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DEWPython: A Python Implementation of the Deep Earth Water Model

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There are two main methods of calculating the thermodynamic properties of water and solutes: mass action (including the Helgeson-Kirkham-Flowers (HKF) equations of state and model) and Gibbs free energy minimization (e.g. [1]). However, the HKF model has certain regions of pressure and temperature where it predicts the speciation and concentration of solutes inaccurately(e.g. [2]). The Deep Earth Water (DEW) model is a series of HKF-type equations used to calculate the properties of water and solute concentrations at high temperatures (373.15 – 1473 K) and pressures (100 – 6,000 MPa) (e.g. [3]; [4]). The DEW model is synthesized in an Excel spreadsheet and calculates ΔG_f, ΔV_f, and equilibrium constants of reactions. We validate DEW water properties against SeaFreeze, which computes properties for water and ice polymorphs Ih, III, V and VI at 220-500K and 0 – 2300 MPa [5], and solute properties against SUPCRT96 [6]. Combining a different model for the properties of water alongside DEW could prove robust in determining the composition and properties of high-pressure fluids in icy ocean worlds such as Jupiter's moons Europa, Ganymede and Callisto, and Saturn's moon Titan. We present an object-oriented Python implementation of the DEW model, called DEWPython. Our model expands on DEW by increasing efficiency, streamlining and automating the input process, and incorporating SUPCRT in-line. We constructed DEWPython to allow for high-resolution grid calculations of both SUPCRT and DEW data, enabling robust new visualizations. Additionally, our model incorporates minerals and aqueous species from the thermodynamic database slop16.dat [7]. We also present a set of reactions relevant to icy ocean world interiors calculated with the DEWPython and their likelihood of formation.

[1] Leal et al., 2016. Adv. Water Resour. 96, 405–422. [2] Miron et al., 2019. Geofluids 2019, 1–24. [3] Huang and Sverjensky, 2019. Geochim. Cosmochim. Acta 254, 192–230. [4] Pan et al., 2013. Proc. Natl. Acad. Sci. USA 110, 6646. [5] Journaux et al., 2020. J. Geophys. Res. Planets. 125, e2019JE006176. [6] Johnson et al., 1992. Comput. Geosci. [7] Boyer, 2019 https://gitlab.com/ENKI-portal/geopig/blob/master/slop/slop16.dat

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