ANALYSIS OF PEAR ESTER FLAVORING SAMPLES USING BROADBAND ROTATIONAL SPECTROSCOPY

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Pear ester (ethyl decadienoate, $C_{12}H_{20}O_2$) is a molecule used in perfumes and as a food flavoring. It can be obtained from both natural and synthetic sources. The motivation for this study was the interest of a local distillery (Vitae Spirits) in understanding differences in the composition of pear ester samples that might cause off flavors in their spirits. Different samples were analyzed by broadband rotational spectroscopy in the attempt to identify possible impurities. The measurement uses a head space sampling approach where the liquid sample is held in a reservoir and heated. The vapor pressure above the sample is entrained in inert neon gas, and this gas mixture is injected into the spectrometer using a pulsed valve. One challenge in the analysis of chemical mixtures using broadband rotational spectroscopy is that the measured spectrum contains overlapping rotational spectra of each mixture component, making it difficult to isolate the spectral pattern of a single chemical species. To aid the analysis, a version of temperature programmed spectroscopy was performed, where the head space spectrum was acquired for a series of sample reservoir temperatures. This measurement method produces characteristic intensity vs. temperature profiles for transitions from a single species. This makes it possible to separate the overall measurement into spectra arising from different species and is an analysis process that can be fully automated. The analysis of different pear ester samples will be summarized including the ability to identify impurity species, like n-hexanal. The identification of pear ester posed challenges in its own right due to the conformational flexibility of the molecule. The approach to obtaining accurate quantum chemistry estimates of the rotational spectrum parameters for pear ester, so the molecule can be identified in the broadband rotational spectrum, will also be described.