

## **The Structure of alkali-silicate glasses: high frequency Raman bands and the Si-O-Si intertetrahedral angle**

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The structure of silicate glasses is often probed using Raman spectroscopy. The 900-1300  $\text{cm}^{-1}$  region is particularly sensitive to vibrations associated with  $Q^n$  ( $n = \#$  of bridging oxygens and ranges from 0-4) species. Curve fitting the high frequency envelope with Gaussian bands is used to determine the relative numbers of Q species in the glasses. Unfortunately, the number of Gaussian bands often exceeds the number of possible  $Q^n$  species present and the widths of the peaks can be highly variable and unrealistic. We have recently shown that the  $Q^n$  ( $n=0-3$ ) bands are predominantly Lorentzian in character; their full width at half maximum (FWHM) is similar at  $\sim 35-55 \text{ cm}^{-1}$ ; Raman cross-sections for the different Q species are comparable, and the  $Q^3$  band (and possibly the other  $Q^n$  bands) is asymmetric due to the presence of bridging oxygens (BO) associated with alkali cations. These findings enable quantification of the different  $Q^n$  species from fitting of Raman spectra. The close proximity of Na also appears to have an influence on the Si-O-Si intertetrahedral angle. The angle is significantly reduced when an alkali is attached to the BO and this appears to be reflected in the behaviour of the D1 and D2 Raman bands as alkali is added.