Applications of High Field Solid State NMR Techniques to Examine Problems in Geochemistry

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There has been much progress in the methodology for solid state NMR, with one of the key drivers being the advances associated with experimental hardware such as the availability of high field magnets and fast magic angle spinning. The new information these developments can provide for geochemistry will be examined via three case studies:

1. The development of ^{17}O to examine atomic scale ordering and connectivity between different components within oxide-based materials.

2. ^{33}S studies of glasses. High magnetic fields have allowed nuclei, especially those with quadrupole moments to become more tractable to study. An example of this is ^{33}S which has traditionally been regarded as a difficult nucleus for solid state NMR study. New work has shown for some cases that sufficient NMR signal can now be generated to make this a useful approach. NMR spectra show that sulphates, thiosulphates and sulphides can be readily distinguished. Some preliminary results for the dissolution mechanism of sulphur in aluminosilicate glasses are given.

3. Intracrystalline partitioning of Al in pyroxenes. The presence of water in the Earth's mantle has wide ranging implications and a detailed picture of the spatial and temporal distribution of water in the mantle is needed to be able to understand fundamental global-scale processes. It has been proposed previously that the partitioning of aluminium between octahedral and tetrahedral sites in orthopyroxene has the potential to be used a mantle geohygrometer. This idea was tested using very high-field ^{27}Al MAS NMR (as the quadrupole interaction is very large at the tetrahedral site). Although the results suggest that Al partitioning is not affected by dissolved water, the results show that NMR studies on nuclei other than ^{1}H open up new possibilities for studying the interaction of water with mantle minerals.

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