ROTATIONAL SPECTROSCOPY OF FLAVOR COMPOUNDS IN PEACH BRANDY FOR PROCESS MONITORING IN CRAFT DISTILLERIES

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The feasibility of using molecular rotational spectroscopy as an on-line monitoring system for brandy distillation has been investigated in collaboration with Monte Piccolo Farm and Distillery. The target product is brandy produced from Indian Blood peaches. A previous study identified key flavor components from 18 peach cultivars, and lactones in the C_8–C_{12} size range appear to produce much of the characteristic peach flavor.[a] These lactones are present in different ratios across peach cultivars and, as a result, these ratios may help identify the ideal peach for brandy distillation. Rotational spectra of octa-, deca-, and dodecalactone isomers were collected to provide a library of possible flavor congeners. Experimental spectra of the lactones were in good agreement with dispersion corrected density functional theory calculations.[b] Despite the lactones possessing long alkyl tails, conformational populations observed in the pulsed-jet expansion were dominated by one or two conformations. A lab-prepared mixture of peach flavor compounds and commercial peach extracts were analyzed to test the ability of the technique to analyze complex mixtures, similar to what would be seen during distillation. These measurements use temperature-programmed broadband rotational spectroscopy to separate the full spectrum of all mixture compounds into a spectrum for each compound. Rapid monitoring of these flavor components with a cavity-enhanced Fourier transform microwave spectrometer using a pre-programmed sample profile has been demonstrated on the commercial instrument from BrightSpec that is based on the NIST compact Balle-Flygare spectrometer design.[c]

[a] Xi, W.; Zheng, Q.; Lu, J.; Quan, J., Horticulture Plant Journal 3, 1-12 (2017).

[b] S. Grimme and M. Steinmetz, Phys. Chem. Chem. Phys. 15, 16031-16042 (2013).

[c] R.D. Suenram, J.U. Grabow, A. Zuban, and I. Leonov, Rev. Sci. Instrum. 70, 2127-2135 (1999).