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Using Monte Carlo Ray tracing to Understand the Vibrational Response of UN as Measured by Neutron Spectroscopy[1] J.Y.Y. LIN, California Institute of Technology, A.A. ACZEL, D.L. ABERNATHY, S.E. NAGLER, Quantum Condensed Matter Division, Oak Ridge National Laboratory, W.J.L. BUYERS, Chalk River Laboratories, Canadian Neutron Beam Center, G.E. GRANROTH, Neutron Data Analysis and Visualization Division, Oak Ridge National Laboratory — Recently neutron spectroscopy measurements, using the ARCS and SEQUOIA time-of-flight chopper spectrometers, [1] observed an extended series of equally spaced modes in UN that are well described by quantum harmonic oscillator behavior of the N atoms. Additional contributions to the scattering are also observed. Monte Carlo ray tracing simulations with various sample kernels have allowed us to distinguish between the response from the N oscillator scattering, contributions that arise from the U partial phonon density of states (PDOS), and all forms of multiple scattering. These simulations confirm that multiple scattering contributes an $\sim Q$-independent background to the spectrum at the oscillator mode positions. All three of the aforementioned contributions are necessary to accurately model the experimental data. These simulations were also used to compare the T dependence of the oscillator modes in SEQUOIA data to that predicted by the binary solid model [2].

[1] A. A. Aczel, *et al.*, Nat. comm. **3**, 1124 (2013).
[2] M. Warner, *et al.* Z. Phys. B **51**, 109 (1983)

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