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

M. ISHIGURO, K. HARADA, K. TANAKA, and T. TANAKA, *Department of Chemistry, Faculty of Science, Kyushu University 33, Higashiku, Fukuoka 812-8581, Japan.*.

The infrared spectrum of fluorobenzene in the CH-stretch region (3040-3120 cm^{-1}) has been observed with a color-center laser spectrometer combined with a pulsed supersonic jet expandion technique. Due to the rotational as well as cooling in the jet, well resolved rovibrational lines were recorded. At least 5 fundamental bands (a_1; $\nu_2, \nu_{13}, \nu_{20a}$ b_1; ν_{7b}, ν_{20b}) are expected in this region according to the opto-thermal Raman conversion dye laser spectroscopy [a]. So far two parallel bands (ν_{13}, ν_{20a}) were analyzed to confirm the vibrational assignments given by the low-resolution spectroscopy.

The rotational constants and band origins were derived from the observed spectra assuming those for ground state to the microwave results [b, c]. The ν_{20a} band were found to be overlapped additionally with the two vibrational bands presumably caused by higher order Fermi interaction, whose inertia defects are small negative about -0.5 amu$\mathring{A}^2$. Their vibrational assignments are obscure yet, but the negative inatria defects imply that they include two or four quanta of low frequency out-of-plane vibrational modes such as $\nu_{11}(\omega = 248\ cm^{-1})$ and $\nu_{16b}(498\ cm^{-1})$.

[a] M. Scotoni, S. Oss, L. Lubich, S. Furlani, and D. Bassi, J. Chem. Phys. 103, 897 (1995)
[b] M. Onda, H. Mukaida, and I. Yamaguchi, J. Mol. Spectrosc. 176, 146 (1996)
[c] L. Nygaard, I. Bojesen, T. Pedersen, and J. R. Andersen. J. Mol. Struct. 2, 209 (1968)