

Supplementray data for

**Room temperature sol-gel synthesis of crystalline Cs[V₃O₈]. Probing the
hydration level of the interlamellar space by ⁵¹V and ¹³³Cs MAS NMR
spectroscopy.**

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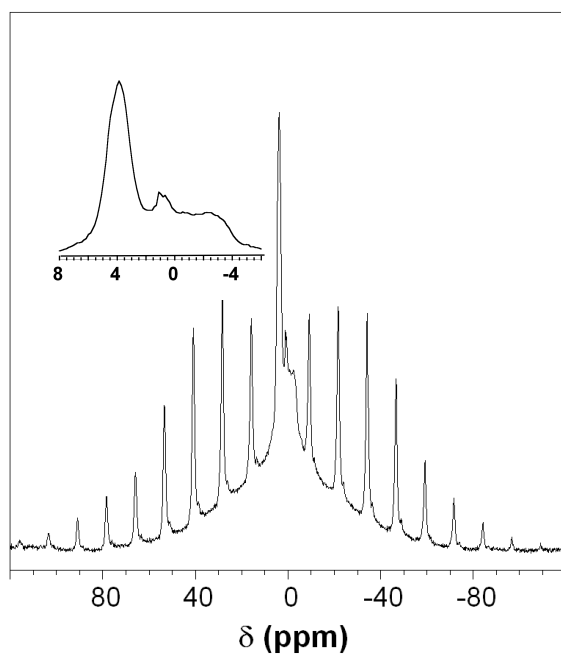


Figure S1: ^1H MAS NMR spectrum of the $\text{Cs}_2[\text{V}_6\text{O}_{16}] \cdot 0.7\text{H}_2\text{O}$ (YOP) spun at 14 kHz and with 4 transients.

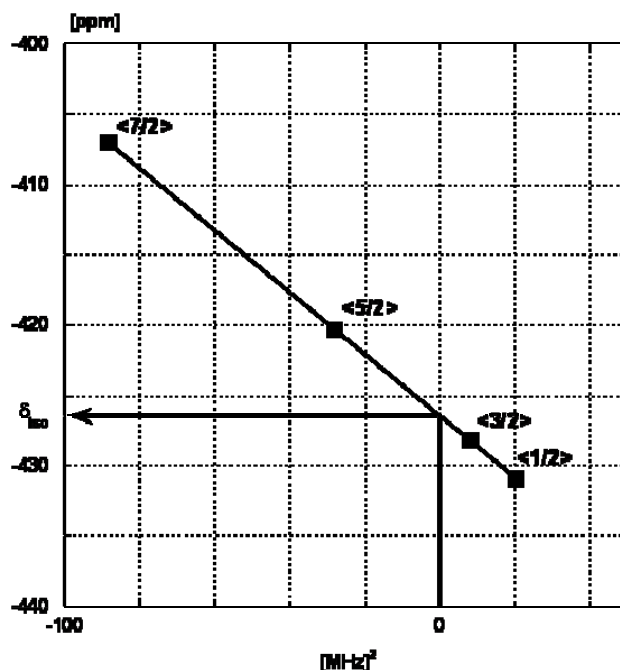
Determination of NMR parameters from the SORGE (Second-Order Graphic Extrapolation) diagram ⁵²

The NMR parameters for the type 3 site were further characterized by using the centre of gravity of the various ⁵¹V transitions. The δ_{iso} and $\nu_Q(\eta_Q)$ values were safely determined by using the so-called Second-Order Graphic Extrapolation or SORGE diagram. $\nu_Q(\eta_Q)$

corresponds to $\nu_Q \left(1 + \frac{\eta_Q^2}{3}\right)^{1/2}$ with $\nu_Q = \frac{3}{2I(2I-1)} C_Q$. It can be shown that the centre of gravity of the various transitions $\langle \pm m, \pm m-1 \rangle$, $\delta_{CG}^{\langle m \rangle}$, δ_{iso} and $\nu_Q(\eta_Q)$ can be related by the following equation:

$$\delta_{CG}^{\langle m \rangle} = \delta_{iso} - [\nu_Q(\eta_Q)]^2 \frac{[I(I+1) - 3 - 9m(m-1)]10^6}{30\nu_0^2}$$

The experimental values of $\delta_{CG}^{\langle m \rangle}$ for $m = 1/2, 3/2, 5/2$ and $7/2$ are plotted versus $\frac{[I(I+1) - 3 - 9m(m-1)]10^6}{30\nu_0^2}$. The slope gives $[\nu_Q(\eta_Q)]^2$ and for “an infinite field”, one derives δ_{iso} .



SORGE diagram

⁵² D. Massiot, D. Müller, T. Hubert, M. Schneider, A. P. M. Kentgens, B. Coté, J. P. Coutures, W. Gessner, *Solid State Nucl. Magn. Reson.* **1995**, 5, 175-180.