ANETHOLE-WATER: A COMBINED JET, MATRIX, AND COMPUTATIONAL STUDY

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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. Previously, we reported the jet-cooled, laser-induced fluorescence (LIF) and single vibronic level fluorescence (SVLF) spectra of anethole.[a] In this work, several weak bands were observed and were tentatively assigned as van der Waals clusters of anethole with water. We have since confirmed this assignment and have conducted a more detailed study to determine the geometry of these clusters. Results from LIF, SVLF, and matrix isolation FTIR[b] spectroscopy, as well as computational results will be presented in this talk.

[a] *J. Phys. Chem. A*, **2013**, 117 (48), 12831–12841

[b] Newly built system at Hobart and William Smith Colleges