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Editorial

Category Theory in Chemistry

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"Mathematical chemistry" as an academic field is said to have been proposed by Weyl in the 20th century as a way of thinking that abstracts and expresses "variables", "symbols" and "functions" [1]. Mathematics in the sense of arithmetic and statistics used to calculate chemical data is excluded here for the time being.

However, "group theory", as well known as the mathematics that describes the three-dimensional shape of compounds, the electronic structure of atoms and molecules, and the geometric structure and symmetry of crystals, is widely used in various fields of material science [2]. Macromolecular substances, which are soft matter, are also objects of symmetry, such as surface arguments, tiling, and non-crystallographic symmetry (such as quasicrystals), even if they do not have crystal-like order [3]. Starting from regular polyhedra, surface curvature is also of mathematical interest [4]. Positive and negative curvature is also connected to rudimentary differential geometry. Regarding shapes, we often hear the word "topology" in chemistry [5]. In addition to using the properties of mathematical topology, there are occasional implications for describing three-dimensional shapes, but with the rise of supramolecular chemistry, it is clear that it is useful for describing shapes of soft molecules and assembly modes. Topology, which is the way the atoms that make up a molecule are connected, can be described and classified by graphs [6].

Furthermore, there are also examples of using more abstract set theory to express and relate chemical content [7]. By introducing a stoichiometric "chemical formula" in set theory notation and patterning it, material transformation was treated mathematically. Attempts to describe the logical structure of set theory in terms of the classification of chemical elements (elements and compounds) and their correlation with physical property values have long been known [8]. Recently, set theory has also been used to formulate ligand-target datasets in drug discovery [9]. Inspired by data science and data-driven research, it should be seen that mathematical methods were used as a means of judgment.

While the application of artificial intelligence to various sciences (such as computing, social networks, and so on) has accumulated achievements, the application of "category theory" to chemistry is regarded as being worthy of attention. Conventionally, a number of differential equations are used to describe chemical reactions (reaction rates). It is a recent mathematical achievement that their topological relationships as networks have been treated by the "cospan" of category theory as open reaction networks [10]. However, theories defining chemical reaction networks as homomorphisms between finitely generated free abelian groups have been developed, and a theorem to know the number of reactions has been discovered [11]. Furthermore, research on the relationships within chemical reaction networks has been further refined in recent years, such as simplification using topology [12].

Besides chemical reactions, composite design may be a notable application of categorical chemistry. There is the problem of determining the conditions necessary to replace one or more basic building blocks with others while preserving overall functionality, which is called the "building block replacement problem" [13]. The mathematical branch of category theory has a formal language at the heart of its methodology. Thus, a theoretical description of hierarchical material categories is possible: (1) a method of providing a mathematical tool

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that can replace one component with another to achieve substantially the same function; (2) how to use them to model and design seemingly different physical systems in a consistent mathematical framework. The utility of such approaches was demonstrated by using algebraic techniques to predict the specific conditions required for the exchange of building blocks.

In addition, the structure of the "ontology log" [14] is based on a branch of mathematics called category theory, which is a category that models a particular real-world situation. The authors of [15] stated that the data from sciences should be organized in such a way that this work is reusable, transferable, and comparable to the work of other scientists. In combination with category theory, which is strong in describing relationships, there are studies that also apply graph theory to chemical reactions [16] and molecular structures [17].

The mainstream of chemical research is the accumulation of experimental facts by synthesizing new compounds and reporting their properties, and this will continue to be the case. However, today, when methods such as theoretical calculation and data science are mature and available, the information derived from experimental facts and its use will also increase in importance. In the midst of this trend, it is to be expected that category theory has been attracting attention recently.

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