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# *Ab Initio* Calculations of NMR Chemical Shielding

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Nuclear Magnetic Resonance is the most widely used structural tool in modern chemistry and biochemistry. In spite of the large amount of empirical information accumulated over the years, correct signal assignment and the understanding of the relationship between molecular structure and isotropic chemical shifts may be difficult at times. *Ab initio* NMR calculations are now attainable and accurate enough to be useful exploring the relationship between chemical shift and molecular structure. The calculated $^{13}C$ chemical shifts, in particular, appear to be accurate enough to aid in experimental peak assignments. A comparison of the experimental and theoretical spectra can be very useful in understanding the basic chemical shift-molecular structure relationship.

A number of methods have been developed for the calculation of molecular second-order magnetic response properties. It is generally accepted that accurate prediction of these properties within the finite basis approximation, requires gauge-invariant procedures. We will focus on predicting NMR chemical shifts and shielding tensors of silatranes and liquid crystalline polymer using one of these procedures, namely GIAO(Gauge Including Atomic Orbitals) at both the Hartree-Fock and DFT levels of theory.