

# Editorial

---

## Journal to Publish Data Calculated from Computer Simulations and Molecular Mechanics

The 21st century has heralded in the electronic age, and the calculation of physical properties from either potential functions or molecular mechanics has become accepted by the scientific community. In keeping with that sentiment, the Journal will now accept papers containing molecular simulation and molecular mechanics calculations provided the emphasis is on the calculation of properties of pure materials and/or mixtures. In particular, the Journal wishes to encourage the submission of papers containing reference type data useful for benchmarking and testing programs and papers that provide reliable property values when experimental data do not exist or are difficult to measure. Large amounts of data and computer codes as ASCII files that are not acceptable for publication can be archived in the Supporting Information of the Journal, which is available free of charge.

From second quarter 2001, the Journal will move rapidly to a Web-based manuscript submission processing system. Authors will be able to submit their manuscript to an ACS Web site, and it will be converted to a pdf file. Reviewers who agree to review a manuscript will be given an access code to download the manuscript, and they can submit their review to the Editor through the Web. Revised manuscripts can be resubmitted and galley proofs reviewed via the Web site through access codes provided. The traditional method of handling manuscripts will remain an option.

NIST, IUPAC, CODATA, and DIPPR are involved in a joint effort to develop an electronic archival database for published property data. This endeavor will require the cooperation of authors and editors of journals. In the longer term, this initiative will provide immeasurable benefits to researchers, data evaluators, and data users. From mid-2001 authors of selected property data will be informed on how to submit their data through the Web to the archival database. This will eventually be extended to all property types as additional Web entry routines are developed.

In September 2000, the Thermodynamics Research Center (TRC), previously a center of the Texas Engineering Experiment Station, at Texas A&M University, College Station, became part of the Physical and Chemical Properties Division of the National Institute of Standards and Technology in Boulder. TRC will be the lead group in the NIST initiative to host the electronic archival database.

Journal space remains at a premium. Manuscripts dealing solely with data on densities and speed of sound in limited temperature and pressure ranges will not be accepted unless the authors provide a convincing case that the results are of real theoretical interest, are of use in industrial design, or are presented in support of a wide ranging correlation or predictive scheme. Otherwise, to be considered for publication such data must be accompanied by measurements on other useful properties.

**Kenneth N. Marsh**, *Editor*

JE000490A