

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Thermodynamics of Supercooled Water VINCENT HOLTEN, CHRISTOPHER BERTRAND, MIKHAIL ANISIMOV, JAN SENEGERS, Department of Chemical and Biomolecular Engineering and Institute for Physical Science and Technology, University of Maryland, College Park, MD 20742 — We present the currently available experimental information for the thermodynamic properties of supercooled ordinary and heavy water and the possibility of modeling these thermodynamic properties on a theoretical basis. Part of the interest into the thermodynamic behavior of supercooled water is caused by an anomalous temperature dependence of the heat capacity, the compressibility and the thermal expansivity. We show that by assuming the existence of a virtual liquid–liquid critical point in supercooled water, the theory of critical phenomena can give an accurate account of the experimental thermodynamic-property data up to a pressure of 150 MPa. In addition, we show that a semi-empirical extension of the theoretical model can account for all currently available experimental data in the supercooled region, up to 400 MPa. Critical-point thermodynamics describes the available thermodynamic data on supercooled water within experimental accuracy, thus establishing a benchmark for any further developments in this area.

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Date submitted: 26 Nov 2011

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