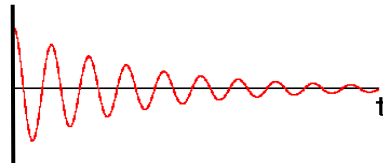


11. The Fourier transform



1768 - 1830

Classical mathematical transformation applied to the transverse magnetization : $M_t = M_0 \exp(-t/T_2) \exp(2i\pi\nu t)$



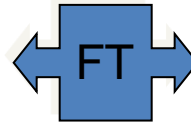
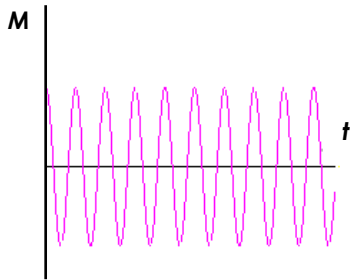
$$TF(M_t) = \int_0^{\infty} M_t(t) \exp(-2i\pi\nu t) dt$$

- Changes seconds to Hertz
- Frequency Analyzer.
- Used from the mid-60s

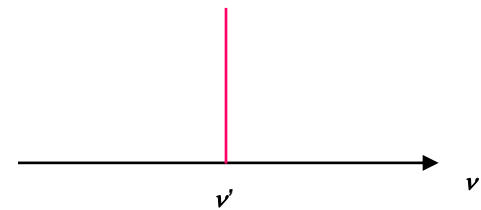
11. The Fourier transform

Examples

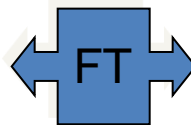
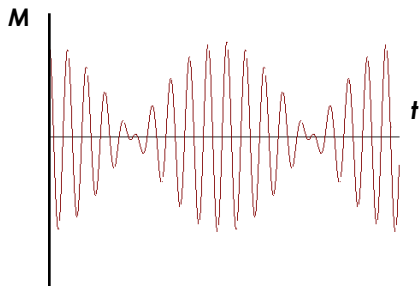
Cosine
 $\cos(2\pi\nu t)$



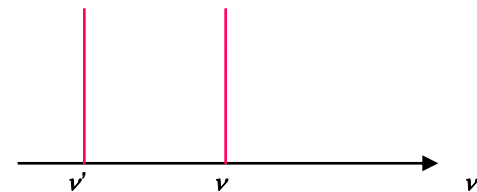
Peak infinitely thin



Deux cosines of two different frequencies
 $\cos(2\pi\nu t) + \cos(2\pi\nu' t)$



Two peak infinitely thin

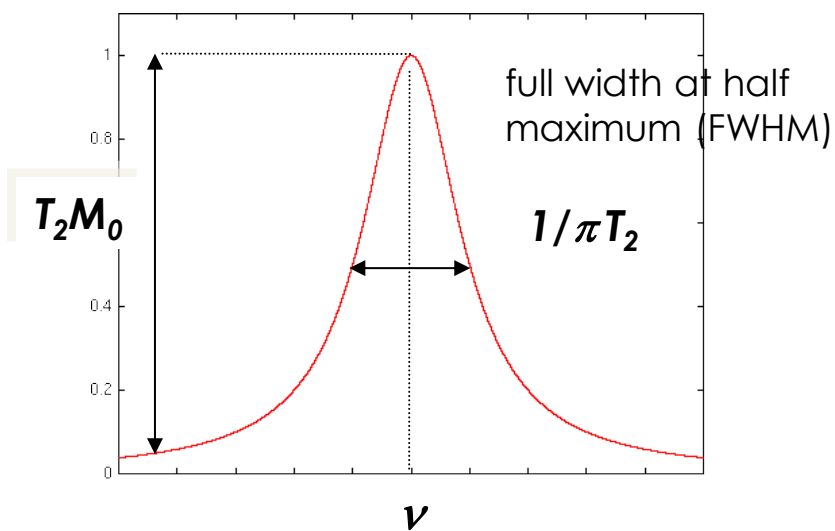
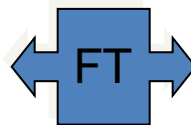
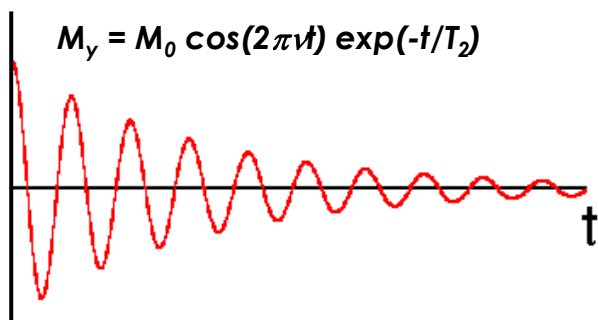


FT acts as a frequency analyzer

11. The Fourier transform

Case of the NMR signal (FID)

Resonance of a **Lorentzian lineshape**



If thermodynamic equilibrium is reached, the area under the Lorentzian corresponds to the total amount of spins.

NMR can be quantitative.

12. The chemical shift δ

The B_0 value is not the same for all the nuclei : small perturbations !

$$\nu_0 = \frac{\gamma B_0}{2\pi}$$

→

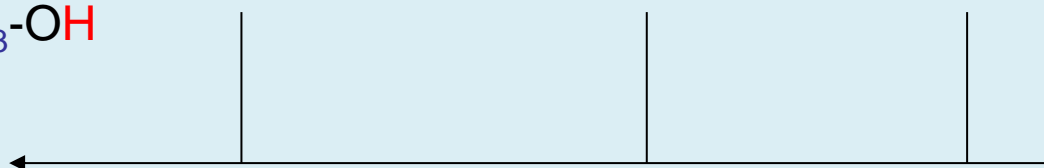
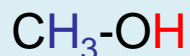
$$\nu_0 = \frac{\gamma(1 - \sigma) B_0}{2\pi}$$

σ : perturbation coefficient $\sim 10^{-6}$

Example :

$$B_0 = 2,35 \text{ T}$$

$$\nu_0(^1\text{H}) = 100 \text{ MHz}$$



$$\nu = 100 \text{ MHz} + 400 \text{ Hz}$$

$$\delta = 4 \text{ ppm}$$

$$100 \text{ MHz} + 130 \text{ Hz}$$

$$1.3 \text{ ppm}$$

$$100 \text{ MHz}$$

$$\text{"0 ppm"}$$

Very small difference but measurable !

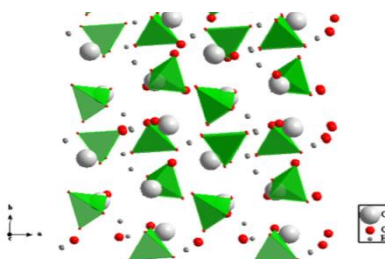
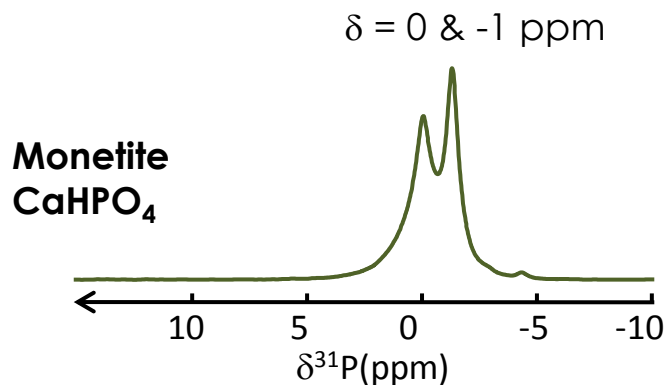
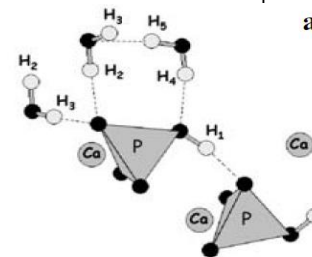
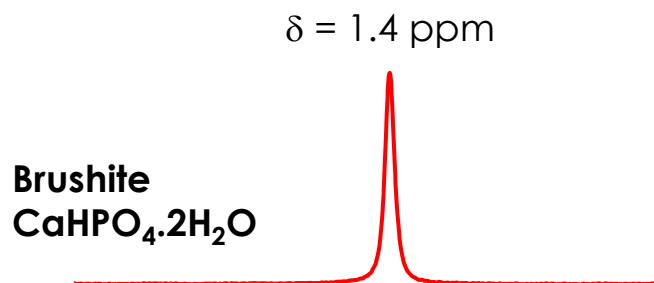
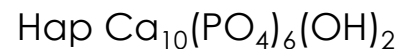
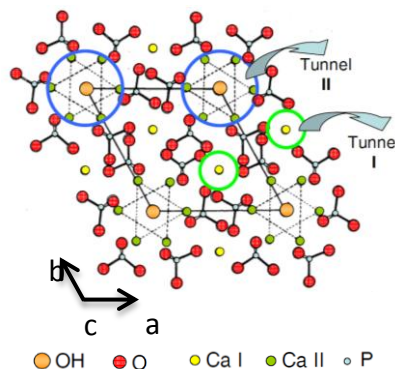
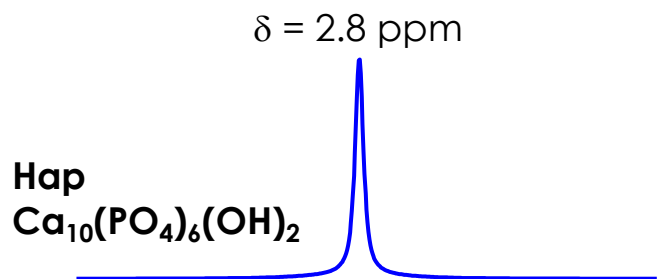
$$\begin{aligned} 100 \text{ MHz} + 130 \text{ Hz} &= 100 \cdot 10^6 \text{ Hz} + 130 \text{ Hz} \\ &= 100 \cdot 10^6 \times (1 + 1,3 \cdot 10^{-6}) \text{ Hz} \\ &= 100 \times (1 + 1,3 \cdot 10^{-6}) \text{ MHz} \end{aligned}$$

The correction is $1,3 \cdot 10^{-6}$ compared to the principal magnetic field:

$$1,3 \cdot 10^{-6} = 1,3 \text{ part per million} = 1,3 \text{ ppm}$$

13. Identification of mineral phases

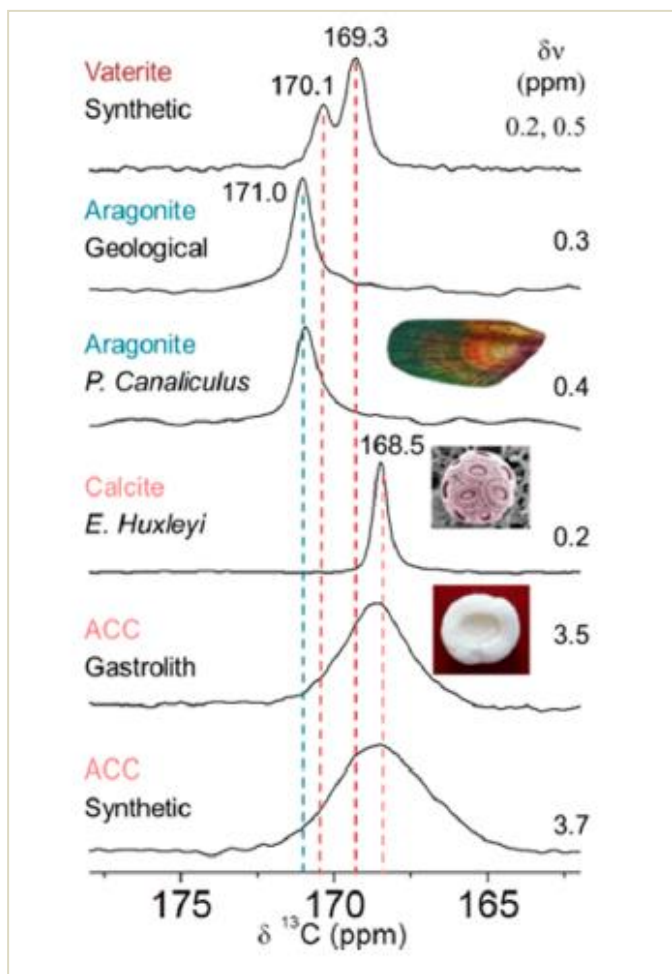
➤ Identification of calcium phosphate phases through ^{31}P NMR



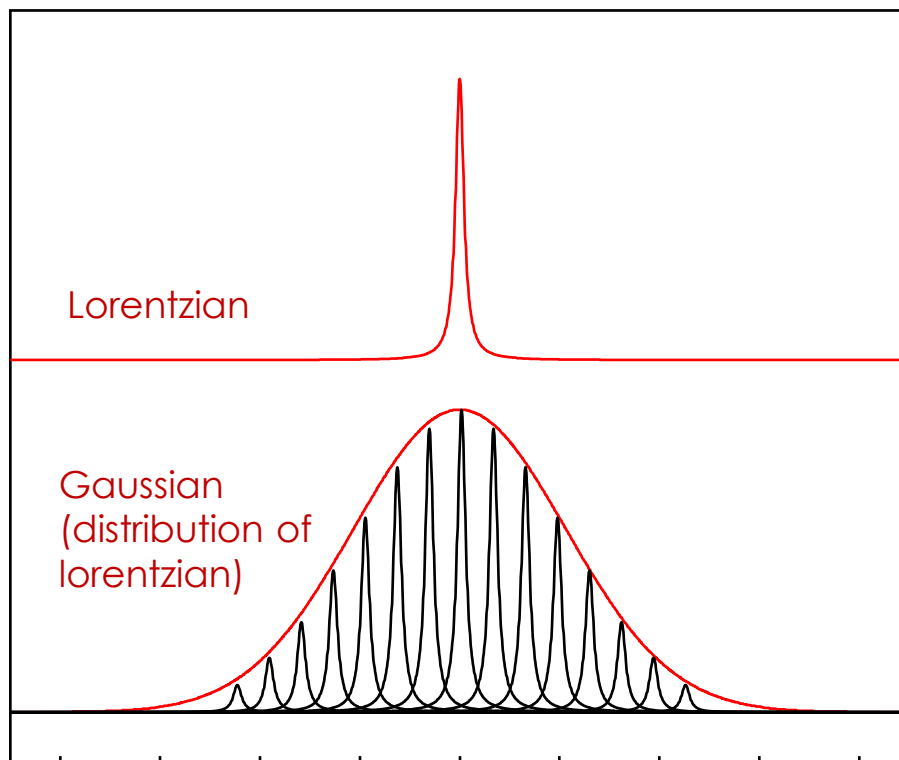
- Number of resonances
- Number of crystallographic sites

13. Identification of mineral phases

➤ Identification of calcium carbonates phases through ^{13}C NMR

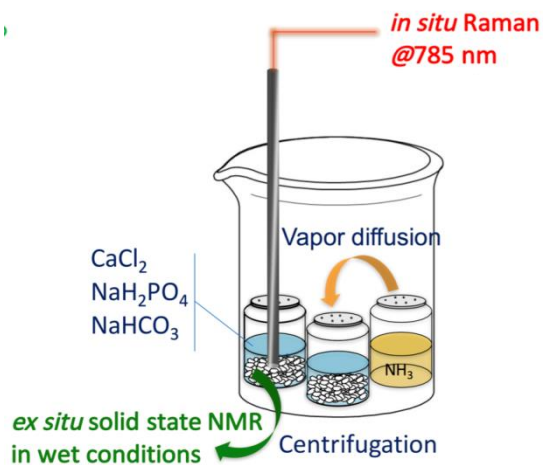


➤ Differentiation crystalline vs amorphous

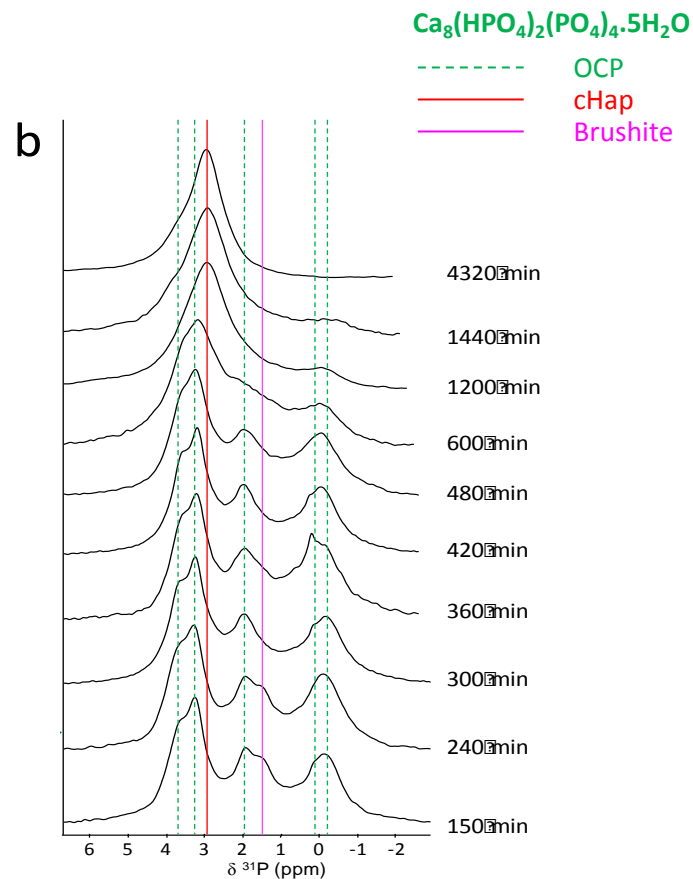


14. Identification of mineral phases

- Precipitation of Hap through NH_3 vapor diffusion
- *Ex situ* ^{31}P NMR



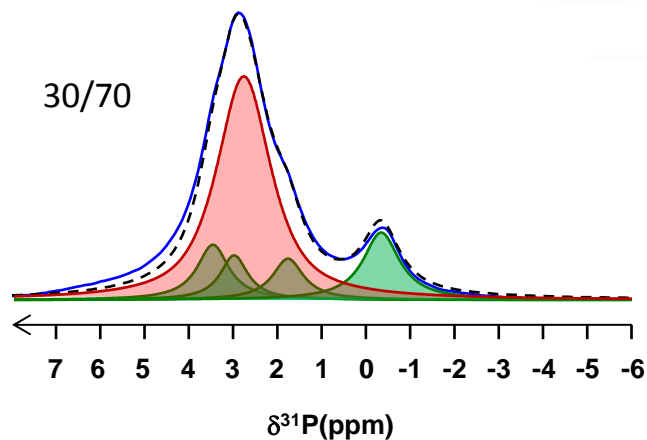
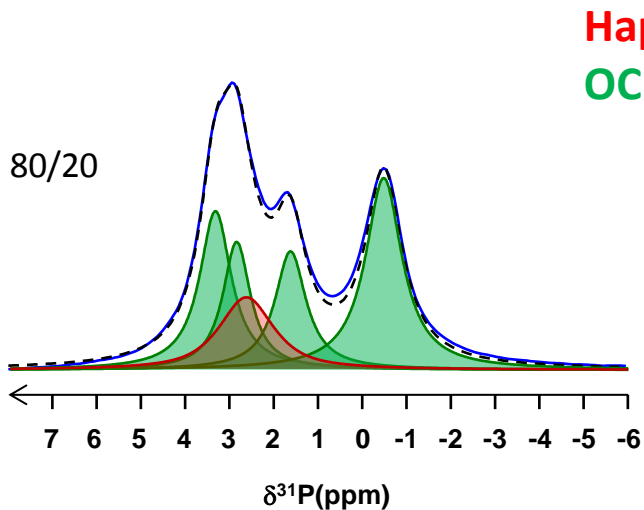
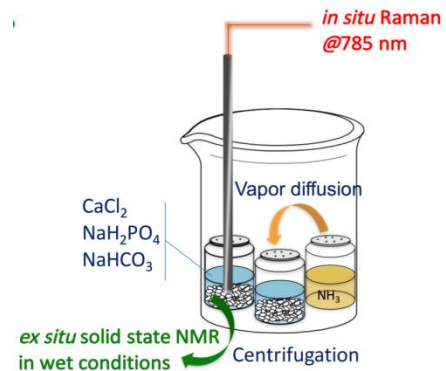
Nassif *et al. Chem. Mater.* 2010



Robin *et al. CrystEngComm* 2020

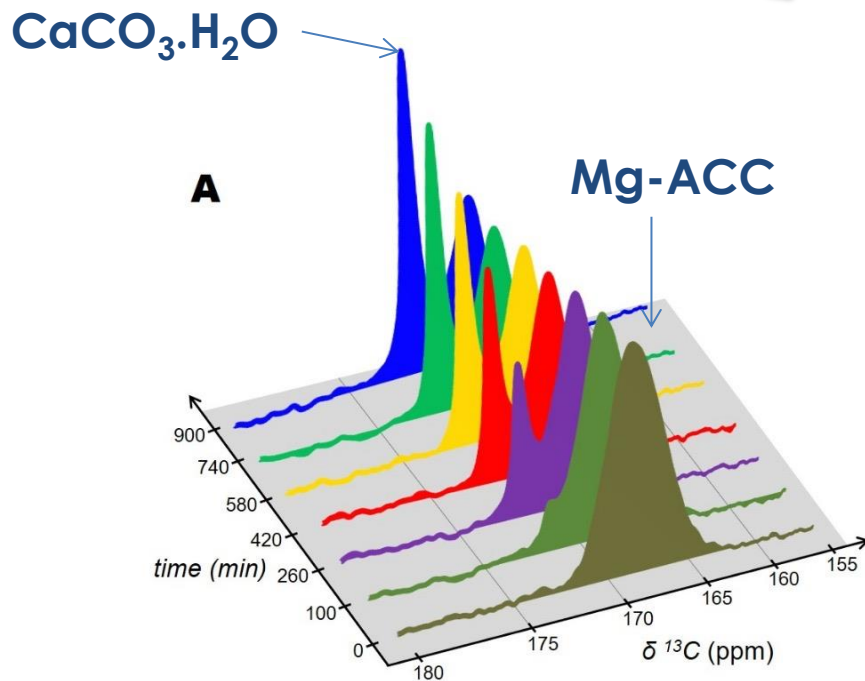
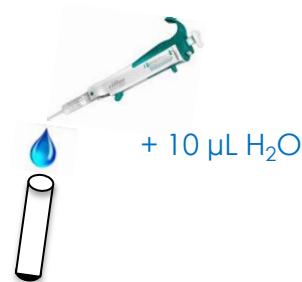
14. Quantification of mineral phases

➤ Only if T_1 relaxation is respected

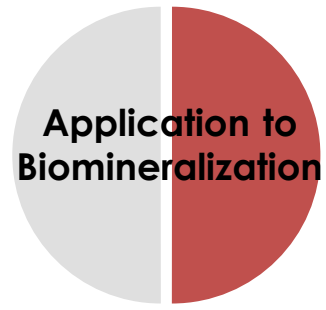


14. Identification of mineral phases

- In Situ transformation of Mg-ACC into monhydrocalcite

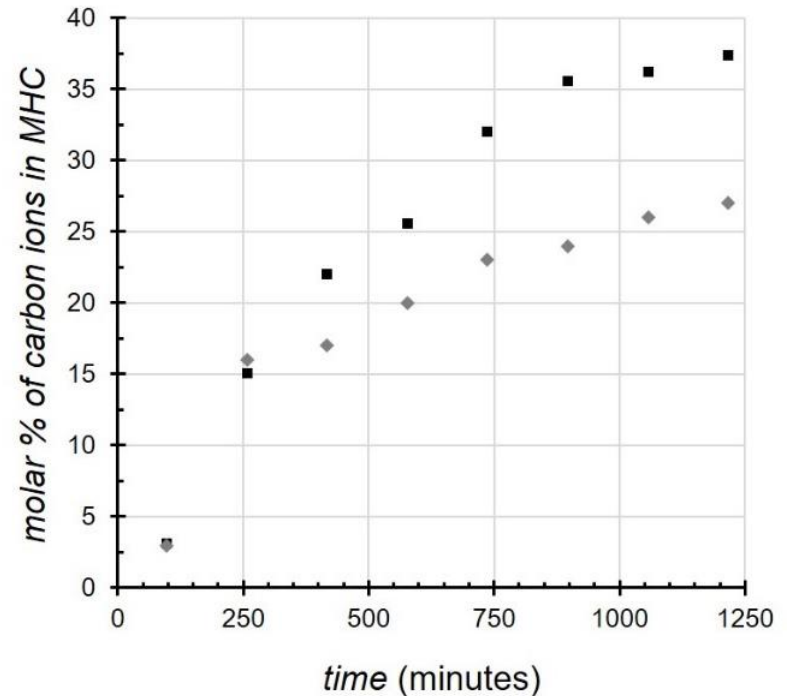
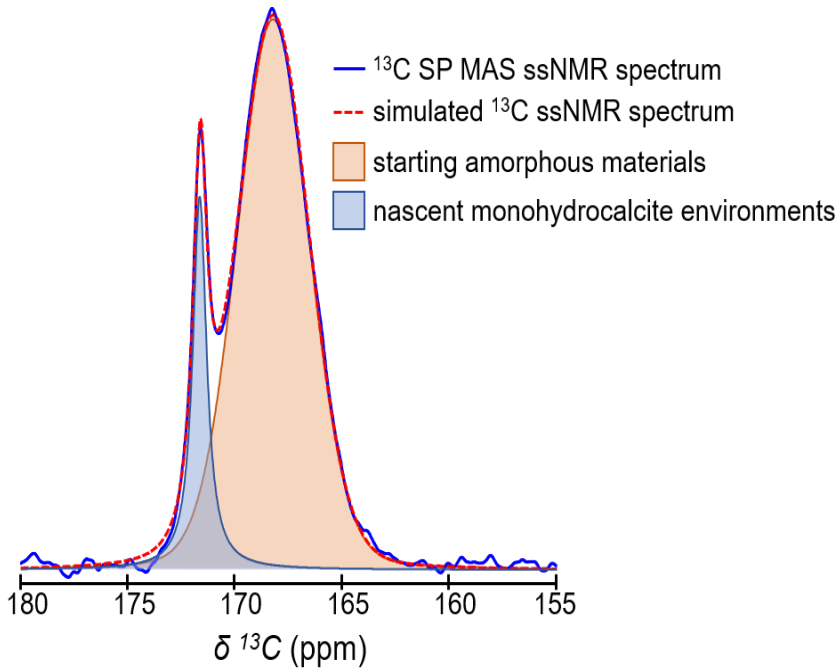


Von Euw *et al.* submitted



14. Quantification of mineral phases

➤ Only if T_1 relaxation is respected



Von Euw *et al.* submitted