Proton chemical shift anisotropy measurements of hydrogen-bonded functional groups by fast magic-angle spinning solid-state NMR spectroscopy

Luminita Duma, Daniel Abergel, Piotr Tekely* and Geoffrey Bodenhausen
Département de Chimie, associé au CNRS, Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France.

Supporting Information

Fig. S1 400 MHz $^1$H MAS NMR spectrum of octosilicate recorded at a spinning frequency of 10 kHz. The low field isotropic peak at 15.98 ppm represents siloxyl protons involved in strong hydrogen bonding, the high-field signal corresponds to water molecules.

Fig. S2 (left) $^1$H rotary resonance profile of siloxyl protons in octosilicate at 10 kHz MAS and 400 MHz resonance frequency. The spin-lock duration was set to 1 ms. The profile was obtained by varying the spin-lock RF field amplitude $\omega_{rf}$ in steps of 0.5 dB from 11 to 30 dB attenuation. (middle) Temporal evolution of the signal as a function of spin-lock time $\tau$ at $n = 1$ and 2 rotary resonance conditions. (right) Fourier transformations giving rotary resonance fingerprints.