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Title:Collective mode frequency shifts in L-serine and a series of isotopologues in the terahertz regime
Authors:Hufnagle, David C. (1); Taulbee-Combs, Anita R. (2); Spendel, Wolfgang U. (2); Pacey, Gilbert E. (2)
Author affiliation:(1) Department of Chemistry and Biochemistry, Miami University, Hughes Hall, Oxford, OH 45056, United States; (2) Ohio Wright Center for Innovation, Institute for the Development and Commercialization of Advanced Sensor Technology (IDCAST), Dayton, OH 45402, United States; (3) University of Dayton, Research Institute, Dayton, OH 45469, United States
Corresponding author:Hufnagle, D.C.(hufnagdc@gmail.com)
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Abstract:Terahertz (THz) time-domain spectroscopy was used to monitor collective mode shifts in L-serine, L-serine-2,3,3-d<inf>3</inf>, L-serine-d<inf>4</inf>, and L-serine-d<inf>7</inf> at both room and liquid nitrogen (LN<inf>2</inf>) temperatures. Increasing the molecular mass by deuteration caused an expected absorbance red-shift; however, the magnitude of the displacement could not be predicted using normal mode analysis. Both modes at 67.8 cm⁻¹ and 91.4 cm⁻¹ demonstrated a greater peak shift upon deuterium substitution at non-hydrogen bonding sites than at sites that participated in hydrogen bonding. This is evident in the larger peak shifts observed in L-serine-d<inf>3</inf> than in L-serine-d<inf>4</inf>, despite a smaller increase in mass. This leads to the conclusion that both peaks present in the room temperature spectra of L-serine likely arise primarily from other intermolecular interactions with <50% contribution from hydrogen bonding. This goes against the prediction that peaks in the THz spectra of amino acids are predominantly due to the hydrogen bonding network that makes up the crystal lattice.
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