

The local structural state of a kimberlitic grosspydite garnet using paramagnetically shifted ^{27}Al and ^{29}Si MAS NMR resonances

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Most rock-forming silicates are solid solutions and much research has been done to determine their crystal chemical properties. Garnet solid solutions (i.e. $\text{X}_3\text{Al}_2\text{Si}_3\text{O}_{12}$ with $\text{X} = \text{Mg}, \text{Fe}^{2+}, \text{Mn}^{2+}$ and Ca) have random long-range X-cation disorder in space group *Ia-3d*. However, the structural state of Fe-bearing garnets at the local scale is not known.

Garnet from a grosspydite xenolith from the Roberts Victor kimberlite, S. Africa was studied by ^{27}Al and ^{29}Si MAS NMR spectroscopy. Paramagnetically shifted resonances were measured to determine the local structural state of the X-cations. The crystals have the formula $\text{Grs}_{46.7}\text{Prp}_{30.0}\text{Alm}_{23.3}$. The composition, the lack of measurable zoning, as well as the mode of occurrence, make this garnet a key sample for investigating the possible presence of short-range X cation order.

The ^{27}Al MAS NMR spectrum shows a very broad asymmetric resonance located between 100 and -50 ppm. It consists of a number of individual closely overlapping paramagnetically shifted resonances. The ^{29}Si MAS NMR spectrum shows two resonances. S0 is located between about -60 and -160 ppm and S4 is centered at roughly 95 ppm. Both are composite resonances containing many overlapping peaks. S0 contains local information for SiO_4 groups that do not have any edge-shared Fe^{2+} -containing dodecahedra. S4 involves various local configurations where there is one edge-shared dodecahedron containing Fe^{2+} . The measured intensity of S0 and S4 are roughly similar to calculated intensities assuming random Fe^{2+} -cation mixing. These first results do not indicate any overt short-range X-cation order in grosspydite garnet.