Hydrogen-Bonding in the Enol Tautomer of 1,3-Diketones: Insights from $^{2/1}$H Isotope Effects on NMR Parameters in the Solid State as well as Computational Chemistry

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The literature dealing with hydrogen bonding is enormous, with numerous published review articles, and with several textbooks containing "Hydrogen Bonding" in the title; however, debates about the nature of the hydrogen bond continue. A classic example is acetylacetone where microwave spectroscopy indicates a C_{2v} structure[1] while ultrafast electron diffraction[2] and quantum chemistry computations[3] indicate C_s symmetry. We will present detailed solid-state NMR data for a closely related molecule, tetraacetylethane (3,3'-bis(acetylacetone)), and the enol tautomer of several other 1,3-diketones. Tetraacetylethane is an ideal model compound as its structure has been studied as a function of temperature by neutron and X-ray diffraction.[4] We have measured $^{2/1}$H isotope effects on isotropic chemical shifts of several 1,3-diketones in the solid-state and the insights that such measurements together with computation chemistry provide concerning hydrogen bonding will be discussed.

References
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