NMR CRYSTALLOGRAPHY OF MOLECULAR SOLIDS

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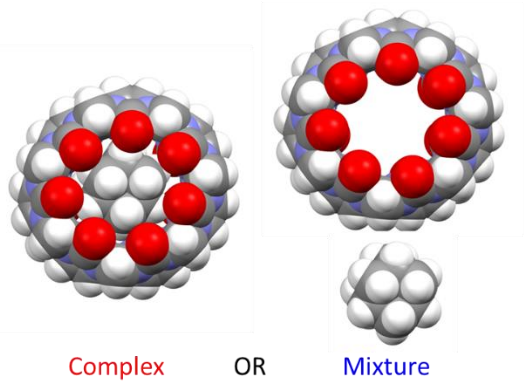
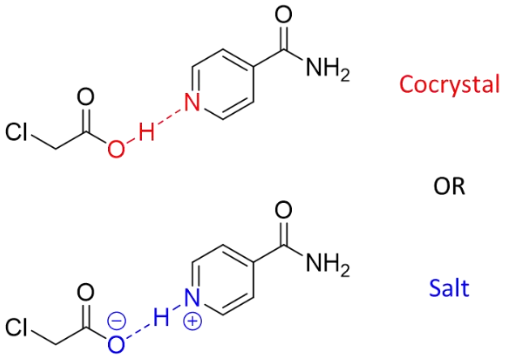
Modern chemistry, biology and materials science are based on the knowledge of structure on the molecular level. X-ray crystallography is the most widely used technique for determination of structures with atomic resolution. Single crystal X-ray diffraction (XRD) has been called the “gold standard” for solid-state structure determination,[1] which has been central to many achievements in chemistry and biology. However, there are two major limitations of this method. First, hydrogen atoms are very difficult to characterize by this technique. Another well-known limitation of XRD is that it requires a highly ordered crystalline sample and is inherently limited in the structural characterization of disordered or amorphous samples.

An alternative experimental technique for atomic-level characterization of solids is solid-state NMR spectroscopy (SS-NMR). NMR spectroscopy is very sensitive to the local environment of hydrogen atoms. Furthermore, SS-NMR does not require a long-range order in the studied materials and is, therefore, suitable for characterization of disordered and amorphous samples. The progress of SS-NMR methods has led to the development of NMR crystallography, which combines experimental SS-NMR data with theoretical simulations to obtain otherwise inaccessible insights into the structure and dynamics of solid materials.

Here, several recent examples of NMR-crystallography studies overcoming the limitations of XRD will be discussed, such as investigation of mechanochemically prepared 2D and 3D arrays of molecular machines[2,3] or investigation of temperature-induced salt-to-cocrystal transformation of pharmaceutical solids.[4] We will also discuss the importance of nuclear quantum effects for the structure of solids with short hydrogen bonds.





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