

FTIR SPECTROSCOPY OF THE ν_4 BANDS OF $^{14}\text{NO}_3$ AND $^{15}\text{NO}_3$

R. FUJIMORI, N. SHIMIZU, J. TANG, K. KAWAGUCHI, *Department of Chemistry, Faculty of Science, Okayama University, 3-1-1, Tsushima-Naka, Okayama 700-8530, Japan*; T. ISHIWATA, *Graduate School of Information Sciences, Hiroshima City University, 3-4-1 Otsuka-Higashi, Hiroshima 731-3194, Japan*,.

High-resolution Fourier transform infrared spectra of the NO_3 ν_4 bands of ^{14}N and ^{15}N isotopic species were observed in the 365 and 360 cm^{-1} region. Observed lines were used to determine $\Delta K=3$ combination differences of the ground state coupled with transition frequencies of the ν_3 hot band $\nu_3 + \nu_4 - \nu_4$ in 1127 cm^{-1} region^a and $\nu_3 + \nu_4$ band in 1492 cm^{-1} region, which made it possible to determine the rotational C_0 constants of 0.228 6321(67) cm^{-1} and 0.228 674(11) cm^{-1} for $^{14}\text{NO}_3$ and $^{15}\text{NO}_3$, respectively. Inertial defects of several vibrational states were calculated by using a formula of Jagod and Oka^b and compared with the observed values. Although the observed Coriolis coupling constants $\zeta_4=-0.188$ ($^{14}\text{NO}_3$) and -0.156 ($^{15}\text{NO}_3$) are largely different from the expected value of -0.7 from a force field calculation, observed inertial defects are in good agreement with calculated values, for example, $\Delta_{obs}(\text{Gr.})=0.206$ [0.223] $\text{amu}\text{\AA}^2$, ($\nu_4=1$) 0.434 [0.437] $\text{amu}\text{\AA}^2$ etc, where calculated values are given in square brackets.

^aK. Kawaguchi, N. Shimizu, R. Fujimori, J. Tang, T. Ishiwata, and I. Tanaka, *J. Mol. Spectrosc.* **268**, 85 (2011).

^bM.-F. Jagod and T. Oka, *J. Mol. Spectrosc.* **139**, 313 (1990).