

In this issue

Parallelized chemistry software

Chemists have long been major users of computers. Improvements in hardware resources are rarely seen as adequate since the problems investigated get scaled more rapidly. The development of parallel computers represents a possible solution. Indigenous efforts are being eagerly followed. However, usage will ultimately be determined by efficient software developed on these machines.

Current Science has periodically carried articles describing the development and usage of parallelized versions of programmes to carry out electronic structure calculations at the LCAO-MO and post-Hartree-Fock levels. In this issue, Paithankar *et al.* (page 585) provide details of a Molecular

Dynamics Simulation package for a transputer network. The efficiency of the programme is illustrated with an illustrative simulation on liquid water.

It is hoped that a full complement of computational chemistry software optimized for indigenous parallel computers becomes widely available in the near future.

J. C.

Fullerenes from camphor

The initial spark for the current excitement in fullerenes was provided by the dramatic structural proposed of Smalley and Kroto for the carbon cluster of mass 720. However, experimentalists got fully involved only after a simple preparative procedure for C₆₀ from graphite

became available. Alternative starting materials, including benzene, have been suggested. There is continued scope for developing newer preparative methods, purification techniques, etc. in fullerene chemistry.

K. Mukhopadhyay *et al.* (page 602) discuss a hot filament CVD method starting from a readily available source, viz. camphor. While the methodology is unlikely to convince organic chemists as a ready source of pure C₆₀, the experimental results are of general interest. FAB mass spectrometry and scanning electron micrography have been used to demonstrate the formation of C₆₀ as well as a host of smaller fullerenes. Interestingly carbon tubules of various sizes have also been produced.

J. C.