



Journal
of The
Chemical
Society

Perkin Transactions II

5
1978

NOTICE TO AUTHORS—No. 12/1977

Publication of Theoretical and Computational Papers

The Primary Journals Committee has been considering future policy towards the publication of papers with a heavily computational content, particularly where these involve standard methods, such as semi-empirical or *ab initio* calculations of molecular electronic properties using readily available computer programmes. Many such papers report what would be considered 'routine work' in other areas of chemistry, and have often included extensive detail.

A specialist sub-committee formulated a set of proposals which were circulated to a large representative sample of theoretical chemists and met with general acceptance. These, with the comments on them, form the basis of this notice.

The Primary Journals Committee recognises that computational work can play a valuable role in chemistry, and will probably continue to do so on an increasing scale. It accepts the time-honoured principle that the first criterion for publication of a paper by the Society should be the worthiness of the chemical problem considered, rather than the particular techniques employed by the author. For example, the use of a new computing algorithm, or the modification of a programme, would not usually, on its own, provide sufficient justification for publication.

The Primary Journals Committee recommends to authors the following guidelines for the preparation of computational papers, so that the material can be presented concisely and effectively.

- (i) Papers should be submitted to the appropriate journal: a paper containing innovations in theory to *Faraday Transactions II*, one in which the computations are incidental to the chemistry to *Perkin, Dalton, or Faraday I Transactions*. Papers concerned mainly with computational details are unlikely to be accepted.
- (ii) The purpose of the paper and the precise ob-

jectives of the calculations performed should be clearly stated: the results obtained should be reported only in so far as they relate to those objectives.

- (iii) Many papers use a routine procedure based on a well documented method, be it semi-empirical or *ab initio*. It is then sufficient to name the particular variant, referring to key papers in which the method was developed, to cite the computer programme used, and to indicate *briefly* any modification made by the author. A review of theoretical background would be out of place, but an author should say why he considers the method adequate for his purposes.
- (iv) Extensive tabulation of numerical results, such as the magnitudes of atomic orbital coefficients, electron populations, contour maps of molecular orbitals and electron densities, and peripheral material of a similar nature, is normally unnecessary. Lengthy line-by-line discussion of such material is, as a general rule, quite unacceptable. Where an author considers that there is a special need to make such material available to other workers, as with highly accurate computations, for example, then this may be deposited with the British Library as a Supplementary Publication. Such material should be submitted with the main paper, clearly distinguished from it, and referred to in the main text.

Guidelines can never provide sufficient criteria for acceptance or rejection of a paper. Critical assessment of the theoretical methods used in a computation, and of their suitability for the purpose in hand, will continue to be entrusted to specialist referees who must also decide whether the results are new and advance science.