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Neutron Scattering Kernels for Methane I & II and Ethane III

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We present new scattering kernels for two materials of interest as cold and very cold neutron moderators: solid Methane in phases I & II and solid Ethane in phase III, based on simple models that include the main dynamical features of those three systems and the effect of spin correlations.

Inelastic neutron scattering experiments were performed using the TOSCA spectrometer at the ISIS pulsed neutron source (Experiment Number: 2000128) on samples of solid CH₄ and C₂H₆ and mixtures of them over a range of temperatures down to 13 K. From the measured INS spectra we derived preliminary Density of State (DOS) for Methane I & II and Ethane III, over the range of energy transfers where the translational and rotational degrees of freedom control the molecular dynamics. In addition, proton spin correlations as a function of temperature were also accounted for, involving all four protons in the methane molecule, and the three protons in each methyl group of the ethane molecule.

In the case of methane, the model predictions of the total cross sections are in good agreement with a quantum mechanical calculation over the limited range where the latter was formulated, and with available experimental information over the complete thermal energy range.

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