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Phase relations, Fe partitioning, and density changes in pyrolite under the lower mantle P-T conditions

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Phase transitions in pyrolite composition have been studied at pressures to 47 GPa and temperatures along an adiabatic geotherm, using multianvil techniques combined with in situ X-ray observations and other spectroscopic measurements. On the basis of electron microprobe analysis of the recovered samples, we noted a significant increase of the Fe-Mg partition coefficient (KD) between silicate Mg-rich perovskite (Pv) and magnesiowustite (Mw) with increasing pressure to 30 GPa, suggesting the coupled substitution of Mg2+ and Si4+ by Fe3+ and Al3+, consistent with earlier studies. In contrast, KD was found to decrease substantially with pressure above about 40 GPa. EELS and Mossbauer measurements on some recovered samples suggest that the Fe3+/(Fe2++Fe3+) values in both Mw and Pv do not change in this pressure range: iron in Mw is essentially ferrous, while about 60% of iron in Pv is in the ferric state at these pressures. The relative enrichment of iron in Mw above 40 GPa may be related to the electronic high-spin to low-spin transition in ferrous iron in Mw at these pressures, as suggested by some recent theoretical and experimental studies. The density changes determined by a combination of the P-V-T and chemical composition data on individual phases agree well with the typical seismological models, suggesting that pyrolite is a good model composition for the upper to middle parts of the lower mantle.

Keywords: pyrolite, density, iron partitioning, spin transition, lower mantle