RAMAN SPECTRAL SIGNATURES AS CONFORMATIONAL PROBES OF BIOMOLECULES

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A first application of ionization-loss stimulated Raman spectroscopy (ILSRS) for monitoring the spectral features of four conformers of a gas phase neurotransmitter (2-phenylethylamine) is reported. The Raman spectra of the conformers show bands that uniquely identify the conformational structure of the molecule and are well matched by density functional theory calculations. The measurement of spectral signatures by ILSRS in an extended spectral range, with a relatively convenient laser source, is extremely important, allowing enhanced accessibility to intra- and inter-molecular forces, which are significant in biological structure and activity.