

Structural probing of flexible molecules

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The development and application of ionization-loss stimulated Raman spectroscopy (ILSRS) for monitoring the spectral features of flexible molecules, over a wide frequency range and with high resolution, is reported.¹ The bands observed in the Raman spectra of two conformers of 2-phenylethanol (PEAL) uniquely identify their structure, and are in accord with anharmonic results obtained by density functional theory calculations. Obtaining the spectral signatures by ILSRS in expanded spectral range and at uniform resolution (see Fig. 1) with relatively convenient laser sources, is extremely important, allowing enhanced accessibility to intra- and inter-molecular forces, which are significant in biological structure and activity. The results of the present work indicate that ILSRS could be a powerful conformational probe in biomolecules.

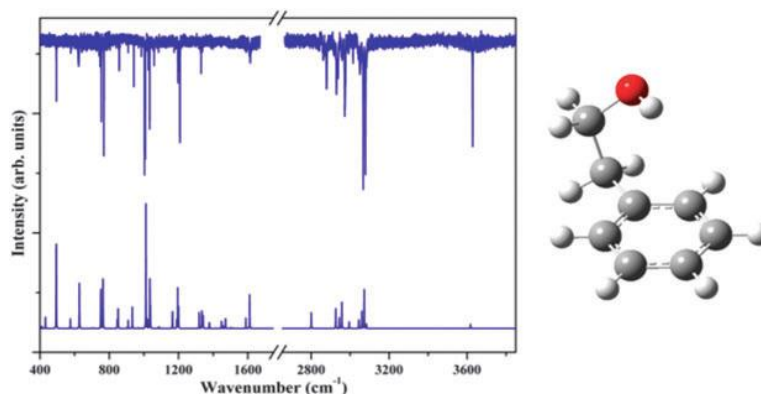


Fig. 1. Ionization-loss stimulated Raman spectrum of conformer **A** of PEAL. Below the experimental spectrum a computed spectrum that exhibits the closest agreement to it, is displayed. The electronic ground state, S_0 , structure of PEAL is shown in the right part.

¹ N. Mayorkas, I. Malka and I. Bar, *Phys. Chem. Chem. Phys.* 13, 6808 (2011).