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Crystal-chemical controls on trace element partitioning between garnet and anhydrous silicate melt

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ABSTRACT

We performed experiments at 3.0 GPa and 1530–1565 °C to investigate the effects of crystal composition on trace element partitioning between garnet and anhydrous silicate melt. Bulk compositions along the pyrope (Py: $Mg_3Al_2Si_3O_{12}$)-grossular (Gr: $Ca_3Al_2Si_3O_{12}$) join, doped with a suite of trace elements (Li, B, K, Sc, Ti, Sr, Y, Zr, Nb, Cd, In, REE, Hf, Ta, Th, and U) produced homogeneous garnets, ranging in composition from $Py_{84}Gr_{16}$ to Py_9Gr_{91}, in equilibrium with melt.

Trace element partition coefficients (*D*-values), measured by SIMS, depend greatly on the Mg/(Mg + Ca) of garnet. For example, from Py_{84} to Py_9, D_{La} increases from 0.004 to 0.2, whereas D_U increases from 0.029 to 0.42. These variations can be explained by the lattice strain model of Blundy and Wood (1994), which describes trace element partitioning of an element *i* in terms of the ionic radius of *i* (r_i), the size of the lattice site on which *i* partitions (r_0), the Young's modulus of the site (*E*), and the (theoretical) partition coefficient D_0 for an ion of radius r_0.

For trivalent cations substituting in the garnet X-site (Y, REE, Sc, and In), apparent values of r_0 fitted to our data vary systematically from 0.935 ± 0.004 Å (Py_{84}) to 0.99 ± 0.01 Å (Py_9), a trend consistent with variations in the size of the X-site. Values of D_0 show an increase from Py_9 ($D_0 = 2.8 \pm 0.1$) to Py_{84} (4.8 ± 0.1) and Young's modulus *E* varies from 257 ± 20 GPa for Py_{60} to 590 ± 40 GPa for Py_{84}. These results allow a quantitative assessment of the influence of crystal chemistry on garnet-melt *D*-values, thereby forming the basis for a predictive model similar to that recently developed for clinopyroxene-melt partitioning by Wood and Blundy (1997). Our new data emphasize the importance of taking into account crystal composition when modeling trace element behavior in natural systems.