FTIR SPECTRUM AND PERTURBATION ANALYSIS OF THE ν_2 BAND OF $^{15}NO_3$

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In 1987, Friedl and Sander[a] reported observation of the FTIR spectrum of the ν_2 band of $^{14}NO_3$ in 762 cm^{-1} region, and rotational analysis was carried out for only transitions with K=3. The obtained negative centrifugal distortion constant D_N implied presence of perturbation from other states, but the perturbation analysis has not been carried out. In the present study, the ν_2 band of $^{15}NO_3$ was first observed in 742 cm^{-1} region. In contrast to the case of $^{14}NO_3$, rotational assignments were carried out for K=0, 3, 6, 9, 12, and 15, and transitions with N$\leq$12 were fitted with usual energy level expression for D_{3h} molecule. However, when we included higher N transitions up to N=22, an effect of Coriolis interaction from v_4=2 appeared in negative D_N for K=0 and staggering in K=3. An energy matrix including ℓ=0 and ℓ=$\pm$2 of v_4=2 and ℓ=0 of v_2 =1 was used to obtain the energy values of v_2 =1 , including the Corilis and ℓ-type resonance terms. From the determined interaction constant between v_2 =1 and v_4=2 , anharmonic constant k_{444} was estimated, by assuming a mixing of v_4=1 and v_4=2.

[a] R. R. Friedel and S. P. Sander, *J. Phys. Chem.* **91**, 2721 (1987).