EPSC Abstracts
Vol. 12, EPSC2018-579, 2018
European Planetary Science Congress 2018


# Comprehensive high-pressure ices EoS for icy world interior

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## Abstract

New X-Ray diffraction (XRD) volume data on ice III, V and VI were collected in-situ in the 200-1800 MPa and 220-300 K range. The accuracy and density of the data allow to derive Mie-Gruneisen equations of state (EoS), providing other thermodynamic parameter such as their thermal expansion coefficient, bulk modulus or heat capacity as a function of pressure and temperature. These new comprehensive EoS enable accurate thermodynamic calculation of ice polymorphs in a framework directly usable for planetary interior modelling.

## 1.Introduction

Water is distinguished for its rich pressure (P) – temperature (T) phase diagram: currently, in which 17 polymorphs of ice have been experimentally identified. Some of these high-pressure forms are believed to be present in icy worlds like Europa, Ganymede, or Titan and newly discovered ocean exoplanets **[1,2]**. These icy satellites can be covered by a hydrosphere up to 900 km thick. These hydrospheres are probably separated into a sequence of concentric shells of high-pressure polymorphs depending on the depth and the temperature profile. In icy satellites like Titan or Ganymede, ice III, ice V and ice VI are likely to be major components **[3]**. Precise knowledge on elastic properties and thermodynamics of these ice phases as a function of P and T is essential to perform modelling of geological structure and evolution of these satellites.

Surprisingly, despite the high planetary relevance, there are very scarce compressibility data on ice III, V and VI. For ice III, only a few data points using volume measurements **[4,5]** exist and there is no *in-situ* single crystal refinement for pure $H_2O$. Ice V appears to have been even less investigated: the only X-ray diffraction experiment has been performed on recovered quenched sample at ambient pressure **[6]**. Ice VI has been also poorly investigated, and even if recent work has determined its compressibility above 300K **[7]**, lower temperature data are still very sparse.

## 2.Experimental approach

To complete the lack of volume data for high pressure ices, we performed *in-situ* single-crystal and powder X-ray diffraction experiment on ices III and V and VI grown in a cryostat cooled diamond anvil cell (DAC) at the ID15B beamline of the European Synchrotron Research Facility. We were able to obtain many volume pressure-temperature data in the 200-1800 MPa and 220-300 K range for ice III, ice V and ice VI. This dataset surpasses in number and accuracy all of the combined data points previously published for each of these ice polymorphs, which allow to derive precise equations of states.

## 3.Data analysis and results

From our data and previously published PVT data, we derived complete Mie-Gruneisen EoS and thermodynamic properties as a function of P and T for ice III, V, and VI, such as their thermal expansion coefficient, bulk modulus or heat capacity. We combined those with liquid water local basis function Gibbs energy representation **[8]** to provide a comprehensive description of equilibriums of pure water, aiming at providing a solid thermodynamic framework for the description of ices and aqueous solutions when solutes are present.

The measured volumes are significantly lower than previous theoretical EoS by up to 8% for ice III and V, which results in a significant increase of their density, important to predict interior structure and buoyancy relations with salty brines. Other thermodynamic parameters such as the thermal expansion coefficient, bulk modulus, or heat capacity are also obtained for the first time for ice III and V as function of pressure and temperature, as illustrated on figure 1 for ice V.

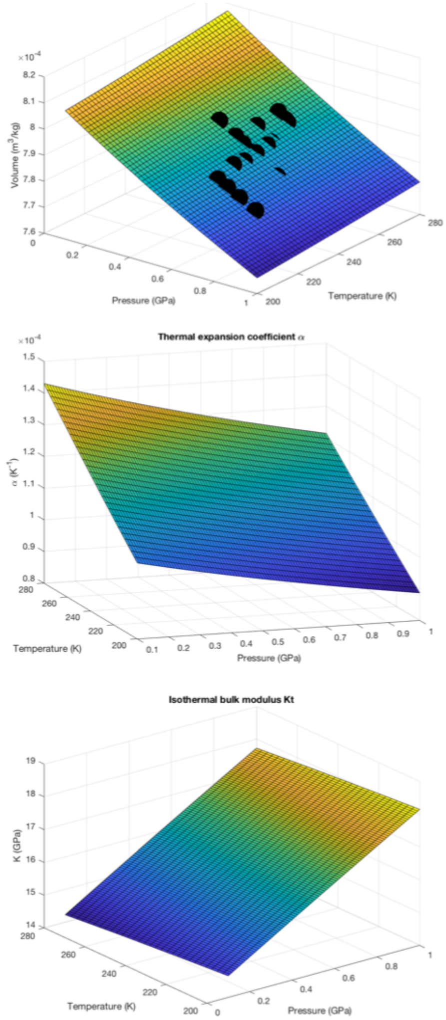


Figure 1: Top, fitted PVT equation of state for ice V, with the data represented as black dots. Middle and bottom, Thermal expansion coefficient and isothermal bulk modulus derived from the fitted PVT-EOS.

# 4.Summary and Conclusions

New volume data were collected in-situ for ice III, V and VI using single crystal and powder XRD. These data enable for the first time to derive accurate equations of states and subsequent thermodynamic parameters such as thermal expansion coefficient and the isothermal bulk modulus. This provide the most comprehensive thermodynamic representation to date of ice III, V and VI, and will lead toward more realistic modelling of icy world interior, as well as water systems at high pressures.

# Acknowledgements

We thank Steve Vance, Evan Abramson, Olivier Bollengier and Tiziana Boffa-Ballaran for helpful discussion and comments on planetary implications, thermodynamic models and XRD measurements.

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