Journal of Mathematical Chemistry 16 (1994) 93–114

Symmorphy transformations and operators in the repeat space $X_r(q)$ for additivity problems

Shigeru Arimoto [1] and Paul G. Mezey

Department of Chemistry, University of Saskatchewan, Saskatoon, Saskatchewan, Canada S7N OWO

Received 17 May 1993

A theoretical framework has been presented, which links two diverse molecular problems: the study of symmorphy transformations of molecular shape analysis (further developed in the present paper) and that of additivity of the zero-point vibrational energy of hydrocarbons and the total pi-electron energy of alternant hydrocarbons. The linkage, using fundamental tools of (general) topology and algebra, makes it possible to mutually introduce the methodologies used in fields hitherto separately investigated. By establishing this linkage, topological patterns described by symmorphy groups can be treated by the algebraic methods developed for the above additivity problems. The linkage also brings forth new techniques of topologizing the repeat space $X_r(q)$ for the additivity problems. Moreover, this connection paves the way to analyzing molecular homologous series and their properties by means of associating sequences of molecular structures with elements of a repeat space equipped with a topology.

1. Introduction

The recognition of pattern, shape, and form in the varieties of chemical structures is one of the fundamental cognitive processes in the investigation of molecular science and engineering.

Perceptual recognition of pattern, experience, and intuition have been, and will remain, vital forces to correlate and organize the wealth of chemical structures and phenomena. On the other hand, formal, algorithmic recognition of the morphological characteristics by means of a mathematical language is essential to develop a more universally applicable theory, to reach a deeper understanding of given structures and phenomena, and further, to gain an insight into the process of molecular recognition.

Although the modes of investigation corresponding with these two types of recognition are of importance on their own right, while complementing each other, the latter mode of research has a special advantage over the former, when a linkage between two or more morphological approaches comes into question. In particular, when the language of a mathematical structure (such as a topological space) is

[1] On leave from: Institute for Fundamental Chemistry, 34-4 Nishihiraki-cho, Takano, Sakyo-ku, Kyoto 606, Japan.

explicitly used, the latter can efficiently assess if there exists an interrelationship with another morphological approach that uses a similar mathematical structure, and in addition, if it is possible to mutually introduce the methodologies.

The main objective of the present paper is to establish a linkage between two molecular morphological studies, which originate in different regions of chemistry but exhibit noteworthy parallels both in the recognition of molecular structures and in the use of mathematical structures. Namely, we shall connect the theory of symmorphy transformations [1,2], reviewed and further developed in section 2, with the theory of polynomial operations for the additivity problems of hydrocarbons [3–7], briefly reviewed and linked in section 4 with the former theory.

Section 3 is devoted to preparing the linkage tools, which are closely related with the techniques in the theory of the quotient topological space [8–13] originated by Alexandroff [11,12], and Moore [13]. The linkage provides an interesting method of topologizing the repeat space $X_r(q)$ [3–7] which is a basic notion of the morphological approach to the additivity problem. The linkage also indicates that the category theoretical techniques of diagrams [14] are helpful: (i) in the study of symmorphy transformations, and, possibly, in the molecular morphological investigations [15–17] related to it, and (ii) in other researches [18] related to linear operators representing chemical network systems.

Diagrams of arrows that succinctly represent transformations acting on abstract spaces often serve as effective tools to reveal a linkage of mathematical theories. We shall use them frequently in the subsequent sections.

2. Symmorphy transformations

In this section, we review earlier results on symmorphy [1,2], and rephrase these results in a context suitable for the development of new results presented in sections 3 and 4.

We shall begin by reviewing symmorphy transformations [1,2] (which we rephrase in proposition 1 and in what follows thereafter). There are several equivalent methods of introducing this and related notions. Among them are algebraic, geometric, and operator theoretical methods. However, we shall here concentrate on an algebraic method using diagrams of arrows, which is most suitable for our later purpose of linking the two morphological studies mentioned in the previous section. By establishing this linkage, topological patterns described by symmorphy groups [1,2] can be treated by the algebraic methods with category theoretic techniques developed for the additivity problems [3–7]. The reader is referred to [14] and references therein for the notion of commutative diagrams and related category theoretic techniques, and to ref. [6] for their applications to the additivity problems. (In the present paper, however, the reader is not required to be familiar with the techniques of commutative diagrams. Since our argument frequently provides supplementary derivations in order to minimize the preliminaries for the techniques.)

Let $\mathbb{R}^3 = (\mathbb{R}^3, \|\cdot\|)$ denote the three-dimensional Euclidean space equipped with the usual norm $\|\cdot\|$, let $G = G(\mathbb{R}^3)$ denote the group of all homeomorphisms t: $\mathbb{R}^3 \to \mathbb{R}^3$, and let ρ: $\mathbb{R}^3 \to \mathbb{R}$ be an arbitrarily given function.

Consider the following diagram:

$$\begin{tikzcd} \mathbb{R}^3 \arrow[rr, "t"] \arrow[dr, "\rho"'] & & \mathbb{R}^3 \arrow[dl, "\rho"] \\ & \mathbb{R} & \end{tikzcd}$$

Diagram I

Define a subset $g_\rho \subset G$ by

$$g_\rho = \{t \in G\text{: Diagram I is commutative}\}. \tag{2.1}$$

Then, the following proposition, which rephrases the corresponding statements in refs. [1,2], is valid.

PROPOSITION 1

g_ρ forms a subgroup of G.

Proof

This is an immediate consequence from the fact that $t_1, t_2 \in g_\rho$ implies $t_1 t_2, t_1^{-1} \in g_\rho$, i.e., if $t_1, t_2 \in g_\rho$, then the above diagram with t being replaced either by $t_1 t_2$ or t_1^{-1} is commutative. □

An element t of group g_ρ was called a symmorphy transformation of ρ.

To recall the motivation for the terminology "symmorphy transformation", let us now consider the case in which ρ: $\mathbb{R}^3 \to \mathbb{R}$ denotes the molecular charge density function and visualize ρ by assigning a colour with magnitude $\rho(r)$ to each point $r \in \mathbb{R}^3$.

Recall the definition of g_ρ and note that a homeomorphism t: $\mathbb{R}^3 \to \mathbb{R}^3$ is an element of g_ρ if and only if

$$\rho(t(r)) = \rho(r) \tag{2.2}$$

for each $r \in \mathbb{R}^3$. From this, we can easily infer that the totality g_ρ of the symmorphy transformations of the molecular charge density function ρ coincides with the set of all homeomorphisms t: $\mathbb{R}^3 \to \mathbb{R}^3$ that keep the colour distribution of ρ, or the appearance of ρ, invariant.

Thus, g_ρ is a group whose elements are selected from the group G by the criterion of the invariance of the appearance of ρ.

However, g_ρ possesses excessive informations if the behavior of ρ is considered to be irrelevant on the outside (on the complement S^c) of a suitably prescribed subset S where the ρ maintains a conspicuous shape. This is usually the case.

For example, the unbounded region of $\mathbb{R}^3$ in which the molecular charge density function takes the values $\rho(r) \leqq \epsilon(\doteqdot 0)$ is of little significance for the morphological characterization of ρ and the molecule. To deal with this situation, one may divide $\mathbb{R}^3$ into two complementary parts, the relevant part S_ϵ and the irrelevant part S_ϵ^c for the morphology of the molecule:

$$\begin{aligned} \mathbb{R}^3 &= S_\epsilon \cup S_\epsilon^c , \\ &= \{r \in \mathbb{R}^3 \colon \rho(r) > \epsilon\} \cup \{r \in \mathbb{R}^3 \colon \rho(r) \leqq \epsilon\} , \end{aligned} \tag{2.3}$$

and construct a simplified group h_ρ using g_ρ and S_ϵ in the following manner.

Henceforth, we shall fix a relevant set $S \subset \mathbb{R}^3$ such that

$$t(S) \subset S \tag{2.4}$$

for all $t \in g_\rho$, i.e., such that $t(r) \in S$ for all $r \in S$ and $t \in g_\rho$.

The process of simplifying g_ρ consists of three steps:

First, introduce an equivalence relation m_ρ to the underlying set of the group g_ρ which is defined by

$$t_1 m_\rho t_2 \Leftrightarrow t_1|_S = t_2|_S , \tag{2.5}$$

where $t_i|_S$ denotes the restriction of the mapping t_i to the set S. The relation m_ρ is clearly reflexive, transitive, and symmetric, thus it is an equivalence relation.

Second, partition the underlying set of the group g_ρ by the above defined equivalence relation m_ρ. Each equivalence class is called a symmorphy class, and two elements in a symmorphy class are said to be symmorphic to each other.

Third, define the symmorphy group h_ρ as the quotient group of g_ρ with respect to the symmorphy equivalence:

$$h_\rho = g_\rho / (m_\rho \text{ equivalence relation}) , \tag{2.6}$$

where elements of h_ρ are symmorphy classes.

One can directly verify that the h_ρ is well defined, however, we shall indirectly check this after establishing the following

THEOREM 1

Let X and Y be non-empty sets, and let $\rho\colon X \to Y$ be an arbitrary given mapping. Denote by $B = B(X)$ the group of all bijections $t\colon X \to X$ with the group operation being the composite operation. Let $G = G(X)$ be a subgroup of $B = B(X)$.

Consider the following diagram

$$\begin{tikzcd} X \arrow[rr, "t"] \arrow[dr, "\rho"'] & & X \arrow[dl, "\rho"] \\ & Y & \end{tikzcd}$$

Diagram II

Define a subset $g_\rho \subset G$ by

$$g_\rho = \{t \in G\text{: diagram II is commutative}\}. \tag{2.7}$$

Let S denote a non-empty subset of E such that

$$t(S) \subset S \tag{2.8}$$

for all $t \in g_\rho$, and define a subset $g_{\rho 0}$ of g_ρ by

$$g_{\rho 0} = \{t \in g_\rho\colon t|_S = i_S\}, \tag{2.9}$$

where i_S denotes the inclusion mapping given by $i_S\colon S \ni r \mapsto r \in X$.

Then the following statements are true:

(i) g_ρ forms a subgroup of G.

(ii) $g_{\rho 0}$ forms a normal subgroup of g_ρ.

(iii) In the quotient group $h_\rho := g_\rho / g_{\rho 0}$, coset $[t_1] := t_1 g_{\rho 0}$ coincides with coset $[t_2] := t_2 g_{\rho 0}$ if and only if $t_1|_S = t_2|_S$, i.e.,

$$[t_1] = [t_2] \Leftrightarrow t_1|_S = t_2|_S \tag{2.10}$$

for all $t_1, t_2 \in g_\rho$.

Proof

(i) The proof of part (i) is analogous with that of proposition 1. One easily verifies that g_ρ is closed under the group operation and the inverse operation $(\cdot)^{-1}$. Thus, g_ρ is a subgroup of G.

(ii) $g_{\rho 0}$ clearly forms a subgroup of g_ρ. Hence, it remains to show that $g_{\rho 0}$ is normal. Recall the well-known fact that a subgroup g_0 of a group g is normal if and only if

$$t^{-1} t_0 t \in g_0 \tag{2.11}$$

for all $t_0 \in g_0$ and $t \in g$.

Let $t_0 \in g_{\rho 0}$ and $t \in g_\rho$ be arbitrary.

Then, for each $r \in S$, we have

$$\begin{aligned}(t^{-1} t_0 t)(r) &= t^{-1}(t_0(t(r))) \\ &= t^{-1}(t(r)) \\ &= r\end{aligned} \tag{2.12}$$

by (2.8) and the definition of $g_{\rho 0}$, so that

$$(t^{-1} t_0 t)|_S = i_S. \tag{2.13}$$

From this the conclusion follows.

(iii) By the definition of $[t_1]$, $[t_2]$, and $g_{\rho 0}$, one gets the following necessary and sufficient conditions for $[t_1] = [t_2]$:

$$[t_1] = [t_2] \Leftrightarrow t_1^{-1} t_2 \in g_{\rho 0}$$
$$\Leftrightarrow (t_1^{-1} t_2)|_S = i_S\,. \tag{2.14}$$

Thus, to prove (iii), it suffices to show that

$$(t_1^{-1} t_2)|_S = i_S \Leftrightarrow t_1|_S = t_2|_S \tag{2.15}$$

for all $t_1, t_2 \in g_\rho$.

($\Rightarrow$): Let $r \in S$ be arbitrary, then

$$(t_1^{-1} t_2)(r) = r\,. \tag{2.16}$$

Operating t_1 to both sides, one obtains

$$t_2(r) = t_1(r)\,, \tag{2.17}$$

which implies that

$$t_1|_S = t_2|_S\,. \tag{2.18}$$

($\Leftarrow$): Let $r \in S$ be arbitrary, then

$$\begin{aligned}(t_1^{-1} t_2)(r) &= t_1^{-1}(t_2(r))\\ &= t_1^{-1}(t_1(r))\\ &= r\,,\end{aligned} \tag{2.19}$$

hence, it follows that

$$(t_1^{-1} t_2)|_S = i_S\,. \tag{2.20}$$

This completes the proof. □

In theorem 1, put $X = (\mathbb{R}^3, \|\cdot\|)$, $Y = \mathbb{R}$, and let $G \subset B(X)$ be the subgroup of all homeomorphisms t: $X \to X$. Then, part (iii) of theorem 1 implies that the symmorphy group h_ρ given by eq. (2.6) is meaningful; moreover, the h_ρ can be alternatively defined by

$$h_\rho = g_\rho / g_{\rho 0}\,. \tag{2.21}$$

Suppose ρ: $\mathbb{R}^3 \to \mathbb{R}$ is a molecular charge density function having symmetry elements. Then, g_ρ contains the corresponding symmetry operations, together with other operations such as nonlinear stretchings, warpings, and distortions of the space that preserve the appearance of ρ invariant. We remark that if one replaces G with the subgroup $G_0 \subset G$ of all isometric transformations t: $\mathbb{R}^3 \to \mathbb{R}^3$ (or a suitable subgroup $G_{00} \subset G_0$), then one obtains a group $g_\rho = g_\rho(G_0)$ which is a descriptor of the symmetry of ρ.

Under the hypotheses of theorem 1 together with extra assumptions that
(i) X is a topological space,
(ii) $G \subset B(X)$ is the subgroup consisting of all homeomorphisms t: $X \to X$,
all the conclusions of theorem 1 are, of course, valid. Thus, we can generalize the

notion of the symmorphy transformation and its related notions to those in more comprehensive situations where X is not necessarily a Euclidean space but a topological space.

We shall transfer all terminologies related with the symmorphy transformation, from the special case to a general case. Suppose that the hypotheses of theorem 1 and the above stated extra assumptions (i), and (ii) are fulfilled.

(I) The group g_ρ is called the *symmorphy transformation group of* ρ. Each element $t \in g_\rho$ is called a *symmorphy transformation of* ρ.

(II) The equivalence relation m_ρ defined on g_ρ by either of the following

$$(i)\ t_1 m_\rho t_2 \Leftrightarrow t_1|_S = t_2|_S\,, \tag{2.22}$$

$$(ii)\ t_1 m_\rho t_2 \Leftrightarrow t_1 g_{\rho 0} = t_2 g_{\rho 0}\,, \tag{2.23}$$

is called *symmorph*.

(III) The equivalence classes constructed by m_ρ, i.e., the left cosets $tg_{\rho 0}(= g_{\rho 0}t)$ with $t \in g_\rho$ are called *symmorphy classes*.

(IV) Two elements t_1 and t_2 in the same symmorphy class are called *symmorphic* to each other.

(V) The quotient group $h_\rho = g_\rho / g_{\rho 0}$ is called the *symmorphy (quotient) group of* ρ.

Now we return to theorem 1, and under the assumptions of this theorem, we shall construct an auxiliary group h_ρ^*. The group h_ρ^* is a faithful representation of h_ρ (i.e., isomorphic to h_ρ) and is helpful to clarify the structures of the groups $g_\rho, g_{\rho 0}$, and h_ρ.

To introduce h_ρ^*, we need some preparation.

First, let us consider the canonical homomorphism ϕ: $g_\rho \to g_\rho / g_{\rho 0} = h_\rho$ defined by

$$\phi(t) = tg_{\rho 0}\,. \tag{2.24}$$

The mapping ϕ sends each $t \in g_\rho$ to the equivalence class $[t] = tg_{\rho 0}$ to which it belongs.

Second, we need

PROPOSITION 2

Assume all the hypotheses of theorem 1. Then the following statements are true:

(i) $t|_S$: $S \to X$ is an injection for all $t \in g_\rho$.

(ii) The range of $t|_S$ is S for all $t \in g_\rho$, i.e.,

$$t(S) = S \tag{2.25}$$

for all $t \in g_\rho$.

Proof

(i) By the definition of g_ρ, all $t \in g_\rho$ are injections from which the conclusion evidently follows.

(ii) By the assumed property (2.8) of S, we have only to show that

$$t(S) \supset S \tag{2.26}$$

for all $t \in g_\rho$. But this is clearly true since $r \in S$ implies that $t^{-1}(r) \in S$ by (2.8) and $t(t^{-1}(r)) = r$, so that $r \in t(S)$. □

Third, let $B(S)$ denote the group of all bijections t: $S \to S$. Define a mapping ω: $g_\rho \to B(S)$ by

$$\omega(t) = t| \,, \tag{2.27}$$

where $t|$ denotes an element of $B(S)$ given by

$$t|(r) = t|_S(r) \,, \tag{2.28}$$

$r \in S$. For any $t \in g_\rho$, $t|$ is indeed a bijection from S onto itself by proposition 2, thus, the above mapping ω is well defined.

Finally, we can give the definitions of h_ρ^* and a related notion $g_{\rho 0}^*$.

We define $h_\rho^* \subset B(S)$ to be the image of ω:

$$h_\rho^* = \mathrm{Im}(\omega) = \omega(g_\rho) \,, \tag{2.29}$$

and define $g_{\rho 0}^*$ to be the kernel of ω:

$$g_{\rho 0}^* = \mathrm{Ker}(\omega) = \omega^{-1}(\mathrm{id}_S) \,, \tag{2.30}$$

where $\mathrm{id}_S \in B(S)$ denotes the identity element of the group $B(S)$, i.e., the mapping id_S: $S \ni r \mapsto r \in S$.

Now we are ready to give a theorem which illuminates the structures of $g_\rho, g_{\rho 0}$, and h_ρ.

THEOREM 2

Assume all the hypothesis of theorem 1, and let ϕ, ω, h_ρ^*, and $g_{\rho 0}^*$ be as above. Then the following statements are true:

(i) ω: $g_\rho \to B(S)$ is a homomorphism, i.e.,

$$\omega(t_1 t_2) = \omega(t_1)\omega(t_2) \tag{2.31}$$

holds for all $t_1, t_2 \in g_\rho$.

(ii) h_ρ^* is a subgroup of $B(S)$.

(iii) $g_{\rho 0}^*$ is a normal subgroup of g_ρ.

(iv) $g_{\rho 0}^* = g_{\rho 0}$. (2.32)

(v) h_ρ^* is isomorphic to h_ρ.

Proof

(i) Let $t_1, t_2 \in g_\rho$ and $r \in S$ be arbitrary. Then by the definition of ω, we see that

$$\begin{aligned}(\omega(t_1t_2))(r) &= (t_1t_2)|(r)\\ &= (t_1t_2)|_S(r)\\ &= t_1(t_2(r))\,.\end{aligned} \tag{2.33}$$

On the other hand, by the definition of ω and proposition 2,

$$\begin{aligned}(\omega(t_1)\omega(t_2))(r) &= (t_1|t_2|)(r)\\ &= t_1|(t_2|(r))\\ &= t_1|_S(t_2|_S(r))\\ &= t_1(t_2(r))\,.\end{aligned} \tag{2.34}$$

From eq. (2.33) and eq. (2.34), the conclusion of (i) follows immediately.

(ii) By definition (2.29) and (i) above, h_ρ^* is the image of the group homomorphism ω: $g_\rho \to B(S)$, this h_ρ^* is clearly a subgroup of the group $B(S)$.

(iii) By definition (2.30) and (i) above, $g_{\rho 0}^*$ is the kernel of the group homomorphism ω: $g_\rho \to B(S)$, thus $g_{\rho 0}^*$ is clearly a normal subgroup of the group g_ρ.

(iv) Straight from the definitions of $g_{\rho 0}$, ω, and $g_{\rho 0}^*$, we have

$$\begin{aligned}g_{\rho 0} &= \{t \in g_\rho\colon t|_S = i_S\}\\ &= \{t \in g_\rho\colon t| = \mathrm{id}_S\}\\ &= \{t \in g_\rho\colon \omega(t) = \mathrm{id}_S\}\\ &= \omega^{-1}(\mathrm{id}_S)\\ &= g_{\rho 0}^*\,.\end{aligned} \tag{2.35}$$

(v) Recall the well-known fundamental theorem of group homomorphism, the First Isomorphism Theorem, which implies that if ω: $g \to h$ is a surjective homomorphism of groups, and ϕ: $g \to g/\mathrm{Ker}(\omega)$ is the canonical homomorphism of g onto the quotient group $g/\mathrm{Ker}(\omega)$, then there exists an isomorphism $\bar{\omega}$: $g/\mathrm{Ker}(\omega) \to h$ such that the following diagram commutes:

$$\begin{tikzcd} g \arrow[r, "\phi"] \arrow[d, "\omega"'] & g/\mathrm{Ker}(\omega) \arrow[dl, "\bar{\omega}"] \\ h & \end{tikzcd}$$

Diagram III

Thus, we see that

$$\begin{aligned}h_\rho^* \cong g_\rho/\mathrm{Ker}(\omega) &= g_\rho/g_{\rho 0}^*\\ &= g_\rho/g_{\rho 0} \quad \text{[by (iv)]}\\ &= h_\rho\,.\end{aligned} \tag{2.36}$$

This completes the proof. □

We remark that parts (iii) and (iv) provide another proof of the fact that $g_{\rho 0}$ is a normal subgroup of g_ρ (see theorem 1, part (ii)).

The technique of constructing a quotient structure, such as a quotient group above, through suitable classification and identification of elements in a mathematical structure is among fundamental weaponries in abstract algebra and topology.

In the next section, we shall make use of the well-known notions and techniques in topology, especially those related to the theory of quotient topological space [8–11] for the linkage of molecular morphological studies mentioned in section 1.

3. Preparation of linkage tools

The present section provides three propositions with which to link the aforementioned molecular morphological studies. Both studies involve molecular patterns and the transformations which act upon them and are associated with a topological space, either directly (symmorphy transformations) or indirectly (polynomial operations for additivity problems). This observation is an initial important step for the linkage, which removes a barrier between fields hitherto separately investigated and provides a fresh and deeper insight into both.

For the purpose of the linkage of the theories, we shall consider here abstractly a special topological space (X, τ_κ), and continuous transformations defined on it. In section 4, we shall see that this setting is general enough to embrace fundamental spaces and transformations in both theories. In the present section, we solely concentrate on preparing the linkage tools and postpone till the next section, the explanations as to how these tools are used for our objective.

Let X be a non-empty set equipped with an equivalence relation $\sim$, let $[x]$ denote the equivalence class that contains $x \in X$, let Y denote the set of all equivalence classes on X. Let κ: $X \twoheadrightarrow Y$ denote the canonical mapping defined by

$$\kappa(x) = [x] . \tag{3.1}$$

We shall endow a topology τ_κ to the set X by defining the following closure operator $^-$: $2^X \to 2^X$, (where 2^X denotes the set of all subsets of X, i.e., the power set of X):

$$\bar{A} = \kappa^{-1}(\kappa(A)) , \tag{3.2}$$

$A \in 2^X$.

It is easy to show that the operator $^-$ satisfies the Kuratowski closure axioms [8–10].

PROPOSITION 3

The following relations hold for any $A, B \in 2^X$.

(i) $\bar{\phi} = \phi$. (3.3)

(ii) $A \subset \bar{A}$. (3.4)

(iii) $\bar{\bar{A}} = \bar{A}$. (3.5)

(iv) $\overline{A \cup B} = \bar{A} \cup \bar{B}$. (3.6)

Proof

First, we shall list up some basic facts of the image $f(A)$ and the inverse image $f^{-1}(B)$ of subsets under a mapping f.

Let E, F denote non-empty sets, and let $f\colon E \to F$ be a mapping. Let $A_1, A_2 \in 2^E$, and $B_1, B_2 \in 2^F$ be arbitrary. Then the following relations are valid:

(I) $f(\phi) = \phi, f^{-1}(\phi) = \phi$, (3.7)

(II) $f^{-1}(f(A_1)) \supset A_1$, (3.8)

(III) $f(f^{-1}(B_1)) \subset B_1$, (3.9)

(IV) $f(A_1 \cup A_2) = f(A_1) \cup f(A_2)$, (3.10)

$f^{-1}(B_1 \cup B_2) = f^{-1}(B_1) \cup f^{-1}(B_2)$, (3.11)

(V) $A_1 \subset A_2 \Rightarrow f(A_1) \subset f(A_2)$. (3.12)

Now the proofs of (i), (ii), and (iv) directly follow respectively from (I), (II), and (IV) above.

Thus, it remains to prove (iii). By the definition of the closure operator, the left-hand side of (iii) is expressed by

$$\bar{\bar{A}} = \kappa^{-1}(\kappa(\kappa^{-1}(\kappa(A)))). \tag{3.13}$$

Hence, to prove (iii), it suffices to show that

$$\kappa(\kappa^{-1}(\kappa(A))) = \kappa(A). \tag{3.14}$$

But, one easily verifies that (ii) and (V) imply

$$\kappa(\kappa^{-1}(\kappa(A))) \supset \kappa(A), \tag{3.15}$$

and (III) implies

$$\kappa(\kappa^{-1}(\kappa(A))) \subset \kappa(A), \tag{3.16}$$

so that eq. (3.14) holds. □

Thus, the topological space $X = (X, \tau_\kappa)$, with the closure operator $^-$, is well defined by the well-known theorem of Kuratowski [8–10], and any subset $A \in 2^X$ is called closed if and only if $\bar{A} = A$, and any subset $B \in 2^X$ is called open if and only if its complement B^c is closed.

Note that κ: $X \twoheadrightarrow Y$ is a surjection by the definition of κ, and that if κ is a bijection, then every subset of X is closed and open at the same time, i.e., X is a discrete space.

Also, note that the relation

$$\begin{aligned}\overline{\{x\}} &= \kappa^{-1}(\kappa(\{x\})) \\ &= \kappa^{-1}(\{[x]\}) \\ &= [x]\end{aligned} \tag{3.17}$$

holds for all $x \in X$, i.e., the equivalence class $[x]$ containing x is precisely the closure of the singleton set $\{x\}$ for all $x \in X$.

Thus, bearing in mind that every singleton set in a Hausdorff space is closed, we see that X is, in general, not a Hausdorff space. More precisely, X is a Hausdorff space if and only if κ is a bijection, i.e., if and only if the family of equivalent classes of X coincides with the set X.

REMARK

The topology τ_κ may be alternatively defined to be the weakest topology of X that makes κ: $X \twoheadrightarrow (Y, \tau_d)$ continuous, where τ_d denotes the discrete topology of Y. This is a dual form of the typical argument in the theory of quotient topological space originated by Alexandroff [11,12] and Moore [13]. For practical reasons, however, we used in this section Kuratowski's closure operator and the associated techniques [9] to prepare the linkage tools.

Now we shall define three types of transformations of $X = (X, \tau_\kappa)$; a class preserving transformation, a class permuting transformation, and a class invariant transformation, which will be central in what follows.

First, consider the family X^X of all mappings of X into itself. The X^X obviously forms a semigroup with the composite operation. Next consider three subsemigroups of X^X:

$$\mathcal{G}_0(X, \tau_\kappa) \subset \mathcal{G}(X, \tau_\kappa) \subset \mathcal{G}_1(X, \tau_\kappa), \tag{3.18}$$

where

(i) $\mathcal{G}_1(X, \tau_\kappa)$ denotes the semigroup of all continuous mappings of (X, τ_κ) into itself,

(ii) $\mathcal{G}(X, \tau_\kappa)$ denotes the group of all homeomorphisms of (X, τ_κ) onto itself, and

(iii) $\mathcal{G}_0(X, \tau_\kappa)$ denotes the subgroup of $\mathcal{G}(X, \tau_\kappa)$ of all mappings $t \in \mathcal{G}(X, \tau_\kappa)$, satisfying the condition

$$\overline{\{t(x)\}} = \overline{\{x\}} \tag{3.19}$$

for all $x \in (X, \tau_\kappa)$.

We shall refer to an element of $\mathcal{G}_0(X, \tau_\kappa)$, $\mathcal{G}(X, \tau_\kappa)$, and $\mathcal{G}_1(X, \tau_\kappa)$, respectively, as a class invariant transformation, a class permuting transformation, and a class preserving transformation. The motivation of this terminology will be clear in what follows.

PROPOSITION 4

Let X, κ, τ_κ, and Y be as above. Let t be a mapping of the topological space $X = (X, \tau_\kappa)$ into itself. Consider the following diagram:

$$\begin{tikzcd} X \arrow[r, "t"] \arrow[d, "\kappa"'] & X \arrow[d, "\kappa"] \\ Y \arrow[r, "u"'] & Y \end{tikzcd}$$

Diagram IV

Then the following statements are true:

(i) The mapping t is continuous if and only if there exists a mapping u such that diagram IV is commutative.

(ii) The mapping t is a homeomorphism if and only if t is a bijection and there exists a bijection u such that diagram IV is commutative.

(iii) The mapping t is a homeomorphism and satisfies the condition (3.19) for all $x \in X$ if and only if t is a bijection and diagram IV with $u = \mathrm{id}_Y$ is commutative.

Proof

(i) Suppose that there exists a mapping u such that diagram IV is commutative. Let $A \in 2^X$ be arbitrary. Then, one straightforwardly obtains the relation

$$\begin{aligned} t(\bar{A}) \subset \overline{t(\bar{A})} &= \kappa^{-1}(\kappa(t(\kappa^{-1}(\kappa(A))))) \\ &= \kappa^{-1}(u(\kappa(\kappa^{-1}(\kappa(A))))) \\ &= \kappa^{-1}(u(\kappa(A))) \quad [\text{recall } (3.14)] \\ &= \kappa^{-1}(\kappa(t(A))) \\ &= \overline{t(A)}, \end{aligned} \tag{3.20}$$

which shows that t is continuous.

Conversely, suppose that t is continuous. We claim that the image $t([x])$ of equivalence class $[x]$ is contained in equivalence class $[t(x)]$ for all $x \in X$. In fact, recalling (3.17), by the continuity of t, we have

$$t([x]) = t(\overline{\{x\}}) \subset \overline{t(\{x\})} = [t(x)] \tag{3.21}$$

for all $x \in X$. Therefore, if one defines u: $Y \to Y$ such that

$$\{u(y)\} = \kappa(t(\kappa^{-1}(\{y\}))), \tag{3.22}$$

then diagram IV is obviously commutative.

(ii) Suppose that t is a bijection and there exists a bijection u such that diagram IV is commutative. Then it is readily verifiable that diagram IV, with t and u replaced by t^{-1} and u^{-1}, respectively, is also commutative. Thus, by (i), both t and t^{-1} are continuous, therefore t is a homeomorphism.

Conversely, assume that t is a homeomorphism, i.e., t is a bijection such that both t and t^{-1} are continuous. Again using (i), we see that there are mappings u, v: $Y \to Y$, such that the central rectangular part, and the left and right rectangular parts of diagram V are commutative.

$$\begin{tikzcd}
X \arrow[r, "t^{-1}"] \arrow[d, "\kappa"'] & X \arrow[r, "t"] \arrow[d, "\kappa"] & X \arrow[r, "t^{-1}"] \arrow[d, "\kappa"'] & X \arrow[d, "\kappa"] \\
Y \arrow[r, "v"'] & Y \arrow[r, "u"'] & Y \arrow[r, "v"'] & Y
\end{tikzcd}$$

Diagram V

Note that diagram V itself is commutative. Hence, one easily sees that

$$u \circ v(\kappa(x)) = \kappa(x), \tag{3.23}$$

$$v \circ u(\kappa(x)) = \kappa(x), \tag{3.24}$$

holds for all $x \in X$. But κ was a surjection of X onto Y. Thus, we have

$$u \circ v = v \circ u = \mathrm{id}_Y, \tag{3.25}$$

showing that u is a bijection. Therefore, t is a bijection and there exists a bijection u such that diagram IV is commutative.

(iii) Suppose that t is a bijection and diagram IV with $u = \mathrm{id}_Y$ is commutative. Then we have

$$\kappa \circ t = \kappa, \tag{3.26}$$

hence

$$\kappa^{-1}(\kappa(\{t(x)\})) = \kappa^{-1}(\kappa(\{x\})) \tag{3.27}$$

for all $x \in X$. Recalling the definition of the closure operator, it follows that the condition (3.19) is fulfilled for all $x \in X$. On the other hand, by (ii), t is clearly a homeomorphism.

Conversely, assume that t is a homeomorphism and satisfies the condition (3.19) for all $x \in X$. Then t is obviously a bijection and

$$\kappa(\kappa^{-1}(\kappa(\{t(x)\}))) = \kappa(\kappa^{-1}(\kappa(\{x\}))) \tag{3.28}$$

holds for all $x \in X$, from which eq. (3.26) follows by using eq. (3.14). Thus, t is a bijection and diagram IV with $u = \mathrm{id}_Y$ is commutative. □

Thus, recalling the definitions of a class invariant transformation, a class permuting transformation, and a class preserving transformation, from proposition 4 one easily obtains the following proposition, a sketchy proof of which is given below.

PROPOSITION 5

Let X, κ, τ_κ, and Y be as above. Let t be a mapping of the topological space $X = (X, \tau_\kappa)$ into itself. Consider the following statements:

(i)′ t is a class preserving transformation.

(i)″ For any equivalence class C of X,

$$t(C) \subset C' \tag{3.29}$$

holds for some equivalence class C' of X.

(ii)′ t is a class permuting transformation.

(ii)″ t is a bijection, moreover for any equivalence class C of X,

$$t(C) = C' \tag{3.30}$$

holds for some equivalence class C' of X.

(iii)′ t is a class invariant transformation,

(iii)″ t is a bijection, moreover for any equivalence class C of X,

$$t(C) = C \tag{3.31}$$

holds.

Then the following relations are valid:

(a) (i)′ $\Leftrightarrow$ (i)″,

(b) (ii)′ $\Leftrightarrow$ (ii)″,

(c) (iii)′ $\Leftrightarrow$ (iii)″.

Proof of proposition 5

(a) Note that for any equivalence class C of X, $t(C) \subset C'$ holds for some equivalence class C' of X if and only if there exists a mapping u such that diagram IV in proposition 4 is commutative. The assertion of part (a) follows from the definition of the class preserving transformation and part (i) of proposition 4.

(b) We first verify that (ii)″ is true if and only if the following statement (#) is true.

(#): t is a bijection, moreover t and t^{-1} are both class preserving transformations.

It then remains to prove that (#) $\Leftrightarrow$ (ii)′. But, by the definition of the class permuting transformation and the class preserving transformation, one easily infers that (#) is true if and only if (ii)′ is true.

(c) Note that t is a bijection and $t(C) = C$ for any equivalence class C of X if and only if t is a bijection and diagram V with $u = \mathrm{id}_Y$ is commutative. The assertion of part (c) follows from the definition of the class invariant transformation and part (iii) of proposition 4. □

4. Symmorphy transformations, class preserving transformations, and polynomial operations in the repeat space

In the previous section, we introduced the following three families of transformations:

$$\begin{aligned} &\{\text{class invariant transformations}\} = \mathcal{G}_0(X, \tau_\kappa) \\ \subset &\{\text{class permuting transformations}\} = \mathcal{G}(X, \tau_\kappa) \\ \subset &\{\text{class preserving transformations}\} = \mathcal{G}_1(X, \tau_\kappa), \end{aligned} \tag{4.1}$$

without referring to the notion of symmorphy transformation. Let us now focus attention to the relation between the notion of the symmorphy transformation and that of the class invariant transformation.

The domain of X of the symmorphy transformation $t \in g_\rho(G(X, \tau))$ with ρ: $X \to Y$ does not intrinsically involve any equivalence relation. However, one can introduce a natural equivalence relation $\sim$ to X, by partitioning X into the "contour-surfaces" C, i.e., inverse images of singleton sets $\{y\}$ of Y under ρ:

$$C = \rho^{-1}(\{y\}). \tag{4.2}$$

It is easy to check that the relation $\sim$ defined by

$$\begin{aligned} x_1 \sim x_2 &\Leftrightarrow \exists y \in Y \text{ such that } x_1, x_2 \in \rho^{-1}(\{y\}) \\ &\Leftrightarrow \rho(x_1) = \rho(x_2) \end{aligned} \tag{4.3}$$

is an equivalence relation. (In the case where ρ denotes a molecular charge density function, the equivalence classes C given by (4.2) are isodensity contour surfaces.)

Let κ be the canonical mapping associated with $\sim$. Then, by the definition of the symmorphy transformations, for any equivalence class C in X induced by the above $\sim$ or κ, $t \in g_\rho(G(X, \tau))$ implies that $t(C) = C$. (Indeed, $t \in g_\rho(G(X, \tau))$ clearly implies that $t(C) \subset C$ by the definition of $g_\rho(G(X, \tau))$. On the other hand, for any $r \in C$, we have $t^{-1}(r) \in C$. Therefore, bearing in mind that t sends $t^{-1}(r) \in C$ to r, we see that the image of any "contour surface" C under $t \in g_\rho(G(X, \tau))$ is the C itself.)

Now recalling the definition of $\mathcal{G}_0(X, \tau_\kappa)$, and proposition 5, (c), we obtain the relation:

$$g_\rho(G(X, \tau)) \subset \mathcal{G}_0(X, \tau_\kappa). \tag{4.4}$$

Thus, the symmorphy transformation group is a subgroup of a group of class invariant transformations, and $g_\rho(G(X,\tau))$ can be located as a substructure of the semigroup $\mathcal{G}_1(X,\tau_\kappa)$ of class preserving transformations.

On the other hand, it should be noted that $\mathcal{G}_0(X,\tau_\kappa)$ can be expressed using the notion of the symmorphy transformation group:

$$\mathcal{G}_0(X,\tau_\kappa) = g_\kappa(G(X,\tau_d))\,, \tag{4.5}$$

where τ_d denotes the discrete topology, and $G(X,\tau_d)$ denotes the group of all homeomorphisms of (X,τ_d) onto itself, i.e., the group of all bijections of X onto itself. (equation (4.5) immediately follows from the definition of $\mathcal{G}_0(X,\tau_\kappa)$ and proposition 4, (iii).)

We are now in the position to recall a morphological approach developed in the studies of the additivity problems of the zero-point vibrational energy of hydrocarbons and the total pi-electron energy of alternant hydrocarbons. The reader is referred to refs. [3–7] for the definitions of the repeat space $X_r(q)$, the alpha space $X_\alpha(q)$, the beta space $X_\beta(q)$, the f space $H_f(q)$, and the motivations of constructing these spaces.

The morphological approach to the above additivity problems involves transformations $\hat{\varphi}$ of the infinite dimensional linear space $X(q)$ of all $qN \times qN$ real matrix sequences $\{M_N\}$ $(N = 1, 2, \ldots)$, where q is a fixed positive integer. More explicitly, the transformation $\hat{\varphi}$: $X(q) \to X(q)$ associated with polynomial $\varphi = c_0 t^0 + c_1 t^1 + \ldots + c_n t^n$ was defined by

$$\hat{\varphi}(\{M_N\}) = \{c_0 M_N^0 + c_1 M_N^1 + \ldots + c_n M_N^n\}\,, \tag{4.6}$$

and $\hat{\varphi}$ was called the polynomial operation associated with polynomial φ.

The repeat space $X_r(q)$ with which molecular structures of homologous series are associated is a subspace of $X(q)$, and $X_r(q)$ is closed under any polynomial operation:

$$\hat{\varphi}(X_r(q)) \subset X_r(q)\,. \tag{4.7}$$

In other words, the repeating pattern which characterizes the elements of the repeat space is invariant under any given polynomial operation.

To make an integral representation α^{int} [5] of a fundamental functional α defined (on a suitable real normed space) by

$$\alpha(\varphi) = \lim_{N\to\infty} [\mathrm{Tr}\ \varphi(M_N)]/N\,, \tag{4.8}$$

we introduced the notion of the f space $H_f(q)$, the polynomial operations $\hat{\varphi}'$ which acts on $H_f(q)$, and the mapping Ω: $X_r(q) \to H_f(q)$ defined by

$$\Omega\left(\left\{\sum_{n=-v}^{v} P_N^n \otimes Q_n\right\} + (\text{an element of } X_\beta(q))\right)(\theta) = \sum_{n=-v}^{v} \exp(in\theta)Q_n\,. \tag{4.9}$$

The Ω is a linear mapping such that the following diagram commutes for any pair of polynomial operations $\hat{\varphi}$ and $\hat{\varphi}'$ (cf. theorem II of [5]).

$$\begin{array}{ccc} X_r(q) & \xrightarrow{\hat{\varphi}} & X_r(q) \\ \Omega \downarrow & & \downarrow \Omega \\ H_f(q) & \xrightarrow[\hat{\varphi}']{} & H_f(q) \end{array}$$

Diagram VI

The commutability of the above diagram was a key step in the "approach via the aspect of form" to construct the integral representation α^{int} of the functional α. Using the relation $\Omega\hat{\varphi} = \hat{\varphi}'\Omega$ and some results from the "approach via general topology", we obtained the desired integral representation,

$$\alpha^{\text{int}}(\varphi) = (1/(2\pi)) \int_{-\pi}^{\pi} \operatorname{Tr} \varphi(F(\theta))\, \mathrm{d}\theta\,, \tag{4.10}$$

where $F = \Omega(\{M_N\})$ (cf. [5] for the domain of α^{int}, and the detailed arguments on α^{int}).

Now we wish to have the following theorem which implies that every polynomial operation $\hat{\varphi}$ is a class preserving transformations: $\hat{\varphi} \in \mathcal{G}_1$, as is each symmorphy transformation $t \in g_\rho(G(X,\tau)) \subset \mathcal{G}_0 \subset \mathcal{G} \subset \mathcal{G}_1$. The proof of the theorem makes use of the thought process in the proof of theorem 2 (in the theory of the symmorphy transformations), the above commutative diagram VI, and one of the linkage tools, proposition 4 in the previous section.

THEOREM 3

Let $X_r(q)/X_\beta(q)$ denote the quotient linear space of the repeat space $X_r(q)$ by the beta space $X_\beta(q)$ with block size q. Let κ: $X_r(q) \to X_r(q)/X_\beta(q)$ denote the canonical mapping defined by

$$\kappa(\{M_N\}) = \{M_N\} + X_\beta(q)\,, \tag{4.11}$$

and let τ_κ denote the topology on $X_r(q)$ given by the closure operation, $\bar{A} = \kappa^{-1}(\kappa(A))$, where A is any subset of $X_r(q)$. Let $H_f(q)$ denote the f space with size q, and let Ω: $X_r(q) \to H_f(q)$ denote the surjective linear mapping given by (4.9). Then, we have

(i) $\operatorname{Ker}(\Omega) = X_\beta(q)$,

(ii) $X_r(q)/X_\beta(q)$ is isomorphic to $H_f(q)$,

(iii) Any polynomial operation $\hat{\varphi}$: $(X_r(q), \tau_\kappa) \to (X_r(q), \tau_\kappa)$ is continuous, (i.e., $\hat{\varphi}$ is a class preserving transformation).

Proof

(i) By the definition of the mapping Ω,

$$\begin{aligned}\mathrm{Ker}(\Omega) &= \{\{M_N\} \in X_r(q)\colon \Omega(\{M_N\}) = 0_f\}\\ &= \{\{M_N\} \in X_r(q)\colon \{M_N\} = 0_\alpha + (\text{an element of } X_\beta(q))\}\\ &= X_\beta(q)\,, \end{aligned} \tag{4.12}$$

where 0_f and 0_α denote, respectively, the zero element of $H_f(q)$ and $X_\alpha(q)$.

(ii) The proof is analogous to that of theorem 2, (v): By the well-known theorem of linear mapping, which is similar to the First Isomorphism Theorem of Groups, there is a linear isomorphism $\bar{\Omega}$: $X_r(q)/X_\beta(q) \to H_f(q)$ such that the following diagram VII is commutative:

$$\begin{tikzcd} X_r(q) \arrow[r, "\kappa"] \arrow[d, "\Omega"'] & X_r(q)/\mathrm{Ker}(\Omega) \arrow[dl, "\bar{\Omega}"] \\ H_f(q) & \end{tikzcd}$$

Diagram VII

But by (i), we know that $\mathrm{Ker}(\Omega) = X_\beta(q)$. Thus, the linear space $X_r(q)/X_\beta(q)$ is isomorphic to the linear space $H_f(q)$.

(iii) Let $\hat{\varphi}'$ denote the polynomial operation on $H_f(q)$ which is associated with the polynomial φ. Consider the following commutative diagram, which is made by combining diagram VI and two copies of diagram VII:

$$\begin{tikzcd} X_r(q) \arrow[rrr, "\hat{\varphi}"] \arrow[dr, "\kappa"] \arrow[dd, "\Omega"'] & & & X_r(q) \arrow[dl, "\kappa"'] \arrow[dd, "\Omega"] \\ & X_r(q)/X_\beta(q) \arrow[r, "\hat{\varphi}''"'] \arrow[dl, shift right, "\bar{\Omega}"'] & X_r(q)/X_\beta(q) \arrow[dr, shift left, "\bar{\Omega}"] & \\ H_f(q) \arrow[rrr, "\hat{\varphi}'"'] \arrow[ur, shift right, "\bar{\Omega}^{-1}"'] & & & H_f(q) \arrow[ul, shift left, "\bar{\Omega}^{-1}"] \end{tikzcd}$$

Diagram VIII

where $\hat{\varphi}'' = \bar{\Omega}^{-1} \circ \hat{\varphi}' \circ \bar{\Omega}$. Now focus attention to the upper trapezoidal part of the diagram, and apply proposition 4, (i), then the continuity of $\hat{\varphi}$ follows immediately. □

To have a clear picture of the assertion of theorem 3 and of the notion of class preserving transformations, the reader may take the following steps: (i) select a concrete example of sequence $\{M_N\} \in X_r(q)$ with $q = 1$ from refs. [3–7]. (ii) Set $\varphi = t^n$ and compute the entries of M_N^n for $n = 2, 3$. (iii) Recall the definitions of the mappings in diagram VIII, and calculate the images of $\{M_N\}$ under the composites of mappings in the diagram. (iv) Follow the proof of theorem 3 with the above example in mind.

REMARK

Part (iii) of theorem 3 may also be derived by part (a) of proposition 5 in the present paper and by part (iv) of the Lemma (p. 136) in the ref. [4], which uses a ring theoretical technique.

So far, in the "approach via the aspect of form" for the additivity problems, we solely dealt algebraically with the forms of repeat sequences which represent molecular structures, and we made topological considerations only in auxiliary functional spaces such as $C(I)$, $CBV(I)$, and so on (cf. [3–7]).

The above theorem indicates a way of topologizing subspaces of $X(q)$ (such as $X_r(q)$, $X_\alpha(q)$, or others), and leads one to consider continuous transformations in the spaces, and also continuous mapping from or into the spaces. Through the topologization of the subspaces of $X(q)$, and use of geometric language and picture similar to those in the theory of symmorphy transformations, one obtains a new vision, and more elucidative methods to handle the additivity problems. The details of this development shall be published elsewhere.

5. Concluding remarks

It is profitable to recall, in connection with the quotient mathematical structures $g_\rho/g_{\rho 0}$ and $X_r(q)/X_\beta(q)$, the notion of the shape groups [15–17], which is central to the study of molecular shape using algebraic topology.

The shape groups associated with a given truncated contour surface are defined to be the pth homology groups: $H^p = Z^p/B^p$. The H^p, for fixed surface and p, is a quotient group as is the symmorphy (quotient) group $h_\rho = g_\rho/g_{\rho 0}$. Two elements $x_1, x_2 \in Z^p$ are called homologous to each other, if $x_1 - x_2 \in B^p$. (Recall that two elements $t_1, t_2 \in g_\rho$ are called symmorphic to each other if $[t_1] = [t_2]$, i.e., if $t_1^{-1} t_2 \in g_{\rho 0}$.)

It is also instructive to compare the quotient linear space $X_r(q)/X_\beta(q) \cong H_f(q)$ with the quotient group $H^p = Z^p/B^p$, focusing attention to the geometric implications of $X_\beta(q)$ and B^p. By theorem 3, the $X_\beta(q)$ is the kernel of the homomorphism Ω, which sends each element $\{M_N\}$ in the repeat space $X_r(q)$ onto $H_f(q)$, annihilating the information on the boundary moieties of $\{M_N\}$. The group B^p of all p-dimensional bounding cycles is, on the other hand, the image of the group homomorphism ∂_{p+1} (the boundary operator). Regarding the methodology and the mode of characterizing the molecular structures, one may observe a noteworthy parallel between the morphological studies using the shape group and the repeat space, the detail of which is under investigation.

Finally, we remark that the theoretical tools developed in the present paper are applied to the problems given in [18] which are seemingly unrelated to the symmorphy transformations and operators in the repeat space $X_r(q)$. In fact, the category theoretical devices using diagrams of arrows exploited in the present paper also serve as a technical basis for a series of papers [18], entitled Structural Analysis of Certain Linear Operators Representing Chemical Network Systems via the Existence and Uniqueness Theorems of Spectral Resolution I, II, and III. In this series of papers, the kernels of certain linear operators are analyzed by using tools which are essentially analogous to those employed in the present paper.

Acknowledgements

This work was supported by a research grant from the Institute for Fundamental Chemistry, Kyoto, Japan.

References

[1] P.G. Mezey, Topology of molecular shape and chirality, in: *New Theoretical Concepts for Understanding Organic Reactions*, eds. J. Bertran and I.G. Csizmadia (Kluwer, Dordrecht, 1989) pp. 77–99.

[2] P.G. Mezey, Three-dimensional topological aspects of molecular similarity, in: *Concepts and Applications of Molecular Similarity*, eds. M.A. Johnson and G.M. Maggiora (Wiley, New York, 1990) pp. 321–367.

[3] S. Arimoto, Phys. Lett. A 113 (1985) 126.

[4] S. Arimoto, Phys. Lett. A 124 (1987) 131.

[5] S. Arimoto and G.G. Hall, Int. J. Quant. Chem. 41 (1992) 613.

[6] S. Arimoto and M. Spivakovsky, J. Math. Chem. 13 (1993) 217.

[7] S. Arimoto and K. Taylor, J. Math. Chem. 13 (1993) 265.

[8] J.L. Kelly, *General Topology* (Springer, New York, 1955).

[9] K. Kuratowski, *Topology* (Academic Press, New York, 1966).

[10] W.J. Thron, *Topological Structures* (Holt, Reinhart and Winston, New York, 1966).

[11] P. Alexandroff and H. Hopf, *Topologie I* (Springer, Berlin, 1935).

[12] P. Alexandroff, Math. Ann. 96 (1926) 555.

[13] R.L. Moore, Trans. Am. Math. Soc. 27 (1925) 416.

[14] S. MacLane, *Categories for the Working Mathematician* (Springer, Berlin, 1971).

[15] P.G. Mezey, Int. J. Quant. Chem.: Quant. Biol. Symp. 12 (1986) 113.

[16] P.G. Mezey, J. Comput. Chem. 8 (1987) 462.
[17] P.G. Mezey, Int. J. Quant. Chem.: Quant. Biol. Symp. 14 (1987) 127.
[18] S. Arimoto, K. Fukui, K. Taylor and P.G. Mezey, Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution I, II, and III, to appear.