COLOR-CENTER LASER SPECTRUM OF THIOPHENE OBSERVED WITH THE PULSED SUPERSONIC JET EXPANSION TECHNIQUE

A. OKUMURA, <u>M. ISHIGURO</u>, K. TANAKA, and T. TANAKA, *Department of Chemistry, Faculty of Science, Kyushu University 33, Higashiku, Fukuoka 812-8581, Japan.*

The high resolution infrared spectrum of thiophene in the CH-stretch region (3070-3140 cm⁻¹) has been observed with a color-center laser spectrometer combined with a pulsed supersonic jet expandion technique. Of 4 fundamental bands (a₁; ν_1 , ν_2 , b₁; ν_{12} , ν_{13}) expected in this region, the ν_2 band was analyzed to the confirmation of previous vibrational assignment. ^{*a* b} The rotational constants and band origin were derived from the observed spectra while the ground state constants were fixed at the microwave values. ^{*c*} The ν_2 band was found to be overlapped by an a₁ vibrational band, which is denoted as ν_x . The ν_x band presumably borrows the intensity from the ν_2 band by Fermi resonance. The vibrational assignment of ν_x is not get clear, but the magnitude of the interaction between the ν_2 and ν_x states is calculated to be 0.8 cm⁻¹ from the analysis of the intensity ratio of these bands.

^aT. D. Klots, R. D. Chirico, and W. B. Steele, Spectrochim. Acta. <u>50A</u>, 765 (1994)

^bA. A. El-Azhary, and R. H. Hilal, Spectrochim. Acta. <u>53A</u>, 1365 (1997)

^cB. Pankoke, K. M. T. Yamada, and G. Winnewisser, Z. Naturforsch. <u>49a</u>, 1193 (1994)