Scalar *J*-Couplings in Silicate-based Materials: from Measurements to Structural Interpretations

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It has been demonstrated over the last decades that *J*-coupling based NMR sequences provide a powerful set of tools to analyze the conformation of organic compounds in the solid state. Until now scalar couplings have nevertheless not widely been used in inorganic compounds, and especially in silicate based materials which have significant implications in geochemistry as well as in the field of material science and glass technology. Two examples will be presented here showing that this type of studies can successfully be performed.

We show that with isotopic enrichment the ^{29}Si-O-^{29}Si ^{2}J scalar spin-spin coupling constant, although very small, can be measured in crystalline wollastonite $CaSiO_3$ compounds with an accuracy of ± 0.1 Hz. Strong coupling effects in the *J*-resolved 2D spectra are evidenced along with additional lines in the *J*-resolved spectra. Cluster ab-initio calculations led to a close-to-linear relationship between J_{SiOSi} and the Si-O-Si bonding angle. In the glass, this relationship allowed the analysis of the distribution of angle within each $Q^{(n)}$ species leading to an unexpectedly strong correlation between the bonding at each corner of a given $Q^{(n)}$ unit and the bonding at adjacent corners is found. This analysis is extended to a potassium silicate composition and to pure silica.

The gehlenite $Ca_2Al_2SiO_7$ composition can act as a model compound for the investigation of inclusion of Boron into alumino-silicates since it is expected to form a mixed $Ca_2(Al,B)_2SiO_7$ phase upon boron addition. We first identified the various $Al(Al_nSi_m)$ building blocks in the pure $Ca_2Al_2SiO_7$ system using ^{29}Si/^{27}Al double resonance *J*-based experiments and confront those results to periodic 1st principle calculations. The B/Al and Al/Si substitution behaviour is then investigated in the complex $Ca_2(Al,B)_2SiO_7$ compositions using double- and triple- resonance experiments involving ^{11}B, ^{29}Si and ^{27}Al.

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