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LETTERS

Computer simulation of high-temperature, forsterite-melt partitioning

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ABSTRACT

We report the first atomistic computer simulations of the partitioning of divalent cations between forsterite (Mg_2SiO_4) and coexisting $MgSiO_3$ melt at ~1600 °C and atmospheric pressure. Our results, using new Monte Carlo techniques, are compared with new experimental determinations of forsterite-melt partitioning for the same elements (Ca, Mn, Ni, Co, Cu, Zn, Sr, Cd, Ba) in the same system under identical conditions. Over seven orders-of-magnitude variation in the Nernst partition coefficient (D), experiment and simulation agree typically within a factor of 2 and at worst to within a factor of 4.2 (D_{Sr}). Our simulation techniques therefore herald a novel means of determining crystal-melt partitioning that may be especially valuable under extreme conditions of pressure and temperature not readily amenable to experimentation.