

# NMR: From Molecules to Spectra

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Nuclear Magnetic Resonance (NMR) is one of the most important tools for the structure analysis of molecules and a widely used technique in chemical and pharmaceutical industry. Here I present our approach to calculate NMR spectra starting from the SMILES description or just the name of the molecule. To this end we first determine the 3D structure of the molecule from which we obtain the NMR spin Hamiltonian. Finally we calculate the NMR Spectra from the spin-spin correlation functions.

One of the main challenges in NMR simulations consists in the large variation of energy scales involved. Typically high field proton NMR are performed at frequencies of the order of 700MHz, pulse duration are of the order of  $10\mu\text{s}$  with a band width of a few kHz, while the measured spectra have sub Hz resolution. Since the energy scales of the effective spin Hamiltonian correspond to sub Kelvin temperature and measurements are done at room temperature simulations are in the infinite temperature regime, limiting the number of spins that can be treated in a full diagonalization on standard desktop machines to 20 spins. We discuss the application of symmetries and clustering to achieve these calculations and various approximation schemes to extend the simulations to large systems. Finally I discuss the calculation of NMR spectra on quantum computer and show results obtained on quantum hardware.

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