Editorial

It is with great enthusiasm that I took over as Editor-in-Chief of the *Journal of Chemical & Engineering Data* in November, 2010. With the many global research challenges that face us in energy, water, food, and health that require quality thermodynamic and physical property data from experiment or computation, this is certainly an exciting time for molecular thermodynamics and for the Journal.

This is also a great time to thank Kenneth N. Marsh for his nearly 20 years of dedicated service to the Journal as Editor-in-Chief. He saw the development of the Journal from a quarterly with a publication of just 500 pages per year to a monthly publication of more than 5000 pages per year. He grew the Journal from one to four associate editors and instituted the cooperation with the Thermodynamics Research Center (TRC) of the National Institute of Standards and Technology (NIST) to provide invaluable information to authors, reviewers, and editors on previously published data and the quality of the data presented. I am extremely indebted to Ken for his expert stewardship of the *Journal of Chemical & Engineering Data* over the past two decades, which has made possible this opportunity for me to serve the thermodynamics community. We look forward to honoring Ken with a special issue of the Journal. The deadline for submission to this special issue will be July 1, 2011.

There are a few items of note as we move forward:

(1) We have eliminated two classes of articles: short articles and correlations. While rapid publication of important experimental data, computational data, and correlations would be valuable to the community, it turns out that time to publication for short articles and correlations have actually been longer than regular articles. In addition, we have seen a trend for authors to provide very minimal material and essentially no discussion or interpretation of the results in the short articles. Therefore, we have eliminated both short articles and correlations. Authors of regular articles should make sure that they contain a substantial quantity of high quality results and that they back up their interpretation of the results with quantum calculations and spectroscopic data. As always, uncertainties must be given and all results should be compared with previously published data. Correlations based on published experimental, evaluated, or calculated data that cover the whole thermodynamic surface are welcome as regular articles or, perhaps more appropriately, as reviews.

(2) The procedure by which the TRC of NIST provides input has been modified. First, the authors are no longer required to provide a Data Summary. However, the data tables in the articles should be presented in the format appropriate for the NIST data capture system. This is discussed in the Guide to Authors and examples of acceptable tables can be found at http://trc.nist.gov/JCED-Support.html. Upon submission, NIST will provide a literature report to the authors and reviewers that contain data from the NIST database for the systems under investigation. NIST will conduct the data evaluation at the end of the review process, immediately prior to acceptance of the article, in order to ensure that the data are satisfactory and that all necessary corrections have been made.

(3) The backlog of papers that caused long periods between when articles were published as ASAP articles on the web and when they appeared in the Journal has been largely resolved in 2010. Given the continued growth in submissions to the Journal, we encourage authors to continue to present their results clearly and concisely and to forego the inclusion of nonessential figures and tables.

(4) It is extremely helpful if authors can provide qualified and appropriate suggested reviewers. I remind authors that none of the suggested reviewers can be from your own institution, not more than two can be from the country in which the work was conducted, and they should not include collaborators or former mentors or mentees. It is helpful if the suggested reviewers have published in ACS journals.

(5) While the Journal has accepted computational papers in the past, I would like to put additional emphasis on this method of data production. We are particularly interested in the calculation of thermophysical properties from molecular properties through the use of quantum chemistry, molecular simulation, and molecular mechanics, particularly when they include detailed comparison with experimental data. Calculation of ideal gas properties from the methods of statistical mechanics is also of interest. We anticipate a topical issue focused on simulations that will have a deadline for submission in the second half of 2011.

(6) Decreasing time to publication is an important goal for the Journal in the coming year. Toward this goal, we have decreased the time requested for reviewers to provide their comments and times for authors to provide their revised manuscripts.

Joan F. Brennecke Editor-in-Chief

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