Abstract Submitted
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Thermodynamics of high-pressure H_2O phases[1] VLADIMIR TCHIJOV, GLORIA CRUZ LEON, UNAM, Mexico, RAINER FEISTEL, Baltic Sea Research Institute, Germany — New $P-V-T$ EOS of ices III and V have been derived [1], as well as new isothermal EOS of ices VII and VIII. MD simulations have been carried out to calculate the densities of ices III, V and VIII as functions of pressure and temperature; the TIP4P and TIP5P models have been adopted. A scheme [2] for calculating the heat capacity of ices II, III, V, VI, and VII has been applied. Recently developed new Gibbs thermodynamic potential function of ice Ih [3] has been used to calculate the 100 K Hugoniot of ice for pressures up to 0.5 GPa; the results are in good agreement with experimental data of Stewart [4]. The validity of the existing EOS of liquid water in the metastable region at high pressures has also been investigated. The IAPWS-95 Formulation was found to be the only EOS of liquid water valid in the low-temperature metastable region both at low and at very high pressures. [1] V. Tchijov, R. Baltazar Ayala, G. Cruz Leon, O. Nagornov, J. Phys. Chem. Solids **65**, 1277 (2004). [2] V. Tchijov, J. Phys. Chem. Solids **65**, 851 (2004). [3] R. Feistel, W. Wagner, J. Mar. Res. (2005, in press). [4] S. T. Stewart, PhD Thesis, California Institute of Technology (2002).

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Vladimir Tchijov
UNAM

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