LETTERS TO THE EDITOR

CANONICAL NUMBERING

Dear Sir:

We have been following with some interest the controversy appearing in this Journal regarding canonical numbering and various types of symmetry.[1-4] The first article by Jochum and Gasteiger[1] contains a number of incorrect and misleading statements about both their work and the work of those who preceded them.[5,6] Canonical numbering or naming algorithms ultimately must compare alternate numberings to determine which is "best". In order to reduce the different numberings to a manageable level, Morgan used a simple graph theoretical concept to initially partition the atoms into various ranks. Randic pointed out that the partitioning could be refined with the use of additional graph theoretical concepts.[7] Thus it is possible to shift more of the effort from the comparison step to the partitioning step. This is a trade-off which may or may not reduce the computer time required. Jochum and Gasteiger, however, strongly imply there is some serious problem with the Morgan algorithm (incomplete partitioning) which leads to "ambiguities". There are no such ambiguities. As implemented by the Chemical Abstracts Service, the only ambiguity is that of stereochemistry, and that is resolved in a text descriptor field. Jochum and Gasteiger also strongly implied that they had a "simple" algorithm which gave complete partitioning, eliminating the need for a comparison step. Carhart correctly pointed out that this was not the case.[2] Subsequent publication of the details of Jochum and Gasteiger's indicated that it does contain a comparison step.[3]

It should also be noted that any canonical naming algorithm will detect symmetry at the level of specificity at which it operates, and can also be made to find all lower levels of symmetry. Thus implementations of the Morgan algorithm[5] or the more completely described Jochum and Gasteiger algorithm[3] will detect constitutional symmetry. The stereochemically extended Morgan algorithm[6] can detect configurational symmetry as well. It has been noted that this can easily be extended even to conformational symmetry.[6]

In the same issue of this Journal in which their rebuttal to Carhart's comments appeared, Gasteiger and Jochum[8] address another well-worked-over area, with no remaining major problems, namely ring perception. They again make a number of misleading and incorrect statements. For example, they indicate that all earlier algorithms, "except Fugmann's,[9] have to generate all rings of a given system before selecting their particular set". The Corey and Petersson algorithm[10] does not generate all rings. The Wipke and Dyott algorithm[11] is derided for, of all things, being implemented in Fortran, with a number of small, well-defined assembler routines. This supposedly makes it less portable than their PL/I program. This is an implementation detail, but they might be interested in knowing that the Wipke and Dyott algorithm has been installed on a number of machines, ranging from Modcomp to DEC to IBM. How many machines even have a PL/I compiler? One other implementation detail of interest, the Wipke and Dyott algorithm required 0.20 s on a DEC KA-10 to process Vobtusine[11] compared to 0.52 s on an AMDAHL 470 V6 for the Gasteiger and Jochum algorithm.[8] Since the AMDAHL 470 V6 is roughly 20 times faster than the DEC KA-10, the Gasteiger and Jochum algorithm and/or implementation appear to be about 50 times slower.

On a more general level Jochum and Gasteiger complain that Carhart did not contact them "directly to help him clarify his misunderstanding".[3] Yet it is obvious from the large number of misinterpretations and/or misrepresentations which appear in their work[1,8] that they made no attempt to clarify their misunderstandings by discussing such matters with the original authors. Publishing last on a particular subject accords one considerable power, power that carries with it the responsibility to treat the preceding work with fairness and objectivity.

For ten years now there has been rather intense competition between the research groups involved in computer assisted synthetic design. The advantages, both real and imagined, of each system have been touted without end, but there is too little communication and cooperation. Researchers in one group often are forced to, or just choose to, reinvent algorithms which are only marginally different, let alone better, than those already developed by other groups. Could not the field advance more rapidly if there were more cooperation and communication?

(1) C. Jochum and J. Gasteiger, *J. Chem. Inf. Comput. Sci.*, **17**, 113–117 (1977).
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(4) R. E. Carhart, *J. Chem. Inf. Comput. Sci.*, **19**, 56 (1979).
(5) H. L. Morgan, *J. Chem. Doc.*, **5**, 107–113 (1965).
(6) W. T. Wipke and T. M. Dyott, *J. Am. Chem. Soc.*, **96**, 4834 (1974).
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(8) J. Gasteiger and C. Jochum, *J. Chem. Inf. Comput. Sci.*, **19**, 43–48 (1979).
(9) R. Fugmann, U. Dölling, and H. Nickelson, *Angew. Chem., Int. Ed. Engl.*, **6**, 723 (1967).
(10) E. J. Corey and G. A. Petersson, *J. Am. Chem. Soc.*, **94**, 460–465 (1972).
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THEY SERVE BUT RARELY PUBLISH

Dear Sir:

I am afraid that your May editorial will not help attract analytical chemists as authors for JCICS. In the second and third paragraphs, especially, you described analytical chemists as service people, or "intermediaries between those who are innovative and those who make and sell products". I protest! There are, of course, routine analysts who do strictly service work, just as there are routine synthesists, but these are not the ones who publish research papers.

If you really want to attract innovative papers, you can find some from the analytical community, but only if you demonstrate an understanding of the research role of modern analysis. I know from many personal conversations that you have this understanding, but your editorial did not bring it out.

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Dear Sir:

Your excellent presentation of the role of chemical information specialists (May issue of this Journal, p 2A) could and should reach the users of the information services in a more