

Abstract Submitted
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The Equation of State of Water in the MPa to TPa Regime J.

MICHAEL BROWN, Earth and Space Sciences, University of Washington — The thermodynamic properties of water, in continual refinement on the basis of evolving experimental and theoretical methods, span an enormous range of volume, temperature, and pressure. A current generation equation of state can accurately represent experimental data below 100 MPa but fails to match within experimental uncertainties a body of high-pressure data. B-spline basis functions (piece-wise continuous polynomials) lend themselves to regularized linear and non-linear inverse techniques and can represent equation of state surfaces. Here, a sixth order tensor b-spline for the free energy is used to fit sound speeds, specific heats, densities, and thermal expansivities in accord with estimated uncertainties. This framework for the assimilation of data allows for flexible fitting to arbitrary precision. Once a system is adequately represented, revisions are easily accomplished in the face of new data or revised interpretations. The new equation of state fits low-pressure data as well as static and shock data extending to more than 100 GPa. Since this representation contains no theoretical assumptions, it provides an unbiased estimator for comparisons with theory. For example, super ionic behavior in the fluid phase is evaluated.

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