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Vibrational modes of n-octane: a theoretical comparison to neutron spectroscopy results

A number of different calibration samples are used on the Beryllium Filter Spectrometer on TAIPAN. Normal-octane is used extensively as a calibration sample because of its well known vibrational modes that are clearly and quite regularly spaced apart over the entire energy range that is covered.

On the other hand alkane chemistry presents itself as an interesting solid-state physics problem. Alkanes exist in several different condensed phases, for example for the low-temperature phase for chain lengths between 8 to 21 carbons, even numbers of carbons produce a triclinic phase whilst odd numbers may be either triclinic or orthorhombic. Behaviour and hence crystallography is dependent on both the electronic structure and the dynamics involved between the different possible vibrational modes and excitations.

Neutron spectroscopy is a wonderful tool to study the dynamical nature of materials and in particular alkanes and similar organic compounds. The short-range nuclear interaction introduces isotopic sensitivity to the measurement, which is governed by the weak nucleon-nucleon interaction, and which gives a very large scattering cross section in the case of hydrogen of 82 barn. In this way a weighted vibrational density of states that is highly sensitive to hydrogen in a material may be measured from polycrystalline (powdered) material. Here, neutron spectra are compared directly to force-field calculations, semi-empirical quantum chemistry calculations, and solid-state density functional calculations. Any overview of the theory is given along with the steps required in analysis.

Topic

Physics

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