

42. Title: Terahertz spectroscopy of enantiopure and racemic polycrystalline valine

Author: Williams, MRC; True, AB; Izmaylov, AF; French, TA; Schroeck, K; Schmuttenmaer, CA

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Abstract: Experimental and computational THz (or far-infrared) spectra of polycrystalline valine samples are reported. The experimental spectra have been measured using THz time-domain spectroscopy. Spectra of the pure enantiomers, both D and L, as well as the DL racemate have been taken at room temperature and low temperature (78 K). The spectra of the pure D and L enantiomers are essentially identical, and they are markedly different from the DL racemate. In addition, a temperature-dependent study of L-valine was undertaken in which the absorption maxima were found to red shift as a function of increasing temperature. The vibrational absorption spectra (frequencies and intensities) were calculated using the harmonic approximation with the Perdew-Burke-Ernzerhof (PBE) functional, localized atomic orbital basis sets, and periodic boundary conditions. The calculated and experimental spectra are in good qualitative agreement. A general method of quantifying the degree to which a calculated mode is intermolecular versus intramolecular is demonstrated, with the intermolecular motions further separated into translational versus rotational/librational motion. This allows straightforward comparison of spectra calculated using different basis sets or other constraints.