SPECTROSCOPIC CHARACTERIZATION OF A NATURAL PRODUCT: ANETHOLE

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Anethole [(*E*)-1-methoxy-4-(1-propenyl)benzene] is a natural product molecule that is commonly recognized as the flavor component of anise, fennel, and licorice. Early jet-cooled spectroscopy of anethole showed the existence of two possible conformations, but did not address details of the vibronic structure.[a] Here, we report the jet-cooled, laser-induced fluorescence and single vibronic level fluorescence spectra of anethole. Analysis of the spectra confirms the existence of two rotamers in the expansion that differ by the relative orientation of the methoxy and propenyl groups. The observed vibronic activity is similar to that of styrene and indicates planar symmetry of both rotamers. Vibrational assignments of anethole are assisted by density functional theory calculations and the results are compared with the analogous motions in styrene.

[a] V. H. Grassian, E. R. Bernstein, H. V. Secor and J. I. Seeman *J. Phys. Chem.* **93**, 3470 (1989).