Ionic Graph and Its Application in Chemistry

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Abstract— A covalent compound can be represented by molecular graph but this graph is inadequate to represent ionic compound. In this paper we introduce some graphs to furnish a representation of ionic compounds. We also study mathematically about these graphs and establish some results based on their relations and structures.

Index Terms— Bipartite digraph, Ionic compound, Ionic graph, Graph of an ionic compound, Graph isomorphism, Semi discrete graph, Widen ionic graph.

1 Introduction

Graph theory is one of the most important area in mathematics which is used to study various structural models or arrangements. This structural arrangements of various objects or technologies lead to new inventions and modifications in the existing environment for enhancement in those fields. The field of graph theory started its journey from the problem of Konigsberg bridge in 1735 [3]. Graph theoretical ideas are highly utilized by the applications in computer sciences [10], especially in research areas of computer sciences such as data mining, image segmentation, clustering, image capturing, networking etc. For example, a data structure can be designed in the form of tree. Similarly modelling of network topologies can be done using graph theoretical concepts. In the similar way the most important concept of coloring in graph is utilized in resource allocation, scheduling etc. Also, paths, walks and circuits in graph theory are used in tremendous applications such as travelling salesman problem, database design concepts and resource networking. This leads to the development of new algorithms and theorems that can be used in tremendous applications. In Biology, transcriptional regulatory networks and metabolic networks would usually be modelled as directed graphs. For instance, in a transcriptional regulatory network, nodes represent genes with edges denoting the interactions between them. As each interaction has a natural associated direction, such networks are modelled as directed graphs. Mason and Verwoerd [9] present a survey of the use of graph theoretical techniques in Biology. Especially, they have used graph theoretical techniques in identifying and modelling the structure of bio-molecular networks. Graph theoretical approaches are widely used in Chemistry to study the structures and properties of molecular compounds. This idea makes a bridge between chemistry and graph theory and gave the birth of Chemical graph theory [5]. Chemical graph theory is used to mathematically represent the molecules in order to gain insight into the physical properties such as bonding type, boiling point, melting point etc. of these molecular compounds. This representation is known as molecular graph [1, 2, 4] and is especially true in the case of molecular compounds known as alkenes. Thus a molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory. A molecular graph [1, 2, 4] is defined as a graph whose vertices are corresponds to atoms and edges are corresponds to chemical bonds between the respective atoms. Molecular graphs can distinguish between structural isomers, compounds which have the same molecular formula but non-isomorphic graphs such as isopentane and neopentane. On the other hand, the molecular graph normally does not contain any information about the three dimensional arrangement of the bonds, and therefore cannot distinguish between conformational isomers. Molecular graphs are inadequate to represent ionic compounds. So we have introduced a new family of graphs in such a way that ionic compounds can easily be represented. These newly define graphs are dealing with the outer shell of the atoms those are forming ionic compounds. Some of the mathematical and graph theoretical basis and applications of these graphs are presented in this paper.

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2 Preliminaries

Definition 2.1 A digraph $D(V,E)$ is a combination of a non-empty set V and a subset $E \subseteq V \times V$. The set V is called vertex set and the set E is called (directed) edge or arc set of D. We write $e = uv$ for an edge with initial point u and final point v. The inverse of the edge e is defined as $e^{-1} = vu$. In this case, e and e^{-1} are distinct edges.

Definition 2.2 [7] The indegree and the out degree of a vertex v in a digraph D with vertex set V are defined as

$d^-(v) = |\{e: e = uv, u \in V\}|$ and

$d^+(v) = |\{e: e = vu, u \in V\}|$

Also in [6], $d^-(v) + d^+(v) = d(v),\ \forall v \in V$

Definition 2.3 A digraph D is bipartite digraph if the vertex set V_D can be partitioned into two non-empty disjoint subsets V_1 and V_2 such that any two vertices in the same set are non-adjacent.

Definition 2.4 An oriented graph is a digraph without loops and multiple edges.

Definition 2.5 A graph G on n vertices is called a semi discrete graph if either $d_G^-(v_k) = 0$ or $d_G^+(v_k) = 0$, for $1 \le k \le n$.

Definition 2.6 A graph G is a connected graph if there exist a path between any two vertices of G.

Definition 2.7 Vertex Chromatic number of a graph G is the minimum number of colors required to colour the vertices of G.

Definition 2.8 An isomorphism of graph G onto a graph H is a bijection $f: V_G \longrightarrow V_H$ such that any two vertices u and v of G are adjacent in G if and only if $f(u)$ and $f(v)$ are adjacent in H.

Definition 2.9 The outermost shell of an atom is called the valence shell of the atom.

Definition 2.10 A cation is a positively charge atom or group of atoms obtained by losing some electrons from its valence shell. An anion is a negatively charge atom or group of atoms obtained by gain some electrons and place them in its valence shell. An ionic compound is a chemical compound in which ions are held together by the electrostatics forces between cations and anions, and net positive and net negative charges are equal. For examples, NaCl and AlF_3.

Lemma 2.1 [Theorem 3.1 of [8]] Semi discrete graphs are bipartite digraphs.

Lemma 2.2 [Corollary 3.1 of [8]] Chromatic number of a semi discrete graph is two.

Lemma 2.3 [Theorem 3.2 of [8]] The Square of a semi discrete graph is the graph itself.

3 IONIC GRAPH

Definition 3.1 A graph of an ionic compound C, is a digraph $D(V, E)$ composed two sets, V the set of all atoms in the compound C and $E = \{uv \mid u, v \in V \text{ and } u \rightsquigarrow v\}$. By $u \rightsquigarrow v$ we mean an electron moves from the valence shell of the atom u to the valence shell of the atom v. The graph of an ionic compound C is denoted by $D(C)$.

Definition 3.2 A graph is said to be ionic graph if it is isomorphic to the graph of an ionic compound. Thus a graph G is ionic if there exists an ionic compound C such that $G \cong D(C)$. It is clear from the basic ideas of isomorphism of graphs that a graph may be isomorphic to more than one graph. Thus if a graph is ionic, it may represent more than one ionic compound. This idea leads to the notion of a family of ionic compounds called cographic ionic compounds.

Definition 3.3 Two compounds C_1 and C_2 are said to be cographic if $D(C_1) \cong D(C_2)$.

NOTATIONS: $d^+(v)$: Out degree of a vertex v; $d^-(v)$: In degree of a vertex v; $d(v)$: Degree of a vertex v; V_G : Vertex set of a graph G; E_G : Edge set of a graph G.

According to the terminology of this definition, the compounds aluminium chloride $AlCl_3$ and scandium fluoride ScF_3 are cographic. We think that the class of cographic compounds has some common properties and characteristics. Thus the class of cographic compounds must be of fundamental interest to chemists and graph theorists.

Definition 3.4 A subgraph, S of a graph G is said to be ionic subgraph if there exists an ionic compound C such that $S \cong D(C)$.

Definition 3.5 A graph is said to be widen ionic graph if it has atleast one ionic subgraph. A graph is said to be simple widen ionic graph if it has no ionic subgraph having more than one edge. A graph is said to be strong widen ionic graph if it has atleast one ionic subgraph having more than one edge. One can easily showed that every digraph is simple widen ionic graph but may not be strong widen ionic graph.

Theorem 3.1 The graph of an ionic compound is semi discrete graph.

Proof: Let C be an ionic compound and $D(C)$ be the graph of C. Then

$V_{D(C)} = \{v \mid v \text{ is an atom in } C\}$ and

$E_{D(C)} = \{uv \mid u, v \in V \text{ and } u \rightsquigarrow v\}$.

Thus for any $uv \in E_{D(C)}$, $d^-(u) = 0$ and $d^+(v) = 0$ because of the atom u can only donate electrons and the atom v can only accept electrons. Therefore either $d^-(v) = 0$ or $d^+(v) = 0, \forall v \in V_{D(C)}$. Hence $D(C)$ is semi discrete graph.

Corollary 3.1 An ionic graph is semi discrete graph.

Proof: Let G be an ionic graph. Then there exists an ionic compound C such that $G \cong D(C)$. By theorem 3.1, $D(C)$ is semi discrete and hence G is also semi discrete.

Corollary 3.2 The graph of an ionic compound is bipartite digraph.

The proof follows from theorem 3.1 and lemma 2.1

Corollary 3.3 An ionic graph is bipartite digraph.

The proof follows from corollary 3.1 and lemma 2.1

Corollary 3.4 The chromatic number of an ionic graph is two.

The proof follows from theorem 3.1 and lemma 2.2

Corollary 3.5 The square of an ionic graph is the graph itself.

Proof follows from theorem 3.1 and lemma 2.3

Theorem 3.2 Every digraph with non-empty edge set is a simple widen ionic graph.

Proof: Let D be a digraph with non-empty edge set. Then there exists at least one pair of vertices u and v such that $uv \in E_D$ or $vu \in E_D$. If $uv \in E_D$ then we have a subgraph S of D with vertex set $\{u, v\}$and edge set $\{uv\}$. Similarly if $vu \in E_D$ then we have a subgraph S of D with vertex set $\{u, v\}$ and edge set $\{vu\}$. Clearly the subgraph S is isomorphic to a graph of an ionic compound which is formed by a pair of atoms having the property that one atom can donate an electron to another atom. Thus we arrived at the result.

Note that a digraph may not be strong widen ionic

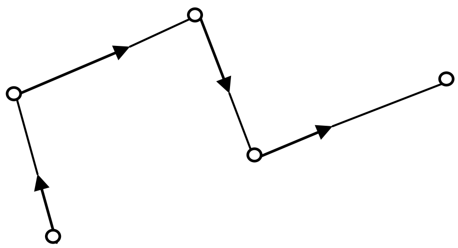
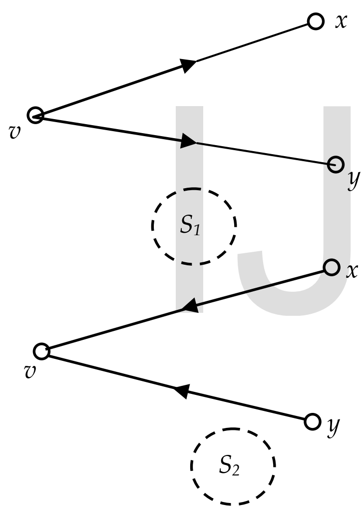


Fig 3.1 An example of digraph which is not strong widen graph

graph. For example, the digraph shown in the figure 3.1 is a digraph but not a strong widen ionic graph. However every digraph is strong widen ionic graph under some certain conditions which leads the following theorem.

Theorem 3.3 A digraph is strong widen ionic if it has atleast one vertex having degree more than two.

Proof: Let D be a digraph and $v \in V_D$ with $d(v)$>2. Then either $d^-(v) \geq 2$ or $d^+(v) \geq 2$. Thus at least one of the following subgraphs is possible



Both the subgraphs S_1 and S_2 are isomorphic to the graph of the ionic compounds $CaCl_2$ and Na_2O respectively. Thus we arrived at the result.

Corollary 3.6 Every connected digraph having more than 3 vertices and a cycle is a strong widen ionic graph.

The proof follows from theorem 3.3

Theorem 3.4 Every connected semi discrete having atleast 3 vertices is strong widen ionic graph.

Proof: Let D be a connected semi discrete graph. Then for any $v \in V_D$, $d^-(v) = 0$ or $d^+(v) = 0$. If $d^-(v) = 0$ then $d^+(v) \neq 0$ and so there exists another vertex $u \in V_D$ such that $vu \in E_D$. Thus $d^+(u) = 0$ and $d^-(u) \neq 0$.

Since $|V_D| \geq 3$, there exists atleast one vertex w distinct from u and v. Again D is connected semi discrete, either $d^-(w) = 0$ or $d^+(w) = 0$ but not both of them are zero.

Now if $d^-(w) = 0$, then $d^+(w) \neq 0$. Therefore $wu \in E_D$ and $d^-(u) \geq 2$. Again if $d^-(w) = 0$, then $d^-(w) \neq 0$. fore $vw \in E_D$ and $d^+(v) \geq 2$.

Similarly if $d^+(v) = 0$, then by interchanging the role u and v, we get either $d^+(u) \geq 2$ or $d^-(v) \geq 2$. By using the proof of the theorem 3.3, we arrived at the result.

4 Representation of Ionic Compounds

Since ionic graphs are isomorphic to the graph of some ionic compounds, these compounds can be characterized with the help of ionic graphs. If D is an ionic graph and C is an ionic compound such that $D \cong D(C)$ then we can easily draw that following conclusions.

(a) The number of vertices of D give the number atoms present in the compound C.

(b) For $u \in V_D$, $d^+(u) > 0$ represents that there exists an atom in C which can donate $d^+(u)$ number of electrons to other atoms of C and thus $d^+(u)$ gives the valency of the corresponding atom.

(c) For $v \in V_D$, $d^-(v) > 0$ represents that there exists an atom in C which can accept $d^-(v)$ number of electrons from other atoms of C and thus $d^-(v)$ gives valency of the corresponding atom.

(d) If $\sum_{u \in V_D} d^+(u) = \sum_{v \in V_D} d^-(v)$, then the compound C is stable.

(e) From the cographic structures, Chemists can retrieve similarity and dissimilarity structures and properties the compounds.

5 Conclusions and Future Works

Molecular graphs are dealing with the study of covalent compounds, particularly alkanes group, but these graphs are inadequate to study ionic compounds. We defined some graphs in such a way that one can easily represent ionic compounds using these graphs. We studied the mathematical structures of these graph and tried to represents some ionic compounds using them. We hope our works will help researchers to get some new ideas about chemical compounds as well as to study some structural models. We will continue our study in structural arrangements of ionic compounds and in characterizing the ionic compounds using these graphs.

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