Inelastic Neutron Scattering (INS) Studies of Framework Materials

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Inelastic Neutron Scattering (INS) is a powerful method that reveals details about the phonon distributions in materials and their vibrational density of states, that, in turn, are related to their thermodynamic properties. In this contribution, INS spectra will be presented for a range of framework materials collected on the spectrometers VISION and SEQUOIA at the Spallation Neutron Source in Oak Ridge National Laboratory (Oak Ridge,TN,USA). These include framework minerals such as the plagioclase feldspar series (albite to anorthite), feldspathoids (sodalite), and zeolites (analcime, heulandite, laumontite, natrolite and stilbite). The latter are compared with zeolitic imidazole framework materials (ZIFs) which are materials that achieve zeolite-type framework topologies by judicious combination of tetrahedral metal nodes and bridging imidazolate linkers in a stoichiometric ratio of 1:2. ZIFs have emerged as a very promising family of microporous metal organic frameworks (MOFs) whose proposed applications cover a wide range of areas (e.g. hydrogen storage, CO_2 sequestration, fuel cell catalysis,light harvesting, etc.). In this talk, results will be presented for ZIF-8, which has the sodalite topology, and its polymorph with the diamondoid topology (DIA), as well as the $Zn(EtIm)_2$ polymorphs with the rho, analcime and quartz topologies [1]. Of special interest in all of the materials studied is the unprecedented detail of the vibrational modes revealed in the INS spectra at low energies between 0 and 25 meV (200 cm^{-1}). These modes are critically important in determining the stability of the phase as they contribute to its low-temperature heat capacity and entropy. This study therefore provides important insights about how the stronger rigid bonds of the framework and weaker, more flexible modes affect the lattice dynamics, energetics and stabilities of the structures.

[1] Friščić *et al.* (2013) *Nature Chem.* **5**, 66-73.