INFRARED OPTICAL CONSTANTS AND ABSOLUTE INFRARED ABSORPTION INTENSITIES OF LIQUID BENZENE-D_1.

JOHN E. BERTIE, YORAM APELBLAT, *Department of Chemistry, University of Alberta, Edmonton, Alberta Canada T6G 2G2*; C. DALE KEEFE, *Department of Physical and Applied Sciences, University College of Cape Breton, Sydney, Nova Scotia, Canada B1P 6L2*.

Quantitative infrared absorption spectra of liquid C_6H_5D at 25°C have been measured between 6250 and 400 cm^{-1} through transmission cells fitted with NaCl and KBr windows. The spectra have been fully corrected for reflection effects and the real, n, and imaginary, k, refractive indices of the liquid have been calculated thoughout this range. To correct for the predictable long-range dielectric effects in the liquid, the Lorentz local field was used to calculate the complex molar polarizability. As has been described previously for liquid methanol [a] and liquid C_6D_6 [b] , the contributions of the different bands to the imaginary molar polarizability spectrum were separated by fitting the spectrum with Classical Damped Harmonic Oscillator bands, and the absolute integrated intensities were calculated analytically from the parameters of the CDHO bands.

The methods used will be illustrated sufficiently to give confidence in the claimed 5 to 10 percent accuracy of the integrated intensities of liquid C_6H_5D, which will be related to those of the gas and to those of C_6H_6 and C_6D_6.

In passing, a noteworthy, but not surprising, similarity will be shown between the first CH overtone spectrum of liquid C_6H_6 at 25°C [c] and that of C_6H_6 in a supersonic beam at a rotational temperature temperature of 5K [d].

[a] J. E. Bertie and S. L. Zhang, J. Mol. Struct. 413-414, 333 (1997).
[b] J. E. Bertie and C. D. Keefe, Fresenius J. Anal. Chem. 362, 91 (1998)
[c] J. E. Bertie and C. D. Keefe, unpublished
[d] R. H. Page, Y. R. Shen and Y. T. Lee, J. Chem. Phys. 88, 4621 (1988).