

# (Slight) Expansion in Scope for JPCRD

Cite as: J. Phys. Chem. Ref. Data 48, 010401 (2019); doi: 10.1063/1.5090506

Submitted: 21 December 2018 • Accepted: 28 January 2019 •

Published Online: 8 February 2019



Allan H. Harvey<sup>1,a)</sup> and Donald R. Burgess, Jr.<sup>2,b)</sup>

## AFFILIATIONS

<sup>1</sup>Co-Editor, Applied Chemicals and Materials Division, National Institute of Standards and Technology, 325 Broadway, Boulder, Colorado 80305, USA

<sup>2</sup>Co-Editor, Chemical Sciences Division, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, Maryland 20899, USA

<sup>a)</sup>Electronic mail: aharvey@boulder.nist.gov

<sup>b)</sup>Electronic mail: dburgess@nist.gov

<https://doi.org/10.1063/1.5090506>

The *Journal of Physical and Chemical Reference Data* (JPCRD) has historically limited its scope to critical evaluations of existing data in a field, producing recommendations for the best available physical and chemical property data, preferably with uncertainty analysis. In early 2018, the scope was expanded to include Review Articles, which might describe and document a reference database, review the data situation in a particular field, provide an overview of a series of JPCRD articles, review reference-quality measurement techniques, or review data evaluation methods.<sup>1</sup>

JPCRD has excluded from its scope original experimental or theoretical work, such as that found in the primary research literature; the only exception is when the experimental or theoretical results are needed to fill a “gap” in the input data for a paper whose fundamental purpose is producing critically evaluated correlations or recommended data.

We are now expanding this scope slightly. While most experimental measurements and theory will still be out of scope, we will publish experimental or theoretical work if—in the judgment of the Editors—it provides definitive “reference data.” By this, we mean data that are clearly the most accurate possible (with small and well-documented uncertainties) and that provide a state-of-the-art standard that is expected to last for many years. Especially welcome are data that can serve as a reference for purposes outside their immediate context, such as calibration of instruments. Examples of past work that could fit in this category include the experiments that established the

0.01 K difference between the ice point and the triple point of water (thus setting 273.15 K as the zero of the Celsius scale),<sup>2</sup> the careful determination of the absolute viscosity of liquid water that has served as a calibration standard for decades,<sup>3</sup> the accurate absolute determination of the dipole moment of the OCS molecule that is a reference for spectroscopic determination of dipole moments,<sup>4</sup> measurements or calculations that establish the energies of key molecules or ions with sub-chemical accuracy for use in a thermochemical network to provide self-consistent energies for related compounds,<sup>5</sup> and the *ab initio* computation of low-density thermophysical properties of helium for use in calibrations and metrology.<sup>6,7</sup>

As always, authors with questions about the suitability of an article for JPCRD are encouraged to contact either of the Editors.

## REFERENCES

<sup>1</sup>A. H. Harvey and D. R. Burgess, Jr., *J. Phys. Chem. Ref. Data* **47**, 010401 (2018).

<sup>2</sup>H. F. Stimson, *J. Wash. Acad. Sci.* **35**, 201 (1945).

<sup>3</sup>J. F. Swindells, J. R. Coe, Jr., and T. B. Godfrey, *J. Res. Natl. Bur. Stand.* **48**, 1 (1952).

<sup>4</sup>J. S. Muentert, *J. Chem. Phys.* **48**, 4544 (1968).

<sup>5</sup>A. Ganyecz, M. Kállay, and J. Csontos, *J. Phys. Chem. A* **122**, 5993 (2018).

<sup>6</sup>J. J. Hurly and J. B. Mehl, *J. Res. Natl. Inst. Stand. Technol.* **112**, 75 (2007).

<sup>7</sup>W. Cencek, M. Przybytek, J. Komasa, J. B. Mehl, B. Jeziorski, and K. Szalewicz, *J. Chem. Phys.* **136**, 224303 (2012).