

Abstract Submitted
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90 K X-ray structure determination and vibrational spectroscopic investigation of L-alanine alaninium nitrate, a homologue of diglycine nitrate¹ MATTHEW HUDSON, DAMIAN ALLIS, Syracuse University, WAYNE OUELLETTE, Research Division, NSWC-IH, BRUCE HUDSON, Syracuse University — The structure of the 2:1 amino acid salt L-alanine alaninium nitrate (LAAN) was determined at 90 K by X-ray diffraction. The vibrational spectrum of LAAN was measured at 25 K by inelastic neutron scattering (INS) spectroscopy and simulated using solid-state density functional theory (DFT). In LAAN, a feature observed at approximately 450 cm^{-1} in the experimental spectrum is noticeably absent in the calculation based on the 90 K X-ray structure. Further investigation of LAAN by Raman spectroscopy reveals spectral differences between the 78 and 293 K spectra. The nature of the spectral changes in LAAN and the disagreement between the INS spectrum and simulation are discussed in relation to a structural change at low temperature which involves the movement of hydrogen-atom(s). This is considered in relationship to the homologous diglycine nitrate, a well characterized ferroelectric material with a $T_c = 206\text{ K}$. doi: 10.1039/b905070a

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Matthew Hudson
Syracuse University

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