# Water Ice Polymorphs Gibbs Energy Local Basis Functions up to 2300 MPa: Reconciling Water Thermodynamics with the Water Phase Diagram

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We developed the first self-consistent Gibbs representation for ice polymorphs using new experimental data that enables predictions of the water phase diagram and water stable phases thermodynamics with unparalleled accuracy [1]. These representations are constructed based on novel crystallographic volume data collected in-situ at high pressures and low temperatures using synchrotron single-crystal and powder X-ray diffraction. We then employed a hybrid approach by combining this data with experimental and theoretical density of states for each polymorph to constrain their vibrational energies and construct a Gibbs energy representation based on the Local Basis Function framework [2]. The resulting surfaces, combined with liquid $H_2O$ Gibbs representation, provide the first internally self-consistent representation of water, its phase diagram, and metastable properties in the 0-500 K and 0.1-2300 MPa range. This comprehensive description offers a new avenue for exploring water thermodynamics and allows for the quantification of crucial parameters previously unconstrained or uncharacterized, such as pressure-temperature and phase-dependent changes in entropy, volume, latent heat, or coordinates of triple points (II-V-VI; Ih-II-XI; II-VI-XV).

## References

1. Journaux, B., J.M. Brown, A. Pakhomova, I. Collings, S. Petitgirard, P. Espinoza, J. Ott, F. Cova, G. Garbarino, M. Hanfland (2020) Gibbs energy of ices III, V and VI: Wholistic thermodynamics and elasticity of the water phase diagram to 2300 MPa, J. Geophys. Res. Planets, 125, doi: e2019JE006176
2. Brown, J.M., (2018) Local basis function representations of thermodynamic surfaces: Water at high pressure and temperature as an example, Fluid Phase Equilibria, 463C, 18-31 doi:10.1016/j.fluid.2018.02.001