# Silicate garnet: A micro to macroscopic (re)view

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### ABSTRACT

Silicate garnets, general formula $E_3G_2Si_3O_{12}$, form an important class of rock-forming minerals and, in nature, most are solid solutions. Their crystal-chemical and solid-solution properties are sometimes interpreted in terms of the widely used Pyralspite-Ugrandite classification scheme, and this can lead to erroneous conclusions. In this study, published data are reviewed and analyzed to achieve a synthesis of relevant experimental and computational results and to construct a working "crystal-chemical model" for describing aluminosilicate garnet, $E_3Al_2Si_3O_{12}$, over different length scales. The pyrope-grossular (Py-Gr) solid solution is given special attention, because it has received a great deal of study. It also shows interesting crystal-chemical and thermodynamic mixing behavior. Computational and experimental investigations made on Py-Gr garnets indicate that the shorter Ca/Mg-O2 bond lengths appear to remain roughly constant in length across the binary and can be described as showing "Pauling limit-type" behavior. The longer Ca/Mg-O4 bonds behave differently, because they lengthen with increasing Gr component in the solid solution. Bond behavior in almandine-spessartine (Al-Sp) garnets appears to be partly different, because both Fe/Mn-O2 and Fe/Mn-O4 bonds show "Pauling limit-type" behavior. $E$-O bond-length variations are continuous. The bonding type in all aluminosilicate garnet end-members is similar. An analysis shows that various computational simulations on Py-Gr solid solutions are consistent with each other with respect to $E$-O bond behavior and also with experimental IR, Raman, NMR spectroscopic, and X-ray diffraction results, but not completely with XAS studies made at the Ca edge. Ca/Mg-O4 bond behavior can be used to explain, partly, the nature of various micro/nanoscopic crystal-chemical and strain properties and macroscopic excess thermodynamic mixing behavior of Py-Gr garnets. Micro/nanostrain for the Py-Gr binary is asymmetric in nature, as are the various thermodynamic mixing functions $\Delta H^{ex}$, $\Delta S^{ex}$, and $\Delta V^{ex}$. The widely cited Pyralspite-Ugrandite classification scheme has limited use in terms of explaining many physical and chemical properties of garnet and it should not be used to predict or describe, for example, solid-solution behavior.

**Keywords:** Garnet, bonding, crystal chemistry, thermodynamics, spectroscopy, X-ray diffraction, computations, strain and solid solutions