NEUTRON SCATTERING FOR MOLECULAR SPECTROSCOPY: INTRODUCTION, SCOPE OF TECHNIQUES AND RECENT DEVELOPMENTS

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Neutrons interact only with the nuclei of molecules so the intensity of an inelastic neutron scattering event depends only on the motion of the nuclei of a molecule. This permits the computation of the full inelastic neutron scattering spectrum from a computation of the normal modes (or, in general, the anharmonic wavefunctions or the classical trajectory) without any need for knowledge of the response of the electrons to the nuclear motion. Applications of ab initio and DFT harmonic analysis to vibrationally inelastic neutron scattering spectra will be presented. Primary emphasis will be placed on molecular solids containing hydrogen where incoherent hydrogen atom scattering dominates the spectra. This greatly simplifies the spectral computations. Examples include highly symmetric molecules where vibrations that are forbidden by optical selection rules are strong in the INS spectra, a variety of hydrogen bonded systems including those with short, strong symmetric hydrogen bonds, charge transfer complexes, stable organic radicals, and some simple ionic species such as the alkali BH4 salts. Coherent scattering for C6F6 and metal carbonyls will also discussed. Some of these cases are presented in a recent review on inelastic neutron scattering: J. Phys. Chem. A 2001, 105, 3949-3960. The current status of periodic DFT methods will be discussed.