Solid state NMR: a powerful tool to characterize substituted hydroxyapatites

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Apatites $Ca_{10}(PO_4)_6(F,Cl,OH)_2$, are a complex and diverse class of materials which have gained increasing importance due to their biological role. One of the main constituents of bones and hard tissues in mammals is a calcium phosphate mineral whose structure closely resembles hydroxyapatite (HA), $Ca_{10}(PO_4)_6(OH)_2$. The so-called biological apatite refers to poorly crystallized non-stoichiometric carbonate-substituted HA.
Hydroxyapatite is also found in pathological calcifications. Indeed, the very first steps of the formation of kidney stones can involvenanocrystalline carbonated-hydroxyapatite deposits, commonly named Randall's plaque, which is considered as a nucleation center for the deposit of kidney stones.
Growth of apatite can also be promoted by bioactive synthetic materials used as implants and these biomaterials have a major role in the manufacture of artificial bone material and as coating on surgical implants.
In all these examples, the apatite phase is nanocrystalline or amorphous with a chemical composition that varies due to the ability of the structure to accommodate a large number of cationic or anionic substituents. This structural versatility allows a fine tuningof the properties in terms of bioactivity, but makes the structural characterization of such substituted apatitesrather difficult.
This presentation will highlight how the use of multidimensional solid-state NMR techniques combined with DFT calculations, allows to better characterize synthetic or biological carbonated apatites.

References

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