Aaron Germuth UNBC

Investigation of Switching Behavior in Hydrocarbons with 4-ports Attachments
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Summary: A common trend among organic molecules such as cyclic unsaturated hydrocarbons is the alteration of single and double bonds. It is postulated that such alternating paths have the ability to conduct electric current [1,4]. This is an essential characteristic that opens up the possibility to design molecular computing elements using unsaturated hydrocarbon molecules. When electricity is conducted, the path is toggled – every double bond is converted to a single bond, and vice versa. At certain atoms, called *ports*, of these molecules other molecules can be attached to make changes and observe their behaviour. The proposed project is interested in developing algorithms to investigate the behaviour of 4-ports unsaturated hydrocarbon molecules. Consequently, we intent to design a software framework where such behavioural studies of 4-ports unsaturated hydrocarbon molecules can be conducted systematically.

Importance of this research: As computers and their circuitry gets smaller and smaller, eventually computation must be achievable at the molecular level. One such possibility is to store information within a molecule based on the configuration of its covalent bonds [3]. Not only will many molecules be able to store useful information, but they can be processed by suitably controlling electricity through these molecules. This suggests the possibility to use individual molecules as computational elements. We can use computer programs to design and then synthesize such molecules.

State of the art: The literature related to the study proposed in this project is very recent and limited. Particularly, a limited but innovative work by Prof. W.H Hesselink's group [1-3] is the most relevant literature to our research. Their work has planted the seed of using graph theory to model cyclic unsaturated hydrocarbons and then study their switching behaviour. In their model, nodes represent atoms, edges represent their covalent bonds, and certain special nodes are labelled as ports that will act as junction to the external world. Anything can be attached to a port, as it does not affect the interchanging of bonds, and does not have to contain a double bond. Prof. Hesselink has shown the switching behaviour of bonds is decided entirely by the configuration of the ports. Each possibility is called a cell, and the work is devoted to discovering which cells of all possible ones are Kekule cells. Kekule cells correspond to perfect matches in graphs. This means every node will have a double and single bond (other than the ports), which corresponds to real aromatic molecules with all their electrons paired (stable). Each Kekule state represents a resonance structure of its corresponding molecule, and therefore the more Kekule states that are found, the more stable that molecule.

Motivation for our work: This area of research is relatively new, and of the few studies that have been done, none of them have restricted the atoms to only allow 4 connections. Carbons (the skeletal backbone of organic molecules) electron configuration (valency) only allows for up to 4 single bonds. In order for the results obtained by Prof. Hesselink to be chemically applicable, they must have this limitation. Our goal is to first confirm, and then advance his results by adding this vital restriction and coming up with a set of Kekule cells that match carbon's valency.

References:

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[4] A.J. Heeger, S. Kivelson, J.R. Schrieffer, and W.-P Su. Solitons in conducting polymers, *Rev. Mod. Phys.*, 60:781, 1988.