NMR Diagnostics of Hydrogen Bond Energy and Geometry

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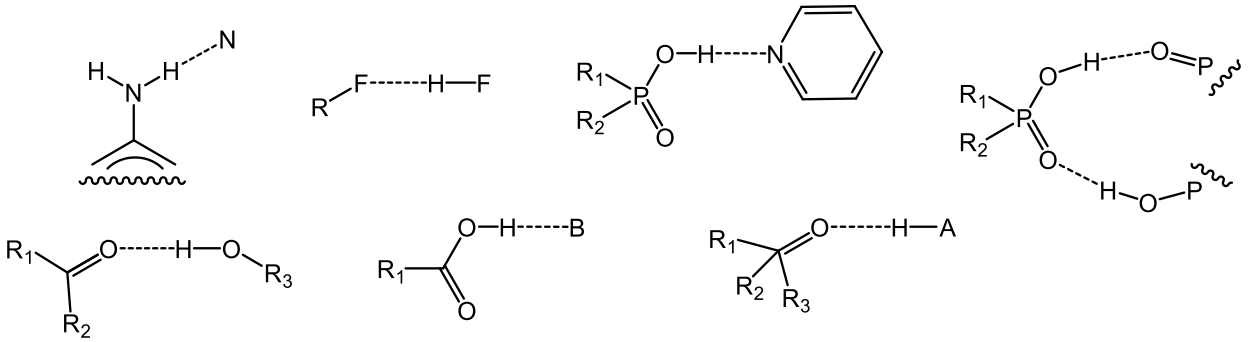
Hydrogen bonds are ubiquitous non-covalent interactions present in all states of the matter: from the gas phase to solutions and liquids, to soft-matter (polymers, glasses, various other disordered solids), to crystals. Despite typically being weaker than covalent bonds, hydrogen bonds stabilize a wide variety of structural motifs and determine physical and chemical properties of many condensed matter systems. For the characterization of an A–H···B bridge, which is essentially a three-center four-electron chemical bond, usually one would like to know i) interatomic distances (A…H, H…B and A…B) and ii) the energy of the interaction. In order to access this information, for disordered and weakly-ordered systems, when the crystallographic data is hardly available, one often has to rely on spectroscopic data.

In this presentation we overview literature data and our own results concerning the interpretation of the NMR spectroscopic data in terms and hydrogen bond geometry and energy. A number of hydrogen bond correlations linking spectroscopic observables with the interactomic distances and complexation energies will be presented. While being established for simple model systems of low molecular weight, such correlations are robust in a sense that they could be applied to more complicated systems as well, such as polymers.



In the figure above some examples of the types of hydrogen bonds considered in this work are presented. The main NMR observables which will be discussed and which might be used as spectroscopic markers of hydrogen bonds are the chemical shifts of atoms participating in the hydrogen bond of neighboring to it: δ^{1}H, δ^{19}F, δ^{31}P, δ^{15}N etc.

This work is supported by the RSF grant 18-13-00050.