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NMR crystallography driven structure determination

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Because solid-state nuclear magnetic resonance (ss-NMR) spectroscopy is sensitive to local order and is selective to the nature of the atoms, this technique has emerged as ideally complementary to powder diffraction for structure determination of a wide range of solids. Here, we will illustrate with the example of hybrid solids (aluminophosphates) the role of high-resolution one and two-dimensional solid-state NMR data to drive the search for a structure model from powder diffraction data. Great progresses have been made in the field of ss-NMR in the past few years (higher magnetic field, more robust pulse sequences, etc.) that now allows access to NMR spectra with very high resolution in such compounds [1]. From these NMR data, information about the cations (number, coordination number, etc) and the connectivity between the cation polyhedra are readily available. Such knowledge allows performing a more constraint structure search, thus increasing the chance to obtain a solution [2]. NMR data further provide information about the non-periodic sub-networks in hybrid compounds (water molecules, OH groups, templates…), allowing to draw very detailed pictures of the solids [3].

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