High-pressure order-disorder transition in Mg_2GeO_4 and Mg_2SiO_4: Implications for super-Earth mineralogy

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Variations in the coordination of silicon within minerals impact their density, viscosity, and affinity for other elements. Yet, experimental proof of silicon coordination numbers exceeding six in high-pressure crystalline silicates has not been found. Such higher coordination phases could play a crucial role in the composition of large rocky exoplanets, where mantle pressures may reach up to ~1 TPa. In this study, we investigated the behavior of magnesium germanate under pressures up to 275 GPa and temperatures exceeding 2000 K through laser-heated diamond anvil cell experiments and density functional theory calculations. The X-ray diffraction data revealed a transition to a disordered cubic Th_3P_4-type structure under pressures greater than 190 GPa, with germanium showing an eight-fold coordination with oxygen. Additionally, our simulations employing the special quasirandom structure (SQS) method indicated a partially ordered tetragonal structure, which appeared similar to the Th_3P_4 structure in our experimental observations. Although direct experimentation at the pressures and temperatures required for these phases to stabilize in the silicate system is not currently possible, we have computationally investigated the potential stability of these phases in Mg_2SiO_4. The results from these studies have been used to construct models to understand the structure and dynamics of Super-Earth planets.