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Chemical equation representation as directed graph

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ABSTRACT

One of the major issues in formalizing the dynamics of chemical reactions is that the graph representation of such reactions is not immediate. This is due to the case that chemical equations involve more than one reactants and products can also be more than one. Over the last decade, an increased attention to reaction dynamics, combined with the intensive application of computers, mathematical modeling of chemical processes, has brought graph theory to the forefront of research. It offers an advanced and powerful formalism for the description of chemical reactions and their intrinsic reaction mechanisms. This paper proposes an elegant method of representing a chemical equation as directed graph.

Key words: Chemical Equation, Graph, Directed Graph, Weighted Graph.

INTRODUCTION

Many biology and anatomy and physiology courses begin with chemistry. More than just nutrients, medicines and poisons, everything we do is chemical. Many things that are our in environment are made of chemicals. Many things that we observe in the world are made of chemical effects. Mathematics is used widely in chemistry as well as all other branches of sciences. Mathematics is used to understand the concepts in chemistry. Mathematical calculations are necessary to explore important concepts in chemistry. Without some basic mathematics skills, these calculations, and therefore chemistry itself, will be difficult. Francesc Rossell described Chemical reactions by edge relabeling graph transformation rules, in which a substrate chemical graph is transformed into a product chemical graph by breaking existing bonds and creating new bonds between atoms [1]. Mayur Bapodra derived ordinary differential equations for a chemical reaction, using graph transformation techniques [2]. M. Yamuna proposed a method of converting a chemical equation as a string using HTML codes and periodic table [3]. Sumami Abu Bakar investigated dynamics of the graph using Perron – Frobenius eigen vector of its adjacency matrix [4].

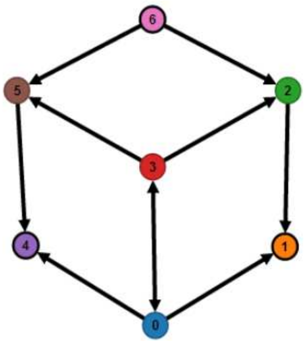
MATERIALS AND METHODS

2.1 Graph

In the most common sense of the term, a graph is an ordered pair G = (V, E) compromising a set V of vertices or nodes together with a set E of edges or links, which are 2 – elements subset of V (that is an edge is related with two vertices, and the relation is represented as an unordered pair of the vertices with respect to the particular edge) [5].

2.2 Directed Graph

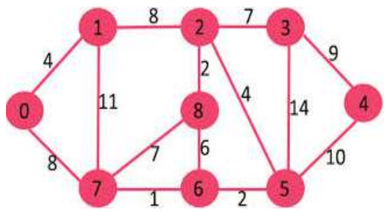
A directed graph is graph, i.e., a set of objects (called vertices or nodes) that are connected together, where all the edges are directed from one vertex to another. A directed graph is sometimes called a digraph or a directed network [6]. Snapshot – 1 [7] provides an example of directed graph.



Snapshot - 1

2.3 Weighted Graph

A weighted graph is a graph in which each branch is given a numerical weight. A weighted graph is therefore a special type of labeled graph in which the labels are numbers (which are usually taken to be positive) [8]. Snapshot – 2 [9] provides an example for weighted graph.



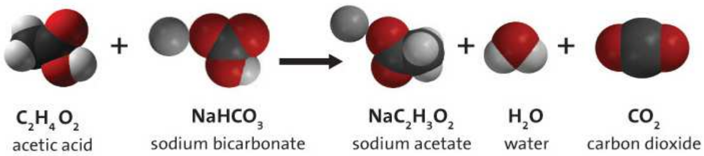
Snapshot - 2

2.4 Chemical Reaction

A process in which atoms of the same or different elements rearrange themselves to form a new substance. While they do so, they either absorb heat or give it off [10].

2.5 Chemical Equation

A chemical equation is the symbolic representation of a chemical reaction in the form of symbols and formulae, wherein the reactant entities are given on the left-hand side and the product entities on the right-hand side [11]. Snapshot – 3 [12] provides an example for chemical equation.



Snapshot - 3

Proposed Method

Construction of the Graph

Consider a chemical equation say for example $CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$.

We now describe the method of constructing a directed graph. Vertices – Number of vertices in G = Number of chemical elements in the equation. In our example the chemical elements are C, H, O. So the number of vertices is 3. Label each vertex by its position in the periodic table. In our example C = 6, H = 1, O = 8. Consider the reactants of the chemical equation. We consider each part of the reactant. In our example reactants are $CH_4 + 2O_2$.

Each part is the combination of chemical elements. Each part of the chemical equation is the combination of numbers and chemical elements. Each element may be prefixed and suffixed by a number.

In our example, consider the part CH_4. Here C is not prefixed or suffixed while H is prefixed by 4. If an element is suffixed assign a suffix value as 1 i.e., CH_4 is consider as C_1H_4. For this part we create partial graph as follows. Label of vertex C = 6 and H = 1. We draw an edge directed from vertex with label 6 to a vertex with label 1. This edge receives weight 1. To represent weight 4 we create a dummy vertex receiving a label 0. Draw an edge directed from a vertex with label 1 to vertex with label 0, whose edge weight is 4. For CH_4 the resulting graph is as seen in Fig. 1.

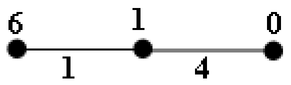


Fig. 1

Second part of the reactant is $2O_2$. For O_2 the resulting graph is as seen in Fig. 2.

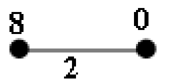


Fig. 2

We need a way to represent the prefix value 2. This we make it possible by using vertex label. The prefix value is 2, so the vertex representing O receives the label as 2.8 where 2 represents the prefix and 8 the position of oxygen in the periodic table. To represent + we use an edge with label 150. So the reactant part is now represented as in Fig. 3.

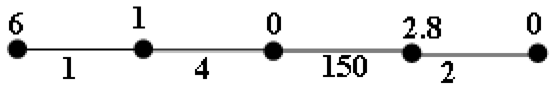


Fig. 3

The same procedure is repeated for products. To differentiate the reactant and product we use edge colours. The reactant part of the reaction is represented with green colour edge products with maroon colour edges. For our example the reactant and product graph as seen in Fig. 4.

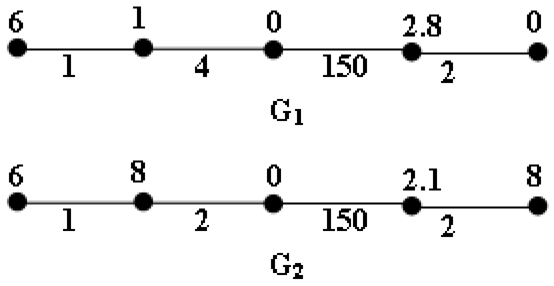


Fig. 4

We now combine both the graphs G_1 and G_2 into single graph G. Number of vertices in G = Total number of elements in chemical equation + a dummy vertex (if necessary).

There is an edge directed between two vertices if there an edge between them either in G1 and G2. The left hand side reaction is represented by green edges and right hand side reaction is represented by maroon edges. The resulting graph for our chemical equation is as seen in Fig. 5.

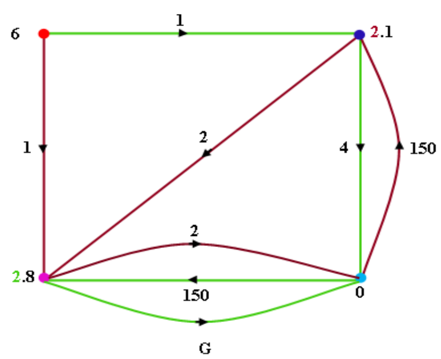


Fig. 5

There may be a chemical equation where on the both sides of the equation the same element receives a prefix number. For example in $P_4O_{10} + 6H_2O \longrightarrow 4H_3PO_4$. H in reactant is prefixed by 6 and the product H is prefixed by 4. In such cases the vertex representing H receives 3 labels 6.4.1. 6 receives green colour to represent the and 4 receives maroon colour to represent the product of the chemical equation. The values are ordered in the way it occur in the equation. The resulting graph for the chemical equation is as seen in Fig. 6.

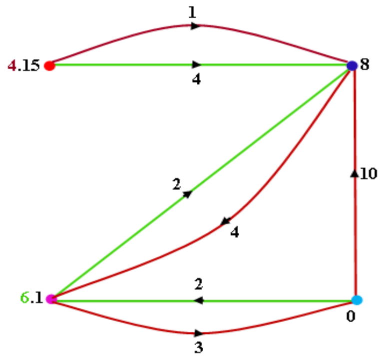


Fig. 6

While representing a reaction as a graph from a single vertex there may be more than one outgoing edges. For example for the chemical reaction $Pb_3O_4 + 8HCl \longrightarrow 3PbCl_2 + Cl_2 + 4H_2O$ the resulting graph is as seen in Fig. 7.

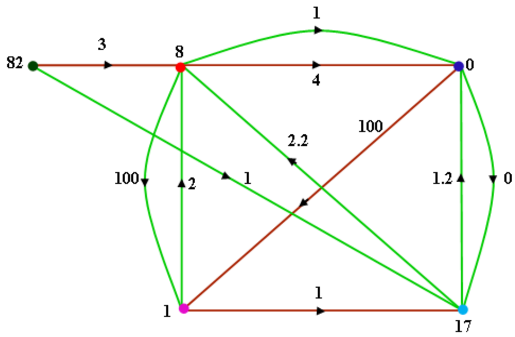


Fig. 7

From vertex 17 there are two outgoing edges with maroon colour. To represent the order of the chemical equation. We assign weights as 1.2, 2.2. This means that edge 1.2 will be traced first and then 2.2 i.e., the first set of values in any edge represent the order in which they appear in the chemical equation.

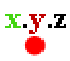
When we receive a graph to recognize the equation we need to know the start vertex. For this purpose we denote a start vertex by red colour other vertices receives random colours.

Summarizing in our graph construction,

 - represents start vertex.

- represents reactant of the chemical equation.

- represents product of the chemical equation.

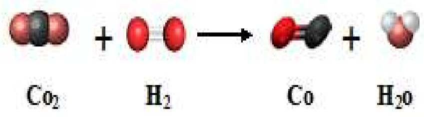
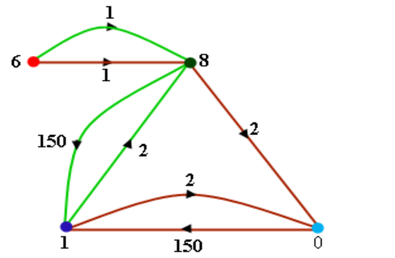
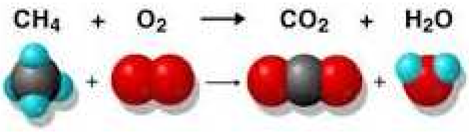
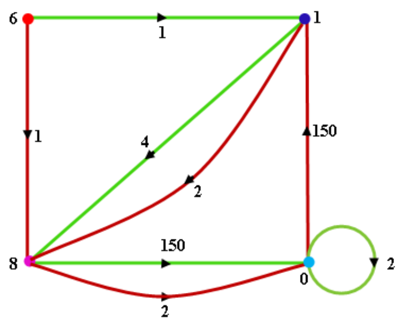
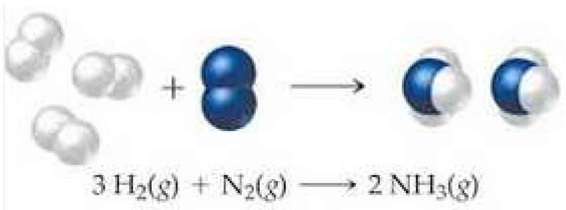
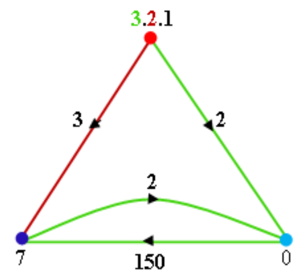
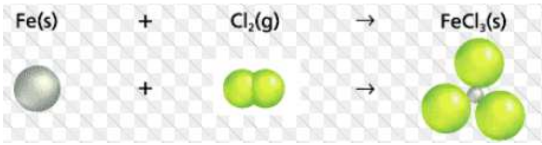
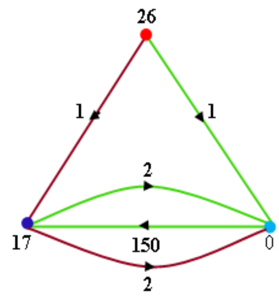


- z represents position of the chemical element in the periodic table.
x represents prefix of z in the reactant.
y represents suffix of z in the product.

- p represents the order of traversal.
q represents suffix of z.

The following table provides some examples of chemical equation, ball and stick representation [13], [14], [15] and their graph representation.

Table – 1

S.No	Chemical Equation	Ball and Stick Representation	Graph Representation
1.	$CO_2 + H_2 \rightarrow CO + H_2O$		
2.	$CH_4 + O_2 \rightarrow CO_2 + H_2O$		
3.	$3H_2 + N_2 \rightarrow 2H_3N$		
4.	$Fe + Cl_2 \rightarrow FeCl_2$		

Suppose the graph representing a reaction is as seen in Fig. 8.

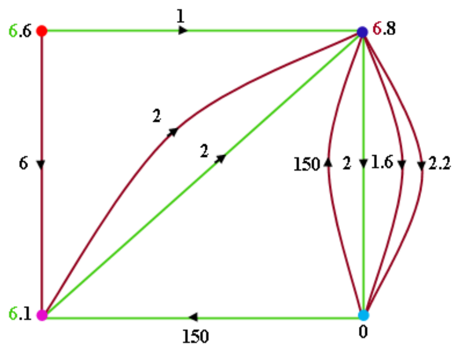


Fig. 8

Since ● represents start vertex and ——— the left hand side reaction. The label of the red vertex is 6.6. The 6 represents the prefix of an element. With a similar representation the reactant traversal is seen in Fig. 9.

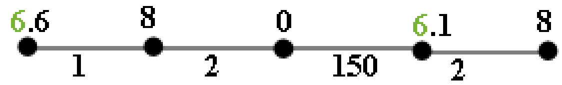
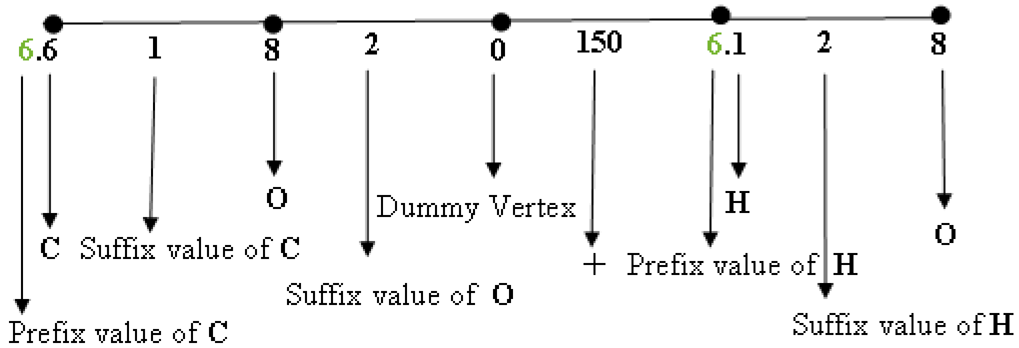


Fig. 9

By our procedure



So the left hand side of the reaction is $6CO_2$ + $6H_2O$. For the product part of the reaction, we have to trace similarly. The partial tracing sequence is seen in Fig 10.

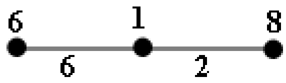
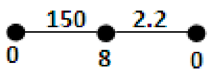
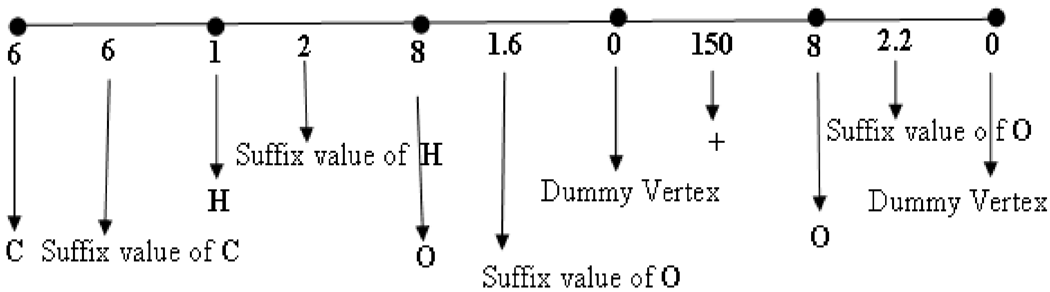


Fig.10

There are two outgoing edges now with label 1.6, 2.2. By our procedure, we have to trace 1.6

followed by  . So the product reaction is $C_6H_2O_6$ +$6O_2$. For our example



So the complete chemical reaction is **$6CO_2$ + $6H_2O$** ⟶ **$C_6H_2O_6$ +$6O_2$**.

CONCLUSION

All materials are made of chemicals. Chemical reactions involve interaction between chemicals such that all reactants are changed into new materials. Humans use chemical reactions to produce a wide range of useful materials including drugs. Chemical equations are symbolic representation of chemical reaction. In this paper we have provided a compact graph theoretical method of representation of balanced chemical reactions. The main challenge of this representation for further research is to use this and hence its matrix representation in chemical property analysis.

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