Crystal chemistry of hydrogen and water storage in planetary interiors

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The crust and mantle of the Earth are made of oxygen minerals. Hydrogen solubility in these minerals controls the abundance of water on the surface and hence the possibility of life on terrestrial planets. Hydrogen can be incorporated in nominally hydrous minerals such as Phase B, superhydrous phase B, phase D, and phase H, or in nominally anhydrous minerals. In the upper mantle and transition zone, the nominally anhydrous minerals may be the principal host phases for H and are capable of incorporating many times the amount of water in the surface oceans.
In the nominally anhydrous minerals at the atomic scale H does not behave like any other cationic substituent. It bonds to a single oxygen with an inter-nuclear distance of less the nominal radius of the oxygen anion to form a hydroxyl anion. Although it does require charge balance, typically a cation vacancy, it does not substitute at cation sites. This has significant impact on elastic properties. The cation vacancies increase the molar volumes and decrease density as well as bulk and elastic moduli. By measurement of the effects of hydration on elastic properties of the nominally anhydrous major minerals of various regions of the mantle it possible to estimate the presence of water. The velocity structure of the Earth is consistent with significant hydration in the upper mantle and transition zone.
In nominally hydrous minerals, with a few notable exceptions, the hydroxyl does not bond to Si, or other high-charge cations, such as C, N, P, or S. In nominally anhydrous minerals, oxygen sites that can be partially protonated to form the hydroxyl can be predicted from Madelung electrostatic site energy calculations. These calculations predict significant hydration in wadsleyite and ringwoodite and limited hydration in olivine. They also predict potential limited hydration in bridgmanite.

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