LETTERS TO THE EDITOR

PERCEPTION OF TOPOLOGICAL SYMMETRY

Dear Sir:

I am delighted to see that my critique[1] appearing in this Journal has encouraged C. Jochum and J. Gasteiger to present[2] previously unreported steps in their algorithm for the canonical numbering of chemical graphs. They refer to these steps as "small details", but in fact they are the very essence of any routine which reliably finds unique numberings for, or perceives topological symmetry of, arbitrary graphs. No matter what set of scoring rules is used to establish a partial ordering among the nodes, one must at some point provide for the node-by-node and edge-by-edge comparison of differently numbered "copies" of the graph being processed. In their latest paper, Jochum and Gasteiger include exactly such a comparison, and I am convinced that as extended their approach is theoretically sound.

However, I did not misunderstand their previous article[3] (unless lack of clairvoyance can be classed as misunderstanding); I simply took it at face value. My critical comments, and the counterexamples I presented, were completely appropriate in the context of that article. In contrast with their latest offering, Jochum and Gasteiger's previous paper did not present a sound and accurate definition of constitutional symmetry, nor did it indicate in any way that crucial steps had been omitted. I am sympathetic with the problems of describing a complex algorithm in the limited space of a journal article, but if space limits the development of a fundamental concept, it is the responsibility of the author to say so, and to indicate that a reader must obtain additional information before he tries to implement the described procedure.

(1) R. E. Carhart, "Erroneous Claims Concerning the Perception of Topological Symmetry", *J. Chem. Inf. Comput. Sci.*, **18**, 108–110 (1978).
(2) C. Jochum and J. Gasteiger, "On the Misinterpretation of Our Algorithm for the Perception of Constitutional Symmetry", *J. Chem. Inf. Comput. Sci.*, paper in this issue.
(3) C. Jochum and J. Gasteiger, "Canonical Numbering and Constitutional Symmetry", *J. Chem. Inf. Comput. Sci.*, **17**, 113–117 (1977).

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INSURANCE FOR DRUG PATENTS

Dear Sir:

Research is expensive; e.g., Cilag-Chemie A.-G.[1] mentioned that from its experience the experiments necessary to develop a new product range between 1000 and 10,000. If the substance is an insecticide many thousands of experiments will be needed. The research expenses for producing a new milk powder range between 20,000 and 500,000 DM. Medical research is extremely expensive because a series of compounds are synthesized and tested in animals, and there is a time lapse between the successful experimentation to patent registration of 2–4 years and from registration to the market of 5–10 years;[1] this means the actual life of the patent is less than that mentioned in the law. A new useful invention can consume 60% of the future profits.

As the development of physical methods now enables researchers to identify the constituents of any drug, the drug, under another trade name with some improvements, may be synthesized by imitating manufacturers. From the legal point of view this does not constitute *infringement* unless the manufacture or use of the product is substantially as claimed by the patent. Whatever the decisions of the patent courts and the effort of patent examiners, infringement is difficult to discover; the new improvements on the invention of the first inventing company enable imitating companies to obtain new patents, especially in the field of steroid drugs where isomerism plays a great role. There is no infringement if any one of the material elements of a combination claim is omitted, even without the substitution of anything equivalent to it.[2] Also "a patent for a process is not infringed by selling the product".[3]

This observation was confirmed by Farbwerke Hoechst A.-G.,[4] which stated that from their experience 1–5% of their patents are directly used; 90% of registered patents lose their value within 5 years, devoid of any applicable value.[4]

Patent insurance may be a suitable solution for the huge losses encountered by drug companies due to infringement, imitation, or invention of another drug with better qualities. Payments would be based on the following: (1) the extent to which the drug is promising, (2) the life history of the drug research company, (3) the prevailing competing drugs in the market and the difference in their advantages, (4) the after-effects of these new drugs in comparison with the old ones, (5) the other patents which were registered by other companies around the date of registration of the new insured drug, and (6) the acceptance of the market for this drug.

In my opinion, the main aim of patent insurance is not to compensate the losses of the drug companies but to encourage them to continue research and compete with other companies to develop better qualities for each drug.

Finally, patent insurance is a simple primitive which warrants study and analysis by specialists in several fields.

(1) Cilag-Chemie A.-G., Schaffhausen, private communication, 1/15/74.
(2) Eames vs. Godfrey, 68 U.S. 78
(3) National Phonograph Co. vs. Lambert Co., 125, F 388,389.
(4) Farbwerke Hoechst A.-G., 6230 Frankfurt am Main, 80, private communication 11/1/74.

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