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SITE PREFERENCE AND PARTITIONING OF SCANDIUM IN SILICATE GARNETS

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Incorporation and site preference of Sc (~ 5 %) in four synthetic garnets (Py, $Py_{60}Gr_{40}$, $Py_{20}Gr_{80}$, and Gr) along the join pyrope-grossular were investigated by a multi-disciplinary experimental–theoretical approach, which combines EMPA, SC and powder XRD, and Sc K-edge XAFS. The XAFS experiments were performed at ID26 (ESRF). The XANES spectra clearly show significant differences in the spectral features of grossular and pyrope, suggesting different local environments for Sc. This finding is supported by the results of the multi-shell fit of the EXAFS signals: Sc is incorporated into the dodecahedral X site in the pyrope-type structure, but in the octahedral Y site in the grossular-type structure. Moreover, a different site-partitioning behaviour is observed for Sc in the solid-solution terms. The first shells contributions of the $Py_{60}Gr_{40}$ EXAFS signal could be obtained by a weighted combination of Sc in tetrahedral (T) and X site, while the first shells fit of $Py_{20}Gr_{80}$ EXAFS signal could be fitted by a weighted combination of single scattering paths calculated for Sc in both Y and T site. In this last case, however, a minor partitioning of Sc also in X site cannot be ruled out. These results are fully compatible with those of the structure refinement of the end-members, which showed (i) higher site-scattering (ss) and ADP values at the X site and lower ss at T in Py; (ii) higher ss and longer mean bond lengths at Y (and T) in Gr. The site partitioning and preference of Sc in garnets is thus dramatically determined by the matrix.