

Publication

An introduction to hydrogen bond scalar couplings

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The hydrogen bond (H-bond) has been recognized in science for more than 80 years as a concept to explain situations where a hydrogen atom is simultaneously binding to two other atoms. Due to the moderate energies necessary for their formation and rupture, hydrogen bonds play a fundamental role in many chemical reactions and most, if not all, interactions involving biological macromolecules. For both proteins and nucleic acids, H-bonds are the essential element in the formation of secondary structures and often they also participate in the stabilization of tertiary structures. Many properties of H-bonds have been studied by a large variety of experimental methods, including NMR spectroscopy. Recently, electron-mediated scalar couplings have been observed which connect magnetic nuclei on both sides of the hydrogen bridge. In contrast to earlier NMR observables, these couplings can be used to "see" all partners of the hydrogen bond, the donor, the proton, and the acceptor in a single COSY experiment. In addition, the size of the coupling constant can be related to hydrogen bond distances and angles. This article should serve as an introduction to these findings and illustrate their use by various examples. (C) 2001 John Wiley & Sons, Inc.

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