Carbon chemistry in Early Earth's magma ocean

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The amount of carbon stored in closed hidden reservoirs, particularly the lower mantle and iron core, is currently unknown, and estimates of the carbon flux between the surface and mantle are model-dependent. To improve our understanding of Earth's global carbon cycle, it is critical to characterize the forms in which carbon existed in the molten early Earth. Here we implement first-principles molecular dynamics to study the evolution of carbon species as a function of pressure (0-140 GPa) and temperature (3000-5000 K) in pyrolite melts with 3.4-6.5 wt.% CO and 5.2-9.8 wt.% CO_2, capturing the range of carbon concentrations in carbonaceous chondrites. Carbon displays a variety of coordination environments, which are affected by the pressure, temperature and oxidation state of the melt. At ambient pressure, carbon exists exclusively as a mixture of CO, CO_2 and CO_3 (unpolymerized carbon) while at higher pressures, the abundance of CO_2 and CO_3 decreases at the expense of CO_4 and complex oxo-carbon polymers (C_xO_y). With increasing pressure, decreasing temperature and decreasing oxygen fugacity, carbon becomes increasingly polymerized, forming multiple carbon-carbon bonds, direct carbon-silicon bonds and complex iron-carbon polymers. The presence of iron-carbon clusters suggests that upon segregation, iron-rich metal may partition a significant fraction of carbon from the silicate liquid, leading to carbon transport into the Earth's core.