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Georges Brunel – A Forgotten Pioneer of Chemical Graph Theory

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Abstract

In the 1890s, the French mathematician Georges Brunel (1856–1900) used graphs in chemistry, considered what nowadays is called "molecular graph", enumerated isomers, and also conceived the adjacency matrix. The life and work of this forgotten pioneer of chemical graph theory is briefly described.

1 Biography of Georges Brunel

Georges Édouard Auguste Brunel was born on September 17, 1856 in Abbeville, France. In the period 1877–1880 he studied mathematics in Paris et the *École normale supérieure*. In 1880/81 he spent a year in Leipzig, Germany, working with Felix Klein. After returning to Paris, in 1881 he became Assistant at the *École normale supérieure*. In 1882 he moved to Algeria, where he was lecturer for mechanics at the *École de Sciences* in Algiers. In 1883 he defended his doctoral thesis on hyperelliptic functions at the *École normale supérieure* in Paris, after which he got a professor position at the *Faculté des Sciencees* in Bordeaux. He held there the chair of pure mathematics (later changed to chair of calculus) until his death. He died on July 24, 1900 in Bordeaux, at the age of 43.

In Bordeaux there was a scientific society called *Société des sciences physiques et naturelles*. This society published a journal: "*Procès–verbaux des séances de la société des sciences physiques et naturelles de Bordeaux*", in which Brunel communicated all his works relevant for chemical graph theory.

Brunel published some 97 mathematical papers, covering such vide fields as analysis, geometry, topology, algebra, number theory, combinatorics, and knot theory. A few are related to graphs (which Brunel called "*réseaux*" = networks) [7].

2 Chemical graph theory of Georges Brunel

In 1894 Brunel got interested to regular graphs [4, 7]. This motivated him to consider graphs pertaining to organic molecules, which he called "*polyméres du carbone*" [5]. These would resemble regular graphs since all vertices corresponding to carbon atoms are of degree 4, *réseaux réguliers à sommets quadrilatéraux*.

In the 1898/99 issue *Procès–verbaux* appeared Brunel's second and last chemical graph theory paper [6]. There he constructed a molecular graph in the (modern–days) usual manner, and then arrived at the skeleton graph by removing the vertices of degree 1 and 2. In this paper he counted the isomers of benzene, i.e., of the chemical species of formula C_6H_6 , i.e., in the notation usual for his time, of formula C^6H^6. His result was 919 possible isomers, quite different from the true value of 217 and 328.[1] In [6] Brunel also counted isomers of alkanes, and corrected some erroneous values earlier obtained by Cayley.

In his 1894 paper [4], Brunel arrived at the concept of adjacency matrix of a graph [7]. This, however, was not used in any of his chemistry–related considerations.

[1] There are 217 distinct molecular topologies consisting of six four–valent carbon and six one-valent hydrogen atoms, thus possessing formula C_6H_6 . If diastereomers and enantiomers are taken into account, then the total number of isomers becomes 328. Most of these "possible" structures are highly strained and unlikely to exist. Only about 80 might be reasonably stable, and less than 40 are known to date [9].

3 Georges Brunel forgotten in chemical graph theory

The author of this article learned about Georges Brunel and his contributions to chemical graph theory from the paper [7], published in a mathematics journal. The fact is that Brunel's papers on graph theory, including [4–6] are listed in the bibliography in the seminal book [3], but otherwise in this book Brunel is not mentioned at all. Neither is there any mention of Brunel in Balaban's famous book [1], in particular not in its Chapter 1 [2]. In his extensive review [10], Rouvray covers in detail the early history of chemical graph theory (in the 18th and 19th century), but fails to mention Brunel. The same omission exists also in the present author's book [8], containing a brief survey of the history of chemical graph theory. The situation is not different in other mathematical chemistry books and papers.

Thus, it may safely be concluded that George Brunel is a completely forgotten pioneer of chemical graph theory.[2] The present text is aimed at helping to ameliorate this sad fact.

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