

# Investigation of Phosphorus Site Condensation in $\text{CaHPO}_4$ by Analysis of $^{31}\text{P}$ MAS-NMR Tensor and X-Ray Powder Patterns

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$\text{CaHPO}_4$  was obtained by slow evaporation at room temperature. Seven samples, obtained at different annealing temperatures, were characterized by X-ray diffraction and  $^{31}\text{P}$  MAS-NMR spectroscopy. All NMR spectra were analyzed using a DMFIT program. At room temperature, the observed  $^{31}\text{P}$  NMR chemical shifts for the title compound were  $-1.59$ ,  $-0.36$  and  $1.26$  ppm with the relative intensities 39%, 10% and 51%, revealing the presence of three non-equivalent phosphorus sites in the structure. The investigation of the NMR tensor shift of all spectra shows that the abounding  $\text{HPO}_4^{2-}$  anion was progressively transformed into  $\text{P}_2\text{O}_7^{4-}$  when the temperature increased.

*Key words:*  $^{31}\text{P}$  MAS-NMR Spectroscopy; Chemical Shift Tensor;  $\text{CaHPO}_4$ .