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Effects of phonon broadening on x-ray near-edge spectra in molecular crystals JOHN VINSON, TERRENCE JACH, NIST, Gaithersburg, MD, TIM ELAM, Applied Physics Laboratory, U. Washington, JONATHON DENLINGER, Advanced Light Source, LBL — Calculations of near-edge x-ray spectra are often carried out using the average atomic coordinates from x-ray or neutron scattering experiments or from density functional theory (DFT) energy minimization. This neglects disorder from thermal and zero-point vibrations. Here we look at the nitrogen K-edge of ammonium chloride and ammonium nitrate, comparing Bethe-Salpeter calculations of absorption and fluorescence to experiment. We find that intra-molecular vibrational effects lead to significant, non-uniform broadening of the spectra, and that for some features zero-point motion is the primary source of the observed shape.

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