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Research Article

AN OVERVIEW ON MATHEMATICAL CHEMISTRY

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ABSTRACT

In this review we have discuss about history and growth of mathematics along with chemistry. Since, chemistry is a practical science and it is focus on synthesis of new compound, hence there is broad scope of mathematics in chemistry and it is also very useful, because among other things, experimental work is guided by models which are produce by mathematics and which target the shortest possible route of experiments. This review also discusses the way of meeting of these two broad areas of sciences. A trial is taken to define mathematical chemistry. Mathematical chemistry is new branch of chemistry. We discuss about several practical ideas in the mathematical way. By discussing Weyl's, Plato's, Geoffroy's, Mendeleev's theory etc we want to highlight more application of mathematical chemistry branch in current scenario.

Keywords: fundamentals of chemistry, fundamentals of mathematics, experimental science, mathematical chemistry journals.

INTRODUCTION

In this review, we try to discuss about important functions of mathematical chemistry. It has been found that on literature survey roots of mathematical chemistry from the 18th century. However, research paper, review, articles etc regarding this field are published in advances specialized journals recently.

Chemical processes are assumed to be probably responsible for Earth's life.[1–3] life means[4] (i) Physical evolution, (ii) Chemical evolution and (iii) Biological evolution. Molecules are of different types some are simple whereas others are highly complex.[5] Because of this thought, chemistry are considered as the core science.[6] Alternatively, mathematics is belongs to intelligent mind.[7] Similarly to chemistry, mathematics has some experimental roots.[8] Nowadays, various kind of chemical techniques available who used to solve mathematical problems.[9] mathematics is a form of language, which is used to exchange ideas about fundamental concepts of abstract which is useful to pertain numbers and space.[10] In early period of time mathematics generally use to count practical human needs. [11] while some anthropologists correlate this counting arose with primitive religious rituals.[12] In early days, people attracted towards number theory which put

affords on growth of the entire field.[13] the sciences of chemistry are also have mental constructs as is mathematics.[14] However, mathematics clear all wrong belief that it offers only certain knowledge.[15] Mathematicians called by so many names[16-18] such as Platonists, formalists some call as logicians, intuitionists etc. All of them explain their role and explain the concepts what they studied [19-20]. Mathematics is nothing more than what mathematicians actually do.[21]

Chemistry is the material science who studies about all the property of molecules, substances and their transformations into new substances.[22] The 19th century is the era of scientific foundation to chemistry.[23, 24] John Dalton (1766–1844) depict the molecular structure[25]. The concept of isomerism given by Jöns Jakob Berzelius (1779–1848)[26]. Pasteur gave spatial aspect theory [27] which turned chemistry into mathematics. Mathematical chemistry concepts were fully realized in the 20th century when quantum chemistry and mathematical chemistry come in front.[28] To mathematize chemistry step is taken by Crum Brown. [29]. Pauling rationalized the tetrahedral carbon model.[30] Johannes Kepler (1571–1630) cataloged Archimedean solids in 1619.[31]

Cayley and Sylvester[32-34] a great mathematicians who first time show interest in chemistry. Further this was explored by Cayley's mathematical work which is based on theorem of Polyá. Polyá theorem further become potential enumeration method to chemists.[35]

Apparently, the Journal of Mathematical Chemistry (MATCH) was first of all initiated by Oskar E. Polanski in year in 1975. This journal has been continuously published paper twice a year till present day. Present editor-in-chief of Mathematical Chemistry (MATCH) is Adalbert Kerber. The title of the journal is Communications in Mathematical Chemistry which is published by J. C. Baltzer AG, Basel in year 1987 because this field is more conservative than other field of science such as physics, biology etc. The first editor of journal was Dennis H. Rouvray a renowned mathematical chemist. Rouvray, mentioned that if mathematical chemistry define not properly, than describe the field rather than editors of Mathematical sciences. In branch of Mathematical chemistry a new application of mathematical methods in chemical processes is to be study. The novelty means the discovery of new chemical theory, new mathematical model, new approach which solve problems that of chemical interest. The most important things in novelty are associated with respect to the chemical problem not mathematics which is under consideration. Until the end of 1989 Rouvray was editor. After Rouvray, the joint editorship of the journal was under Paul Mezey and Nenad Trinajsti till year 1993. Furthet editor-in-chief was Paul Mezey. In year 1991, Mathematical Chemistry in form of Series published by Science Publishers. Further Danail Bonchev and Dennis H. Rouvray put more effort in this and publish many review articles from this journal. This journal has total six volumes. Some more volume now a day which is in real regarding complexity of molecules and reactions is under preparation.

The term mathematical chemistry is fairly new, although, it is worth pointing out that general application of mathematics to chemistry is reported till 19th century. The term mathematical chemistry given on paper which is published in year published in 1928 by John Hasbrouck Van Vleck, who was the Nobel Prize winner for Physics in year 1977. According to him mathematical chemistry is that branch of science in which quantum mechanics measure the chemical heats of reaction. The term mathematical chemistry modified by Van Vleck.

Mathematical chemistry includes the bulk of chemical phenomena to calculation. Gay-Lussac considered the father of theoretical and computational chemistry. Professor André Deriding co-editor of MATCH defines as mathematical chemistry as it is non-trivial mathematical application for chemical problems. This statement is match by statement which is given by editor of JMB for Mathematical chemistry. Apparently, Ouray's attempt discussion some debate about the separation of mathematical chemistry to short out other concepts which kindly explanation what constitutes mathematical chemistry actually. Klein involved in discussions regarding nature of mathematical chemistry. Jerome Karle and Herbert A busy in field to predict out the use of mathematics in chemistry who is also the winner of Nobel Prize for chemistry 1985.

Hauptman who focuses on mathematical solutions of crystal structures said mathematical chemistry is mathematical methods useful for chemical applications. Ivar Ugi stated that it is actually the participation of mathematics in chemistry without the help of physics solution of chemical problems obtained directly by qualitative mathematics.

Thus, mathematical chemistry concerned about theoretical applications of mathematical methods for the chemistry related problems. But the word new and non-trivial which is used by Rouvray in his definition has been left out point of definition. The term new should not imply in is its application in chemistry. There is no need of new definition. The research in chemistry is trivial it not consider subject definition, so merely their results are not so interesting. Therefore, this should not be definition according to mathematical chemistry. Research in this area is closely related to the problems and concepts occurring in chemistry. These are much more from their chemical origins. For example Cayley's, Polya's theory for isomer-enumeration concepts, concept of the energy graph etc serve as typical examples. Sylvester called this branch as 'algebraic chemistry'.

Beside this research of mathematics are includes in mathematical Chemistry and they should not be fully skipped. The core part of chemistry i.e. structural chemistry inserts mathematics into chemistry.

MATHEMATICAL THINKING FOR CHEMISTRY

Mathematical chemistry is also termed as discrete mathematical chemistry. This term is introduced by Villaveces & Restrepo in year 2012. Further in the second half of the 20th century it become as a new sub-discipline area. Instances three scientific journals belong to this area of mathematical chemistry. The creation of IAMC on Mathematical Chemistry is the collectively growing scientific community. This community suggests that the combination of this field i.e. mathematics and chemistry is something very new. The purpose of this review is to highlight the close contact between mathematical and chemical thinking. Several examples to support this statement are discussed as.

Redfield (1927), gave [36–38] combinatorial theory which have use in medicinal chemistry.[39]

Crum Brown's uses graphical notation for molecules [40].

1. In 1940, Hermann Weyl, [41] published a paper entitled variables and functions which consists kind of variables, symbols present variables and functions mapping on one variable upon the other.
2. Plato[42] used geometrical part of mathematics to discuss his chemical ideas in the mathematical way of thinking, which is intiated by Lloyd in year 2007. This idea as follows: (i) Variables such as fire, water. (ii) Symbols as bottom polyhedra. (iii) Functions, hexagoan.
2. Etienne-François and Geoffroy (1672-1731)[43] designed the table which based on mathematical view (i) Variables represented by substances (ii) Mathematical Symbols and (iii) Functions. Table arranges is based upon molecular or substance reactivity with reference to a substance.
3. Lavoisier introduced a language of Algebra[44]for chemistry, which is most adapted as simple, exact, and best manner possible, language for analytical method. There work is kind of nomenclature which easily detect out substances, elements, compounds etc. Lavoisier's work in terms of mathematical thinking is as follows, Variables is chemical elements, Symbols is all chemical symbols which is used and Functions as all elements.
4. Mendeleev's periodic table given by Johann Wolfgang Döbereiner[45] which shows arithmetic relationship for elements. Arithmetic relationship follows a topological structure shown in periodic table. Variables is valence, oxidation state, etc, Functions is atomic weight.
5. Weyl's mathematical way[46] according to his study Mendeleev's periodic table can be summarized as follows: (i) Variables: properties of elements. (ii) Symbols is p1(x), p2(x),…; pi (iii) Function, the function p1(x), characterizes the chemical elements, second p2(x) represent as similarity function between the different properties of the chemical elements.
6. Cayley mathematical theory[4] calculate the number of molecular structures and how to calculate it. Thus in his case Variables is atoms number and bonds. Function is $n \rightarrow t$.
7. Sylvester's algebra[48] and chemistry, he states a similarity in between algebra and chemistry. According to him, chemical substance is same as invariant of a binary system. This idea relating mathematics to chemistry nearby related with identity of atoms in molecules. He map different invariants such as he assume atoms with certain valence is a graph, which correspond to their chemical structure. He said chemistry is the counterpart of algebra. His algebraic mathematical modeling nearly or equally same as that of given by Weyl's (i) Variables is atoms and their valences. (ii) Symbols is chemical element etc
8. Wiener[49], showed how to relation between the molecular structure with their physical property i.e. boiling points. He treats molecular structure in terms of graph and searched some features that estimate their boiling points. Wiener's work based on graphs which mathematically relate the structure of molecule with their macroscopic properties. This idea explores mathematical chemistry broadly which in turn called Quantitative Structure-Activity Relationships or Quantitative Structure-Property Relationships. According to his mathematical way of thinking Variables is the boiling point, Symbols used is TB, and Function is $TB = aw + bp + c$, where a, b, and c are constants.

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CONCLUSION

In this review we have discuss different cases of mathematical thinking for chemical problems. Such as how Weyl's conception of mathematical thinking co-relate to each other. Next Plato's variables are geometrical; they abstract daily transformations observed in nature. It told only some transformations allowed by geometry and some are forbidden. forbidden transformation are not happen. Mendeleev provide wealth of chemical information. Geoffroy's deals with affinity periodic table arranged chemicals elements according to affinity, but Mendeleev's deals periodic law arrange elements in terms of their properties and related them with their atomic weight. Lavoisier's classification of substances coincides with Weyl's mathematical theory which predicts chemical behavior. Cayley and Sylvester works based on mathematical thinking because both were mathematician but problems belong to othere disciplines are quite remarkable. Cayley and Sylvester connect mathematics with chemistry. Cayley, transfers molecular drawings, into mathematics and shows the calculation molecular structures with the help of mathematics, which explore further, as mathematical chemistry. His work is the extension of Wiener's work, who relates structures and macroscopic properties. Sylvester with the help of molecular drawing graph showed chemical information such as the kind of elements, their valences etc. But later on Wiener predicted that chemical structures drawing was not such as their graph, which are complete mathematics which can be explore in same direction. So, further he gives a mathematical concept which originated from graphs and chemical properties. This ignites the search for other functions such as macroscopic properties. This leads to the birth of new fields in area of mathematical chemistry. On seeing all these examples which are based on correlation of mathematics with chemical problems show its long term connection with chemistry before half of the 20th century. It seems that different way of mathematical thinking in chemical science field are available and many more can be found, when one looks for it.

CONFLICT OF INTERESTS

Since in this review t here is single author so there is no any possibility of conflict of interest.

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