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Proton behaviour, structure and elasticity of serpentine at high-pressure MAINAK MOOKHERJEE, Yale University, LARS STIXRUDE, University of Michigan — Serpentine occurs in oceanic crust as the alteration product of ultramafic rocks and is a possible candidate for carrying water to the deep earth. The presence of sub-surface serpentine may be manifested by mud volcanoes, high electrical conductivities, and seismic anomalies. Using density functional theory, we predict a phase transition in serpentine near 22 GPa. The phase transition is caused by a re-orientation of the hydroxyl vector coupled with changes in the di-trigonal rings of SiO_4 tetrahedra. The symmetry of the crystal-structure remains unaffected. Evidence of pressure-induced hydrogen bonding is absent in serpentine, as evident from the reduction of O-H bond length upon compression. Results of compression for the low-pressure phase is well represented by a fourth order Birch-Murnaghan finite strain expression with K_O= 63 GPa, K'_O= 10.2 and $K_O K''_O$ = -120, where K is the bulk modulus, prime indicates pressure derivatives, and O refers to zero pressure. At low pressures, the elastic constant tensor is highly anisotropic with $C^o_{11} \sim 2.4 \times C^o_{33}$, and becomes more isotropic with compression. We find an elastic instability near 36 GPa that may be related to experimentally observed amorphization.

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