. $\underline{m}_t = \sum_{j=1}^k \boldsymbol{\lambda}_{t,j} \cdot \underline{X}_j \in \mathbb{R}^k$ where, of course, $\lambda_{t,j} \in \mathbb{Z}$ for $t = 1, \dots, \ell$ and $j = 1, \dots, k$.[3] The base in this case is $\{\underline{X}_1, \dots, \underline{X}_k\} \subset \mathbb{R}^k$.

Example 2.4 (Measure units). Every (composite) measure unit $M_1, \dots, M_n$ is built up from elementary units $E_1, \dots, E_m$ (such as length, mass, time, etc.) as $M_i = \prod_{j=1}^m E_j^{a_{i,j}}$ where $a_{i,j} \in \mathbb{Z}$ for $i = 1, \dots, n$ and $j = 1, \dots, m$. Clearly we again can assign the measure units M_i to the *vectors* $\underline{M}_i := [a_{i,1}, \dots, a_{i,m}]^{\mathrm{T}} \in \mathbb{R}^m$ since any *product* of the powers of the units M_i corresponds to a linear combination of the vectors $\underline{M}_i$ (see, e.g., the Reynold's numbers).

One could find many more such examples (e.g., how atoms are built up from atomic parts) where our theory below could also be applied.

Let us remark that we have to fix the set of building *components* (atoms/species/reactions) to build more complicated *structures* (as species/reactions/mechanisms) *in advance* since this set gives not only the base of the space but the dimension or even the space itself in which our investigations take place. For our further reference we fix these concepts into a precise definition.

[1] We will not emphasize the difference between the species $\underline{A}_j$ and the vectors A_j.

[2] Moving the terms with negative coefficients $b_{i,j}$ to the left-hand side of the equality (initial materials of the reaction) and leaving the others in the right-hand side (resulting materials) we get the usual form of the mechanism.

[3] Negative coefficients mean that the corresponding reactions take place in reverse order.

Definition 2.5. All the elements of an arbitrary but fixed and finite set $\{C_1, \ldots, C_N\}$ are called *components*, and any (possibly only formal) linear combinations

$$\underline{S} = \sum_{i=1}^{N} s_i \cdot C_i$$

of its elements with arbitrary real numbers $s_i \in \mathbb{R}$ are called *structures*.

At the end of this paper we discuss the case of *subsequent adding* new structures containing new components, i.e. how to extend the dimension of the space we are in and how to continue the calculations in the extended space without giving up our old results.

3. Valuation operators and linearity

We call any linear mapping of real value (i.e., a linear functional) which maps from (the above) structures a *valuation operator*.

Definition 3.1. Any linear mapping (or functional) $\mathcal{L} : \mathbb{R}^n \to \mathbb{R}$ is called a *valuation operator*.

Continuing the above examples in section 2 let us mention some valuation operators on them. These and others are described, for example, in [11] or in Pethö's works, widely used already in practice and are called *estimation and correlation methods of thermodynamic parameters* in thermodynamics and thermophysics.

The *molar volume* of species is usually computed as the sum (i.e. linear combination) of the components' data. This is a typical example where we can assume that the molecular quantitative property (increment) can be added linearly from the amount of that property (increment) of the components (functional groups or bonds). Other examples are the *enthalpy of formation* or the *heat capacity.* Practical methods and applications are described, e.g., in the book [11].

The *standard Gibbs free energy change* ΔG° (or free enthalpy) of a reaction is the sum (linear combination) of the standard chemical potentials μ_i of the components (species) involved in the reaction as

$$\Delta G^\circ = \sum_{i=1}^{n} \nu_i \mu_i^\circ.$$

The *heat of reactions* when studying mechanisms: Hess' well-known law states that the resulting heat is again the sum (linear combination) of the heat of single reactions taking part in the mechanism. (This example is studied in [2,12].)

Clearly, the long list could be continued up to infinity.

For properties which are not linear but multiplicative instead, we can use the logarithm function for getting linear correspondence – among the logarithm of the property of the parts, as we did in example 2.4 in section 2 (see also [1]) or is applied, e.g., in [13] for drawing Pourbaix diagrams.

4. Riesz's theorem

Using our terminology all valuation operators are linear functionals of the form $\mathcal{L}: V \to \mathbb{R}$ for some vector space V, so we can apply the following deep theorem of Frigyes Riesz which (and all the other results cited in the subsequent sections) can be found in any linear algebraic book.

Theorem 4.1 (Representation theorem of F. Riesz). If V is any finite-dimensional linear space with an arbitrary scalar product $\langle\cdot,\cdot\rangle : V \times V \to \mathbb{R}$ then for every linear functional $\mathcal{L}: V \to \mathbb{R}$ there is a (unique) fixed vector $\underline{a} \in V$ (depending only on $\mathcal{L}$) such that

$$\mathcal{L}(\underline{v}) = \langle \underline{a}, \underline{v} \rangle \tag{1}$$

holds for every vector $v \in V$.

Since Riesz's theorem is valid for *any* scalar product $\langle\cdot,\cdot\rangle$ (symmetric, positive definite and bilinear function from $V \times V$ to $\mathbb{R}$) on the space V, for applications we may choose first the Euclidean product

$$\langle \underline{u}, \underline{v} \rangle := \sum_{i=1}^{n} u_i v_i,$$

where $[u_1, \ldots, u_n]^{\mathrm{T}}$ and $[v_1, \ldots, v_n]^{\mathrm{T}}$ denote the coordinates of $\underline{u}$ and $\underline{v}$ with respect to a *fixed* base $B \subseteq V$. (We discuss all the possible scalar products of $\mathbb{R}^n$ and the connections among them in section 6.)

So we get the below special case of Riesz's theorem:

Theorem 4.2. If V is any finite-dimensional linear space with any fixed base $\{\underline{b}_1, \ldots, \underline{b}_n\} \subseteq V$ then for every linear functional $\mathcal{L}: V \to \mathbb{R}$ there is a (unique) fixed vector $\underline{a} \in V$ (depending only on $\mathcal{L}$) such that

$$\mathcal{L}(\underline{v}) = \sum_{i=1}^{n} a_i v_i \tag{2}$$

holds for every vector $v \in V$ where $[a_1, \ldots, a_n]$ and $[v_1, \ldots, v_n]$ denote the coordinates of $\underline{a}$ and $\underline{v}$ with respect to the base B.

Using (2) this latter variant of Riesz's theorem tells us for valuation operators (e.g., in our examples above) the following:

Corollary 4.3. If the linear space $\mathbb{R}^N$ is determined by the components $\{C_1, \dots, C_N\}$ then for any valuation operator $\mathcal{L}: \mathbb{R}^N \to \mathbb{R}$ there is a unique vector $\underline{a} := [a_1, \dots, a_N]^T \in \mathbb{R}^N$ such that $\mathcal{L}$ can be computed as

$$\mathcal{L}(S) = \sum_{i=1}^{N} a_i \cdot s_i \tag{3}$$

for any structure $S = \sum_{i=1}^{N} s_i \cdot C_i$. (Recall definition 2.5 for the notion of components and structures.)

This clearly means that the values of *every* valuation operator on *any* structures in *all of the examples*: not only is determined by the components involved but simply it is *the weighted sum of the numbers of the components in the structure*!

This observation might facilitate the investigations of any valuation operators in any of our (or other) examples. For example, we have to determine only the coefficient vector $\underline{a} \in \mathbb{R}^N$ for the given valuation operator and after this we can trivially count (or further investigate) its value on the basis of (3).

The above result might be not new for chemists: trivially the linearity of $\mathcal{L}$ implies

$$\mathcal{L}(S) = \mathcal{L}\left(\sum_{i=1}^{N} s_i \cdot C_i\right) = \sum_{i=1}^{N} s_i \cdot \mathcal{L}(C_i) \tag{4}$$

which clearly implies (3) choosing $a_i := \mathcal{L}(C_i)$ for $i = 1, \dots, N$. Let us remark here that the above computation assumes that $\mathcal{L}$ can be computed for components C_i on the same way as for structures $\underline{S}$.

However, the real power of Riesz' theorem lies in the fact that it is valid for *any* scalar product on *any* linear space V. We used it only in the very special case of Euclidean scalar product *with respect to* the base $\{C_1, \dots, C_N\}$ of our interested components! The variety of and the connections among different scalar products and bases in $\mathbb{R}^n$ is explained in section 6.

One surprising application of the above results is a one-sentence proof of Hess' law in thermochemistry: if a linear combination of the reactions $X_1, \dots, X_k$ results the zero (or void) mechanism $\underline{\mathcal{M}}$ then the sum (the same linear combination) of the reaction heats $\mathcal{H}(X_j)$ of the reactions X_j will also be 0. This is trivial since if $\sum_{j=1}^{k} \lambda_j X_j = \underline{\mathcal{M}}$ then

$$\mathcal{H}\left(\sum_{j=1}^{k} \lambda_j X_j\right) = \mathcal{H}(\underline{\mathcal{M}}) = 0. \tag{5}$$

□

The following theorem is also well known, using it we can give bounds for the values of $\mathcal{L}(S)$ in advance:

Theorem 4.4 (Cauchy–Bunyakowsky–Schwarz). For any linear space V and scalar product $\langle\cdot,\cdot\rangle : V \times V \to \mathbb{R}$ on V the equality

$$\left|\langle \underline{a}, \underline{x}\rangle\right| \leqslant \|\underline{a}\| \cdot \|\underline{x}\| \tag{6}$$

holds for every vectors $\underline{a}, \underline{x} \in V$ where $\|\underline{x}\| := \sqrt{\langle \underline{x}, \underline{x}\rangle}$ is the norm of all the vectors $\underline{x} \in V$.

Corollary 4.5. For any linear space V with the arbitrary scalar product $\langle\cdot,\cdot\rangle : V \times V \to \mathbb{R}$ on it and for any linear functional $\mathcal{L} : V \to \mathbb{R}$ we have

$$\left|\mathcal{L}(\underline{S})\right| \leqslant c \cdot \|\underline{S}\| \tag{7}$$

for any vector $\underline{S} \in V$ where $c \in \mathbb{R}$ is a fixed constant depending on $\mathcal{L}$, and on the scalar product $\langle\cdot,\cdot\rangle$ only (but not the vector $\underline{S}$ itself).

Using (7) we can estimate the magnitude of $\mathcal{L}(\underline{S})$. For example, if $\langle\cdot,\cdot\rangle$ is the Euclidean (quadratic) scalar product on $\mathbb{R}^N$ then we have

$$|\mathcal{L}(\underline{S})| \leqslant c \cdot \sqrt{s_1^2 + \cdots + s_N^2}, \tag{8}$$

where $c = \sqrt{a_1^2 + \cdots + a_N^2}$ (the quadratic sum of the $\mathcal{L}$-values of the components) and $\underline{a}$ is defined in (2) in theorem 4.2.

5. Direct sums

In all of the above results we had to fix the dimension of the space in advance. This clearly fixes the number of components which can be used.

In this section we explain the possibility of later (subsequent) adding new structures containing new components, i.e., how to extend the dimension of the space we are in, and continue the calculations without giving up the old ones. Though the below results solve this problem we must be careful in practical computations.

Extending the dimension by introducing new base vectors (components in our examples) can be handled with *direct sums* of linear spaces and of linear operators.

Let us recall here that the *direct sum* $V = V_1 \oplus V_2$ means that *each* vector $\underline{v} \in V$ can be written *uniquely* in the form $\underline{v} = \underline{v}_1 + \underline{v}_2$ for some $\underline{v}_1 \in V_1$ and $\underline{v}_2 \in V_2$ (which clearly implies $V_1 \cap V_2 = \{0\}$). Further, $\mathcal{L} := \mathcal{L}_1 \oplus \mathcal{L}_2$ means $\mathcal{L}(\underline{v}) = \mathcal{L}_1(\underline{v}_1) + \mathcal{L}_2(\underline{v}_2)$ for the linear operators $\mathcal{L} : V \to \mathbb{R}$, $\mathcal{L}_1 : V_1 \to \mathbb{R}$, $\mathcal{L}_2 : V_2 \to \mathbb{R}$ and for any vectors $\underline{v}$, $\underline{v}_1$, $\underline{v}_2$ above.

Statement 5.1. If V is any linear space which is a direct sum of the two spaces $V = V_1 \oplus V_2$, then every linear functional $\mathcal{L} : V \to \mathbb{R}$ can be written in the form $\mathcal{L} = \mathcal{L}_1 \oplus \mathcal{L}_2$ where $\mathcal{L}_i : V_i \to \mathbb{R}$ are linear functionals for $i = 1, 2$.

On the other hand, if $\mathcal{L}_i : V_i \to \mathbb{R}$ are linear functionals for $i = 1, 2$ then the functional $\mathcal{L} := \mathcal{L}_1 \oplus \mathcal{L}_2$, $\mathcal{L} : V \to \mathbb{R}$ is also linear.

Using Riesz's theorem 4.1 for all the vector spaces V, V_1 and V_2 separately, clearly we have that $\mathcal{L}(\underline{v}) = \langle \underline{a}, \underline{v} \rangle$, $\mathcal{L}_1(\underline{v}_1) = \langle \underline{a}_1, \underline{v}_1 \rangle$ and $\mathcal{L}_2(\underline{v}_2) = \langle \underline{a}_2, \underline{v}_2 \rangle$ hold for all vectors $\underline{v} \in V$, $\underline{v}_1 \in V_1$ and $\underline{v}_2 \in V_2$ for some fixed special vectors $\underline{a} \in V$, $\underline{a}_1 \in V_1$ and $\underline{a}_2 \in V_2$. Let us emphasize, however, that $\underline{a}$ is *not* the (direct) sum of $\underline{a}_1$ and $\underline{a}_2$ in general. This latter requirement can be ensured, e.g., when the subspaces V_1 and V_2 are *orthogonal* to each other (with respect to the scalar product $\langle \cdot, \cdot \rangle$) which means $\underline{v}_1 \perp \underline{v}_2$ (i.e., $\langle \underline{v}_1, \underline{v}_2 \rangle = 0$) for *all* $\underline{v}_1 \in V_1$, $\underline{v}_2 \in V_2$. We state the exact result below.

Statement 5.2. If $V = V_1 \oplus V_2$ and $\mathcal{L} = \mathcal{L}_1 \oplus \mathcal{L}_2$ are arbitrary as in statement 5.1, $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{R}$ is an arbitrary scalar product such that V_1 and V_2 are orthogonal to each other (with respect to this scalar product) and further the vectors $\underline{a} \in V$, $\underline{a}_1 \in V_1$ and $\underline{a}_2 \in V_2$ satisfy

$$\mathcal{L}(\underline{v}) = \langle \underline{a}, \underline{v} \rangle, \quad \mathcal{L}_1(\underline{v}_1) = \langle \underline{a}_1, \underline{v}_1 \rangle \quad \text{and} \quad \mathcal{L}_2(\underline{v}_2) = \langle a_2, \underline{v}_2 \rangle$$

for all $\underline{v} \in V$, $\underline{v}_1 \in V_1$ and $\underline{v}_2 \in V_2$ then

$$\underline{a} = \underline{a}_1 \oplus \underline{a}_2 = \underline{a}_1 + \underline{a}_2. \tag{9}$$

In order to formulate extensions of valuation operators we need the concept and the notation of *restriction* $\mathcal{L}|_H : H \to W$ of any linear mapping $\mathcal{L} : V \to W$ and subspace H of V (in our applications $V = \mathbb{R}^N$ and $W = \mathbb{R}$). Clearly

$$\mathcal{L} = \mathcal{L}|_{V_1} \oplus \mathcal{L}|_{V_2}$$

holds for any linear mapping $\mathcal{L} : V \to W$ and subspaces V_1, V_2 of V if $V = V_1 \oplus V_2$.

Corollary 5.3. If the vectors $\underline{a} \in \mathbb{R}^N$, $\underline{b} \in \mathbb{R}^M$ are determined by the arbitrary but disjoint sets of components $\{C_1, \ldots, C_N\}$ and $\{D_1, \ldots, D_M\}$ and by the (arbitrary) valuation operators $\mathcal{L}_1 : \mathbb{R}^N \to \mathbb{R}$, $\mathcal{L}_2 : \mathbb{R}^M \to \mathbb{R}$, which are restrictions of the same valuation operator $\mathcal{L} : \mathbb{R}^{N+M} \to \mathbb{R}$, then

$$\mathcal{L}(S) = \sum_{i=1}^{N} a_i \cdot s_i + \sum_{j=1}^{M} b_j \cdot s_{N+j} \tag{10}$$

holds for any structure $S = \sum_{i=1}^{N+M} s_i \cdot C_i \in \mathbb{R}^{N+M}$.

The above result allows us just to add the values of $\mathcal{L}(S_1)$ and $\mathcal{L}(S_2)$ to get the value of $\mathcal{L}(S)$ if $S = S_1 + S_2$ is *any* but disjoint partitioning (concerning the involved components) of the structure S. In other words, applying newer components (either atoms or species or reactions, etc.) we are allowed just only to extend our previous databases, the *linearity* of $\mathcal{L}$ ensures that *no* new data or computational methods are necessary.

6. Scalar products

We give here a brief summary of scalar products in any finite-dimensional linear space, revealing both the variety and boundary of them and also the connections among them. This helps us to find the exact role of the Euclidean scalar product we used in section 4 for a fixed base of the space. All notions and results can be found in any standard graduate level linear algebraic textbook.

First we have to clarify some notions.

Definition 6.1. The matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ is *symmetric* if $\mathbf{A}^{\mathrm{T}} = \mathbf{A}$, in other words $a_{i,j} = a_{j,i}$ for $i, j = 1, \dots, n$ where $a_{i,j}$ are the entries of $\mathbf{A}$.

For $i \leqslant n$ the ith *main subdeterminant* or *main minor* $\mathbf{d}_i \in \mathbb{R}$ of $\mathbf{A}$ is the determinant of the left-upper submatrix of size $i \times i$ of $\mathbf{A}$ formed by the first i many rows and columns of $\mathbf{A}$.

The matrix is *positive definite* iff all its main minors $d_1, \dots, d_n$ have the *same* sign (either all of them are positive or all of them are negative).

In what follows let V be any fixed finite dimensional linear space of dimension $n \in \mathbb{N}$ with any fixed base $B = \{b_1, \dots, b_n\} \subseteq V$. (No special role at all will possess in what follows the base we chose.) In what follows, we will not force any distinction of the vectors $\underline{u} \in V$ and their coordinates $[u_1, \dots, u_n]^{\mathrm{T}} \in \mathbb{R}^n$ with respect to the fixed base B.

Theorem 6.2. The mapping $\mathcal{A}: V \times V \to \mathbb{R}$,

$$\mathcal{A}(\underline{u}, \underline{v}) := \underline{u}^{\mathrm{T}}\mathbf{A}\underline{v} = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{i,j} \cdot u_i \cdot v_j$$

is bilinear for any matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$. $\mathcal{A}$ is symmetric if and only if $\mathbf{A}$ is symmetric. $\mathcal{A}$ is positive definite (i.e., $\mathcal{A}(\underline{u}, \underline{u}) > 0$ for $\underline{u} \in V$, $\underline{u} \neq \underline{0}$) if and only if $\mathbf{A}$ is positive definite.

The below two results together give a complete characterization of scalar products on any finite-dimensional vector space.

Corollary 6.3. The mapping $\mathcal{A}: V \times V \to \mathbb{R}$, $\mathcal{A}(\underline{u}, \underline{v}) = \underline{u}^{\mathrm{T}}\mathbf{A}\underline{v}$ is always a scalar product on V for any symmetric and positive definite matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$.

Theorem 6.4. For any scalar product $\mathcal{A}: V \times V \to \mathbb{R}$ there is a (unique) matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ such that $\mathcal{A}(\underline{u}, \underline{v}) = \underline{u}^{\mathrm{T}}\mathbf{A}\underline{v}$.

$\mathbf{A}$ clearly depends on the base $B \subseteq V$ of the space but there are simple formulae for transforming the above matrices of a fixed scalar product $\mathcal{A}$ in *any* different bases. Even special bases can easily be found by the below result.

Theorem 6.5 (Gram–Schmidt). For *any* scalar product $\mathcal{A}: V \times V \to \mathbb{R}$ in *any* finite dimensional linear space V there is a base $F = \{\underline{f}_1, \ldots, \underline{f}_n\} \subseteq V$ which elements are orthogonal to $\mathcal{A}$, i.e., $\mathcal{A}(\underline{f}_i, \underline{f}_j) = 0$ for $i \neq j$.

Corollary 6.6. If $\mathcal{A}$ and F are as in the above theorem then the matrix **A**, corresponding to $\mathcal{A}$ and F, is diagonal with positive entries, that is, for every $\underline{u}, \underline{v} \in V$ we have

$$\mathcal{A}(\underline{u}, \underline{v}) = \underline{u}^{\mathrm{T}} A \underline{v} = \sum_{i=1}^{n} a_{i,i} u_i v_i$$

where the coefficients $a_{i,i} \in \mathbb{R}$ are all positive.

The next (and last) result summarizes the connections among different *scalar products* on a given finite dimensional linear space: there is *no* difference at all among different scalar products on a fixed linear space V – from topological point of view, at least.

Theorem 6.7. For any two scalar products $\mathcal{A}, \mathcal{B}: V \times V \to \mathbb{R}$ there is an automorphism $\mathcal{I}: V \to V$ such that

$$\mathcal{A}(\underline{u}, \underline{v}) = \mathcal{B}\big(\mathcal{I}(\underline{u}), \mathcal{I}(\underline{v})\big)$$

holds for any vectors $\underline{u}, \underline{v} \in V$. Moreover, $\mathcal{I}$ is continuous with respect to the topologies induced by $\mathcal{A}$ and $\mathcal{B}$, i.e., $\mathcal{I}: (V, \mathcal{A}) \to (V, \mathcal{B})$ is a (topological) homeomorphism.

Our first application of the above result is to the Euclidean scalar product, of course. Theorem 6.7 says especially, among other, that any valuation operator can be measured in any measure unit, up to a scalar factor.

7. Conclusions

We presented a theoretical investigation and background for calculation methods already in use concerning valuation operators (increments/linear functionals/quantitative characteristics) in several fields of chemistry and physics.

As direct consequences we proved, e.g., that linear increments really can be computed as weighted sum of the increments of the components (see equation (3) in corollary 4.3), or we presented a one-sentence proof of Hess’ law in thermochemistry in (5), we gave estimates for the magnitude of $\mathcal{L}(S)$ in (8), etc.

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