# Computational insights on carbonate-silicate-metal melt behavior in the lower mantle

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Carbonate melt is an important carbon-bearing phase in the mantle. While its role in the upper mantle has been well studied [1, 2], its importance in the lower mantle is less understood. The behavior of carbonate melt in the lower mantle is complicated by pressure, temperature, and $fO_2$ conditions [3], as well as reactions with common lower mantle phases such as $MgSiO_3$ and metallic iron [4].

We performed *ab initio* molecular dynamics simulations on an $Mg_{24}Si_{12}C_{12}O_{72}Fe_{13}$ melt composition (i.e. 12 $MgCO_3$ + 12 $MgSiO_3$ + 13 Fe) at conditions up to 135 GPa and 4000 K to understand speciation and coordination of carbonate melts in the lower mantle and at the core-mantle boundary. We find a rich diversity of species in our carbonate-silicate-metal melt, with our system displaying various carbon bonding environments. We determine that as the overall coordination of carbon increases with pressure, the abundance of C-C-bonds decreases with pressure and is compensated by an increase in C-Fe and C-Si bonding. We evaluate the implications of these chemical and structural changes for the storage and cycling of carbon in Earth's mantle.

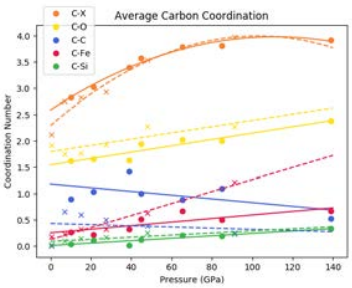


**Figure 1:** The average coordination of carbon bonded to all elements (orange), oxygen (yellow), carbon (blue), iron (red), and silicon (green). This study (solid lines) is compared to Solomatova *et al.* [5] (dashed lines).

[1] Braunger *et al.* (2020) *EPSL* **533**, 116041. [2] Stagno *et al.* (2018) *Chemical Geology* **501**, 19-25. [3] Rohrbach & Schmidt (2011) *Nature* **472**, 209-212. [4] Dorfman *et al.* (2018) *EPSL* **489,** 84-91. [5] Solomatova *et al.* (2019) *Nature Communications* **10**.