Abstract Submitted
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Multiple-Sequence Two-Dimensional Infrared Spectroscopy of *N*-Acetyl-L-Prolinamide[1] SOOHWAN SUL, DENIS KARAISKAJ, YING JIANG, NIEN-HUI GE, Department of Chemistry, University of California at Irvine — Femtosecond nonlinear 2D IR spectroscopy has been applied to study the conformational distribution of a model dipeptide, *N*-acetyl-L-prolinamide, in chloroform. Using rephasing, non-rephasing, and reverse photon echo pulse sequences at several polarization conditions, we resolved new spectral features associated with multiple conformers that were difficult to discern by linear IR spectroscopy. Ab initio calculations in vacuo suggested the existence of a major *trans*-C_7 and a minor *cis* structure. Calculated 2D spectra based on these structures agree reasonably well with experimental spectral features obtained at parallel polarizations, but better agreement between the calculated and experimental cross-peak patterns can be reached if the major conformer takes a structure deviated from the C_7 form. We will discuss our results in relationship with earlier findings from NMR studies and MD simulations.

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