

Editorial

Now that a second series of 25 volumes of Theoretica Chimica Acta is complete, it is once again a particularly appropriate time to thank all those who have contributed to the journal's success: the authors, the co-editors, the referees, the editorial staff, and, last but not least, the publishers.

There have been hardly any changes as far as the scope of the journal is concerned. The portion of theoretical papers not belonging to quantum chemistry has slightly increased, and the extent to which purely computational quantum chemical papers should be considered is still a crucial problem.

The organic chemist, when carrying out a CH analysis with the aid of an automatic analyser, will not claim that the result he obtains is a contribution to research in analytical chemistry. Judging superficially on the basis of this reflection one could feel tempted to conclude that if a computational program is applied to a molecular problem the result will not be a contribution to research in theoretical chemistry. However, this is not quite so, as there is still no theoretically founded mathematical method applied in quantum chemistry the error of which could be estimated from the start. Computational methods used in quantum chemistry are, in the last analysis, empirical, and their applicability can therefore only be ascertained by concrete computations and subsequent comparison with experimental results.

Computational works not concerned at all with the above questions but treating problems of general chemical interest, using well-known "successful" programs, have not appeared in the journal as often as formerly, as they cannot be considered, in the strict sense of the word, contributions of theoretical chemical interest.

All in all, the journal has, in my opinion, continued to be a valuable specialized medium of publication. I hope that this will remain the case in the future.

Hermann Hartmann

Mainz, January 25, 1979

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