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A REPLY TO SOME COMMENTS FROM PROF. DR. H.-H. SCHMIDTKE

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In essence Professor Schmidtke's criticism[1] of the graph-theoretical approach to chemistry is that such an approach enables one at best to cope only with chemical knowledge which existed up to the early part of the present century. Although these remarks were apparently not directed at me specifically and were intended rather as a criticism of the use of graph-theoretical methods in general, I feel that a reply from me may not be out of order, particularly as the comments were appended at the end of a lecture I gave on the chemical applications of graph theory[2].

Professor Schmidtke also makes two rather sweeping predictions in his comments, these being that (i) physical insight will necessarily be lost if graph theory is ever able to treat adequately the phenomena of quantum chemistry, and (ii) graph theory will not in any case be capable of classifying chemical and physical experience. In support of these assertions he cites work on certain compounds synthesized in recent years, which are novel in that they cannot be described by simple constitutional formulae.

In reply to his broad criticism, it must I think be admitted that up to the present time many of the chemical applications of graph theory have been concerned primarily with knowledge obtained up to the early part of this century.

This in itself, however, cannot be viewed as a serious criticism, since, even if it admitted of no exceptions, any new way of approaching and handling existing data is worthy of consideration. It is by no means necessary that the data treated be of the most recent kind. Moreover, the assertion is not in general valid for there are several well-known exceptions.

As examples of these exceptions, mention might be made of the considerable number of theorems obtained within the framework of simple Hückel theory by a host of workers, especially those in the Trinajstić group[3]. These results have at the very least provided valuable insights into the nature and chemical properties of the systems studied. A second example comes from the field of isomer enumeration, which, by the application of straightforward graph-theoretical methods[4], has yielded a great deal of information pertinent to the classification of chemical species[5]. Yet a third example is to be found in a variety of studies which utilize the concept of transferability[6], in particular in studies involving the use of the additivity principle[7] or, more recently, the use of topological indices[8]. As is well-known[9], such studies can lead to very valuable predictions of the physico-chemical parameters of molecular species.

With regard to Professor Schmidtke's first prediction, I am inclined to agree that the phenomena of quantum chemistry can only be described by a somewhat more sophisticated theory of graphs than that used hitherto. This is not to say, however, that all physical insight will necessarily be lost, as Professor Schmidtke seems to think. Recent work reported in MATCH by Graovac and Trinajstić[10] and Polansky[11] already indicates one possible new approach. Both of these contributions have utilized the concept of the weighted graph, the former within the context of simple HMO theory and the latter in a rather broader framework. Extension of both of these approaches

to molecules having heteroatoms is also feasible. I should like to assure Professor Schmidtke that those of us who use graph theory are as anxious as he is to present as accurate a description of nature as possible. Unfortunately neither the Schrödinger equation nor the graph-theoretical approach is capable of doing that adequately at present.

The second prediction that graph theory will not be capable of classifying chemical and physical experience cannot in general be supported. In fact, in many different spheres, graph theory has already been used for just this purpose. As mentioned above, graph theory has been used extensively for the enumeration of chemical species, and more recently for the storage and retrieval by computer of chemical data by means of systems such as the line-formula notational system of Wiswesser[12]. Even species possessed of heteroatoms or multicentre bonds are not necessarily excluded here, since weighted or rooted graphs may be used to represent them.

In conclusion, it should be stressed that, because solutions to difficulties arising from the use of graph theory may not always be immediately apparent, this in no way implies that the discipline has no rôle to play in the interpretation of the physico-chemical world. Furthermore, it should not be forgotten that, even though applications of graph theory in chemistry can be traced back well over a century, the more sophisticated usages are of relatively recent vintage, and accordingly not as well matured at present as one might wish. At this stage therefore it is difficult to make definitive pronouncements on all the points raised here, though in general I foresee an eventual outcome rather different from that envisaged by Professor Schmidtke. If I may, I would suggest to Professor Schmidtke that forbearance on his part may perhaps be the more appropriate course of action, for in the long run this will, I feel sure, be seen to have been justified.

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