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DECODING MOLECULAR PROCESSOR INFORMATION

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Abstract: There are non-imaginable resources of information inherently stored and naturally processed in the physical world. Eliciting and processing information does assume, as usual, the existence of the system (e. g., classic logical gates) suitable for operations or measurements performed. Meanwhile, the powerful chemical and other complex system conversions of information have not used implementation of this kind. Processes in living and non-living physical world run with immediate changes of the properties of objects constituting complex systems. We can detect the features of changing structures and thus to acquire the knowledge about environment. The main part of the structural properties and processes is however hidden though it can underlie important transformations. A massive information which is cumulated and processed in structures of complex systems turns out to constitute a kind of a specific number processor. Thus, the information by which the molecular systems are loaded is to be elicited and transformed to the forms suitable for detection.

1. PRELIMINARY NOTES

What are and what is the role of specific interrelationships between atomic species in the chemical molecule which pre-organize chemical compounds. To answer this question, a recognition of mathematical properties pervading the basic chemical background has been accomplished.

The interest to recognize the principles of chemical structures are entirely justified as the cognitive and technologically applied problem. One of the basic concepts in chemistiy is the notion of the elementary unit called molecule that is difficult to be over-appreciated in the recognition and diversification of chemical substances. These objects and their pertinent features are the goal to investigate them from the viewpoint of mathematical discrete chemistiy approaches. The relatively new idea of self-organization [1,2] has widely been used in the similar concept in the foundations of chemistry. The basic stoichiometry rules and, for example, the phenomenon of saturation cany this out. It could be noted that modern chemistry started to develop on 19th century from the idea of assembling atomic species and giving elementary quantitative characteristics. The result of such self-organization (self-assembly) is distinguishing an elementary unit first described by molecular formula and by the so-called structural formula. Since different compounds can have the same molecular formula, the result of distinguishing a molecular species must be attributed by the self-assembly structure, i. e., by distinguishing some relationships between nuclei. It is supposed that the theory of multiple bonding is not necessary to explain in classic terms, e. g. of the theory of orbitals. The self-assembly phenomenon affords general mathematical entries free of redundant interpretations but not rejecting the core of quantum chemical and empirical results.

Assume the class of objects denoted Obj$\boldsymbol{T}$ (cf. a more advanced view of ref. [3]), i. e., a class of some pairs (A, s) where s is a structure on A, is partitioned by an equivalence relation r. Then a mapping

$$\mathrm{Tp}: \mathrm{Obj}\boldsymbol{T} \rightarrow \boldsymbol{U}$$

which ascribes a set of $\boldsymbol{U}$ to an object of Obj$\boldsymbol{T}$ and such that for two objects X, Y TpX= TpY if and only if pair (X, Y) fulfils r, is said to determine some types of the structures involved. If an operation ♣ is determined on the objects such that X♣ Y=Z where Z is again an object, then it is easy to see that an operation on the types can be induced in this way. Thus, types and the operation induced can be treated as certain specific arithmetic of structural numbers (types). A well-known example is given by the types of well-ordered sets called ordinal numbers [4]. Ordinal number arithmetic is strictly reflecting the corresponding operations on the well-ordered sets. For finite case, it is simply the arithmetic of natural numbers. In general, however, ordinal numbers are not easy to interpret in the physical world. The maximal class of ordinal numbers is not even set. This shows that equivalent transformations of structures and numbers are not always leading to the suitable system to use directly it, e. g., in the nano-processor design. On the other hand, the ordinal number arithmetic remains extremely informative, for example, in the foundations of mathematics in spite of that operating this system is not replaceable by Turing machine (cf. another case [5]). The information obtained by number-type operations is supposed to be more useful and efficient than immediate corresponding transformations on the structured objects similarly as counting on natural numbers is easier than visualizing it, e. g., by handling with concrete things such as small stones. Such improvements in efficiency are considered here as decoding procedures in view of more efficient insights in the nature of systems investigated.

The structures underlying chemical processes are of great interest to answer what would be the kind of information encoded when the new compounds are created, e. g., during the chemical synthesis. To decode this information the procedure for the receiving and rules to operate ordinal numbers determination will be resembled for the case of chemical structures. The concept has been framed particularly in the following way.

For $X1, \ldots, Xn$ reacting substrates operations on number-types: Tp$X1$ + ... TpXn = Tp$Y1$ + ... +TpYm are to be considered. Thus, the information by which the molecular systems are loaded can be elicited and released in the forms suitable for detection. The powerful specific computational processes are to be revealed in this way. A crucial question however remains what are the chemical structures?

2. A CHEMICAL STRUCTURE AND ITS DECODING

A pre-chemical object is a system $(A, \lambda, v, \bullet)$ such that λ (the atomic number operation) maps A into the set of natural numbers N, v (the "bonding force" operation) is a partial mapping with the domain (dom$v$) included in the set of all subsets of A (denoted Pow$A$) into N, and • (the "bonding" operation) is a partial mapping from the Cartesian product of subsets of A

(Pow$A$ x Pow$A$) into N, To obtain commutative "bonding" operation a symmetrized multiplication is useful:

$$u \overset{S}{\cdot} v \overset{\mathrm{df}}{=} \max\{u \cdot v, v \cdot u\}$$

The non-zero values of the "bonding" operation yield the following relationship:

$$\dot{r} \overset{\mathrm{df}}{=} \{(u, v) \in \mathrm{dom} \cdot \mid u \cdot v \neq 0\}$$

There are several groups of conditions that correspond to the operation mentioned or to the pairs of them. As a whole, an axiomatic system has been constituted in this way.

I) *Condition for the underlying set A*

U_1) This group includes only one condition in which finiteness of the set A is postulated, i. e., A has cardinality $n \in N$.

II) *Conditions of the "bonding" operation*

B_1) The condition of the excluded inclusion postulates the null values of the "bonding" operation for such pairs of subsets of A which are related by inclusion. Formally:

$$\dot{r} \cap \left(\subseteq_{\mathrm{Pow}A}\right)^{-}_{\mathrm{SymPow}A} = \varnothing$$

where $\subseteq_{\mathrm{Pow}A}$ denotes the relation of inclusion in Pow$A$ and the whole expression is the closure of this relation under all symmetric relations (denoted SymPow$A$) which embrace it.

B_2) The condition of the one direction of the "bonding" relationship. This statement establishes that if $u \cdot v$ and $v \cdot u$ are different, then one of the values equals 0. Formally:

$$\forall (u, v) \in \mathrm{dom} \overset{S}{\cdot} : (u \cdot v \neq v \cdot u) \Rightarrow (u \cdot v = 0 \vee v \cdot u = 0)$$

III) *Conditions of the "bonding force" operation*

BF_1) The condition of the empty set. It is asserted the exclusion of empty set from the domain of "bonding force" operation. Formally:

$$\varnothing \notin \mathrm{dom}\, v$$

BF_2) The condition of one element classes. In virtue of this axiom, the one element subsets of A (denoted A/I_A) are included into domain of the "bonding force" operation. Formally:

$$A/I_A \subseteq \mathrm{dom}\, v$$

BF_3) The condition of separation. Due to this statement, the multi-element classes of the domain of v are separated. Formally:

$$\forall u, v \in \mathrm{dom}\, v \setminus A/I_A : u \cap v \neq \varnothing \Rightarrow u = v$$

IV) *The condition of the fixed atomic numbers.* This statement assumes the inclusion of the atomic number operation λ in a general function Λ. Formally:

$$\lambda \subseteq \Lambda$$

Function A has been defined on the Grothendieck universes [3] and adopted to the chemical goals

V. *Mixed conditions*

BO_1) The condition of the domain of "bonding" operation. Due to it, the domain of multiplication • includes only pairs from the domain of "bonding force" operation. Formally:

$$\mathrm{dom} \cdot = \mathrm{dom}\, v \times \mathrm{dom}\, v$$

BO_2) The condition of the resultant "bonding force" operation. It is postulated the null value of v for multi-element classes if all the one element classes included are saturated. Formally:

$$\forall u \in \mathrm{dom}\, v \setminus A/I_A : ((\forall v \in \mathrm{dom} v,\ v \subseteq u,\ v \neq u : vv = \mathrm{grad}\, v) \Rightarrow vu = 0\ )$$

$$\text{where for } v \in \mathrm{dom}\, v \ \ \mathrm{grad v} \overset{\mathrm{df}}{=} \sum_{w \in \mathrm{dom}\, v} v \overset{S}{\cdot} w$$

Z_i) The condition of zero atomic number classes. There are no relationships distinguished between forms with zero atomic number and any other. Thus, non-chemical, i. e. particularly belonging to the physics of elementary particles "bonding" relationships are eliminated. Formally:

$$\dot{r} \cap \left(\mathrm{Pow}(\lambda^{-1}\{0\} \times \mathrm{Pow} A\right)^{-}_{\mathrm{SymPow} A} = \varnothing\ .$$

The chemical spaces are determined by the axioms above-mentioned. However, to get an equivalence with compensating systems, the category of chemical spaces and their morphisms is restricted by an additional statement on saturation, i. e. by

SAT_1)

$$\forall u \in \mathrm{dom}\, v : \mathrm{grad}\, u \leq vu.$$

SAC spaces just determined have been used for chemical investigations using the so called set - spectrum method [6].

Since the structures to be transformed to reveal the nature of the inherent information are now already determined, one can immediately ask about its mathematical significance to get solutions how an information can be released. For this aim, the theorem on the unique decomposition of chemical numbers will be used [7]. This holds in HOW - spaces (T, +, •) where (T,+) is a commutative monoid and (T, •) is a commutative semigroup. Thus, the spaces considered are not even integral domains. In spite of this, HOW - numbers can be decomposed only in a unique way, i. e., the following assertion holds.

Any HOW - number o equals a product of certain exponents of prime chemical numbers $\sigma_H^l\, \sigma_O^m\, \sigma_W^n$ where l, m, n are uniquely determined positive integral numbers.

Thus, there exists a one-to-one mapping f which transforms chemical numbers T in the threes ($/$, m, n) of the Cartesian product $N \times N \times N$. This is manifestly also surjective mapping.

$$\mathrm{f}: T \rightarrow N \times N \times N\,.$$

Since the structures can be transported a counterpart of the chemical arithmetic $(T, +, \bullet)$ has been induced on$N$xNxN,*i.* e., an isomorphic arithmetic ($N \times N \times N$,-, +) has been received.

A new situation emerged in this way to elicit the nature of arithmetical operations performed during chemical reactions. The proof leads to the following forms of chemical arithmetic operations:

$$(l, m, n) + (l', m',n') = (l + l', m + m', n + n')$$

$$(l, m, n) \bullet (l', m' n') = (2(\mathrm{qu}(l + l', 2) - \min\{\mathrm{qu}(l + l', 2),m + m'\}) + \mathrm{rem}(l + l', 2),$$

$$(m + m') - \min\{\mathrm{qu}(l + l', 2), m + m'\}, n + n' + 2\min\{\mathrm{qu}(l + l', 2), m + m'\}),$$

where addition of 3-tuples is induced by f as the counterpart of the semigroup $(T, \bullet)$ and multiplication natural number threes means the transformed monoid $(T, +)$ [7],

The result shows that the system does not surpass the usual Turing machine limits as in the case of ordinal numbers. Collapse and creating new molecules during chemical reaction is however the source of a more powerful processing than it could happen by the use of logical gates.

3. CONCLUSIVE REMARKS

The abstract operations on chemical numbers turned out replaceable by combined usual integral number transformations. Thus, the structural information has been essentially converted to the form suitable for nano-scale processing and the traditional logical gate system. To recognize how the structural material information can be released owing to specific number operations is the first class problem for chemical sciences and technology. Besides, a new kind of computer does emerge due to operations on the numbers having direct relevance to the underlying chemical structure conversions.

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